Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 08:24 PM EST

PDB ID	:	3U6N
Title	:	Open Structure of the BK channel Gating Ring
Authors	:	Yuan, P.; MacKinnon, R.
Deposited on	:	2011-10-12
Resolution	:	3.61 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:

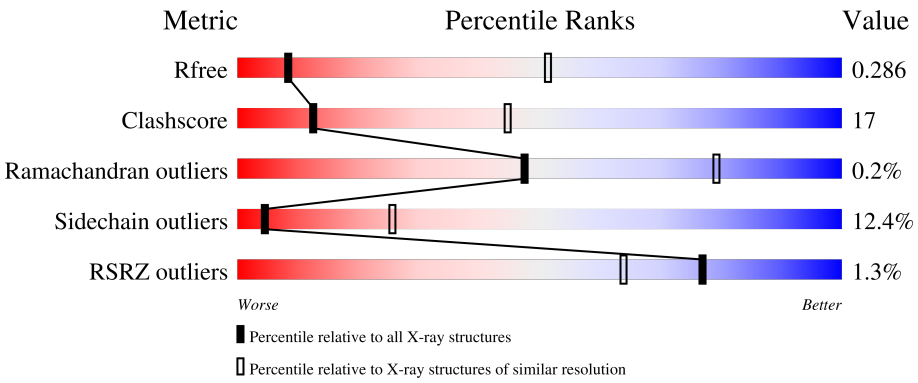
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.61 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	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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	A	696	% 56% 25% • 16%
1	B	696	% 56% 25% • 16%
1	C	696	55% 26% • 16%
1	D	696	% 56% 24% • 16%
1	E	696	% 56% 25% • 16%

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Mol	Chain	Length	Quality of chain
1	F	696	57% 24% • 16%
1	G	696	56% 25% • 16%
1	H	696	56% 24% • 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34504 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 High-Conductance Ca2+-Activated K+ Channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	585	4312	2756	722	800	34	0	0	0
1	B	585	4312	2756	722	800	34	0	0	0
1	C	585	4312	2756	722	800	34	0	0	0
1	D	585	4312	2756	722	800	34	0	0	0
1	E	585	4312	2756	722	800	34	0	0	0
1	F	585	4312	2756	722	800	34	0	0	0
1	G	585	4312	2756	722	800	34	0	0	0
1	H	585	4312	2756	722	800	34	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	MET	-	initiating methionine	UNP B7ZC96
A	578	ARG	-	see remark 999	UNP B7ZC96
A	579	SER	-	see remark 999	UNP B7ZC96
A	580	ARG	-	see remark 999	UNP B7ZC96
A	581	LYS	-	see remark 999	UNP B7ZC96
A	582	ARG	SER	see remark 999	UNP B7ZC96
A	1061	SER	-	expression tag	UNP F1QYL4
A	1062	ASN	-	expression tag	UNP F1QYL4
A	1063	SER	-	expression tag	UNP F1QYL4
A	1064	LEU	-	expression tag	UNP F1QYL4
A	1065	GLU	-	expression tag	UNP F1QYL4
A	1066	VAL	-	expression tag	UNP F1QYL4
A	1067	LEU	-	expression tag	UNP F1QYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1068	PHE	-	expression tag	UNP F1QYL4
A	1069	GLN	-	expression tag	UNP F1QYL4
B	340	MET	-	initiating methionine	UNP B7ZC96
B	578	ARG	-	see remark 999	UNP B7ZC96
B	579	SER	-	see remark 999	UNP B7ZC96
B	580	ARG	-	see remark 999	UNP B7ZC96
B	581	LYS	-	see remark 999	UNP B7ZC96
B	582	ARG	SER	see remark 999	UNP B7ZC96
B	1061	SER	-	expression tag	UNP F1QYL4
B	1062	ASN	-	expression tag	UNP F1QYL4
B	1063	SER	-	expression tag	UNP F1QYL4
B	1064	LEU	-	expression tag	UNP F1QYL4
B	1065	GLU	-	expression tag	UNP F1QYL4
B	1066	VAL	-	expression tag	UNP F1QYL4
B	1067	LEU	-	expression tag	UNP F1QYL4
B	1068	PHE	-	expression tag	UNP F1QYL4
B	1069	GLN	-	expression tag	UNP F1QYL4
C	340	MET	-	initiating methionine	UNP B7ZC96
C	578	ARG	-	see remark 999	UNP B7ZC96
C	579	SER	-	see remark 999	UNP B7ZC96
C	580	ARG	-	see remark 999	UNP B7ZC96
C	581	LYS	-	see remark 999	UNP B7ZC96
C	582	ARG	SER	see remark 999	UNP B7ZC96
C	1061	SER	-	expression tag	UNP F1QYL4
C	1062	ASN	-	expression tag	UNP F1QYL4
C	1063	SER	-	expression tag	UNP F1QYL4
C	1064	LEU	-	expression tag	UNP F1QYL4
C	1065	GLU	-	expression tag	UNP F1QYL4
C	1066	VAL	-	expression tag	UNP F1QYL4
C	1067	LEU	-	expression tag	UNP F1QYL4
C	1068	PHE	-	expression tag	UNP F1QYL4
C	1069	GLN	-	expression tag	UNP F1QYL4
D	340	MET	-	initiating methionine	UNP B7ZC96
D	578	ARG	-	see remark 999	UNP B7ZC96
D	579	SER	-	see remark 999	UNP B7ZC96
D	580	ARG	-	see remark 999	UNP B7ZC96
D	581	LYS	-	see remark 999	UNP B7ZC96
D	582	ARG	SER	see remark 999	UNP B7ZC96
D	1061	SER	-	expression tag	UNP F1QYL4
D	1062	ASN	-	expression tag	UNP F1QYL4
D	1063	SER	-	expression tag	UNP F1QYL4
D	1064	LEU	-	expression tag	UNP F1QYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1065	GLU	-	expression tag	UNP F1QYL4
D	1066	VAL	-	expression tag	UNP F1QYL4
D	1067	LEU	-	expression tag	UNP F1QYL4
D	1068	PHE	-	expression tag	UNP F1QYL4
D	1069	GLN	-	expression tag	UNP F1QYL4
E	340	MET	-	initiating methionine	UNP B7ZC96
E	578	ARG	-	see remark 999	UNP B7ZC96
E	579	SER	-	see remark 999	UNP B7ZC96
E	580	ARG	-	see remark 999	UNP B7ZC96
E	581	LYS	-	see remark 999	UNP B7ZC96
E	582	ARG	SER	see remark 999	UNP B7ZC96
E	1061	SER	-	expression tag	UNP F1QYL4
E	1062	ASN	-	expression tag	UNP F1QYL4
E	1063	SER	-	expression tag	UNP F1QYL4
E	1064	LEU	-	expression tag	UNP F1QYL4
E	1065	GLU	-	expression tag	UNP F1QYL4
E	1066	VAL	-	expression tag	UNP F1QYL4
E	1067	LEU	-	expression tag	UNP F1QYL4
E	1068	PHE	-	expression tag	UNP F1QYL4
E	1069	GLN	-	expression tag	UNP F1QYL4
F	340	MET	-	initiating methionine	UNP B7ZC96
F	578	ARG	-	see remark 999	UNP B7ZC96
F	579	SER	-	see remark 999	UNP B7ZC96
F	580	ARG	-	see remark 999	UNP B7ZC96
F	581	LYS	-	see remark 999	UNP B7ZC96
F	582	ARG	SER	see remark 999	UNP B7ZC96
F	1061	SER	-	expression tag	UNP F1QYL4
F	1062	ASN	-	expression tag	UNP F1QYL4
F	1063	SER	-	expression tag	UNP F1QYL4
F	1064	LEU	-	expression tag	UNP F1QYL4
F	1065	GLU	-	expression tag	UNP F1QYL4
F	1066	VAL	-	expression tag	UNP F1QYL4
F	1067	LEU	-	expression tag	UNP F1QYL4
F	1068	PHE	-	expression tag	UNP F1QYL4
F	1069	GLN	-	expression tag	UNP F1QYL4
G	340	MET	-	initiating methionine	UNP B7ZC96
G	578	ARG	-	see remark 999	UNP B7ZC96
G	579	SER	-	see remark 999	UNP B7ZC96
G	580	ARG	-	see remark 999	UNP B7ZC96
G	581	LYS	-	see remark 999	UNP B7ZC96
G	582	ARG	SER	see remark 999	UNP B7ZC96
G	1061	SER	-	expression tag	UNP F1QYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1062	ASN	-	expression tag	UNP F1QYL4
G	1063	SER	-	expression tag	UNP F1QYL4
G	1064	LEU	-	expression tag	UNP F1QYL4
G	1065	GLU	-	expression tag	UNP F1QYL4
G	1066	VAL	-	expression tag	UNP F1QYL4
G	1067	LEU	-	expression tag	UNP F1QYL4
G	1068	PHE	-	expression tag	UNP F1QYL4
G	1069	GLN	-	expression tag	UNP F1QYL4
H	340	MET	-	initiating methionine	UNP B7ZC96
H	578	ARG	-	see remark 999	UNP B7ZC96
H	579	SER	-	see remark 999	UNP B7ZC96
H	580	ARG	-	see remark 999	UNP B7ZC96
H	581	LYS	-	see remark 999	UNP B7ZC96
H	582	ARG	SER	see remark 999	UNP B7ZC96
H	1061	SER	-	expression tag	UNP F1QYL4
H	1062	ASN	-	expression tag	UNP F1QYL4
H	1063	SER	-	expression tag	UNP F1QYL4
H	1064	LEU	-	expression tag	UNP F1QYL4
H	1065	GLU	-	expression tag	UNP F1QYL4
H	1066	VAL	-	expression tag	UNP F1QYL4
H	1067	LEU	-	expression tag	UNP F1QYL4
H	1068	PHE	-	expression tag	UNP F1QYL4
H	1069	GLN	-	expression tag	UNP F1QYL4

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

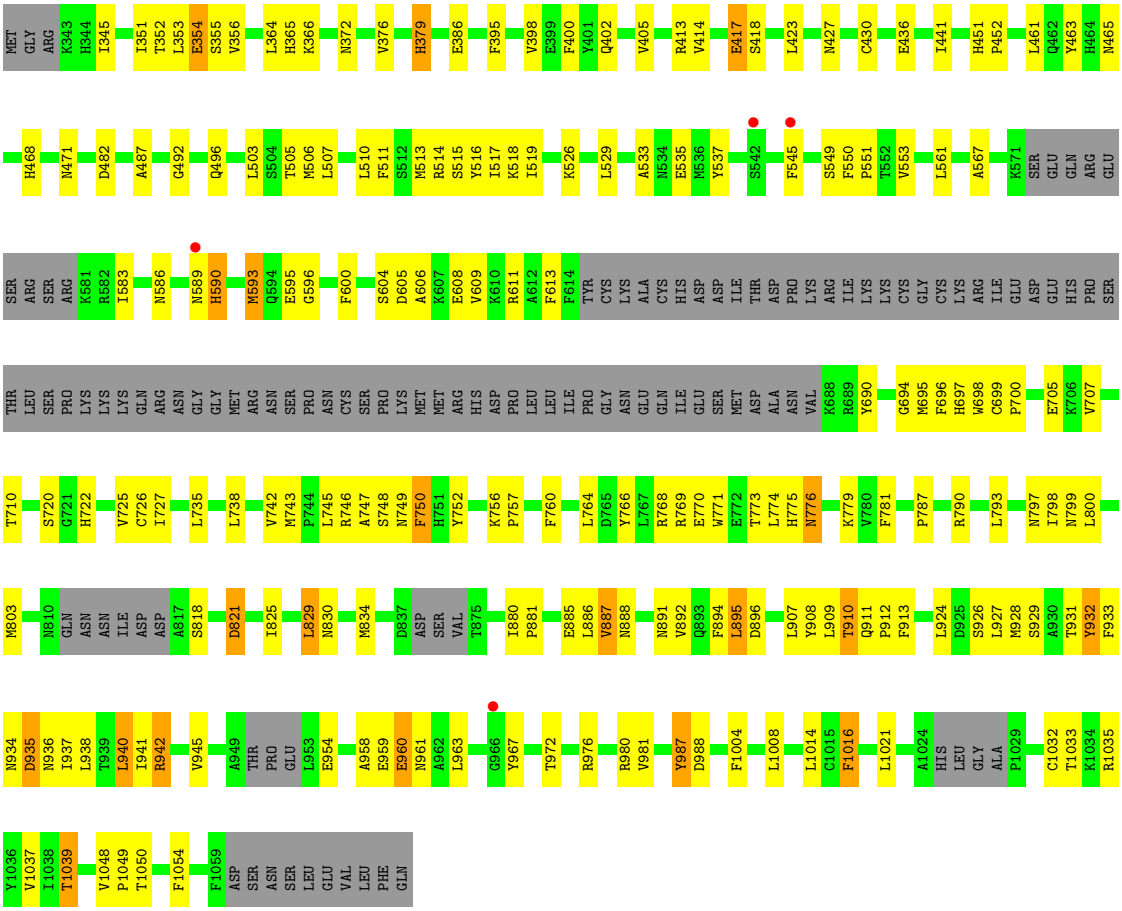
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0

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.

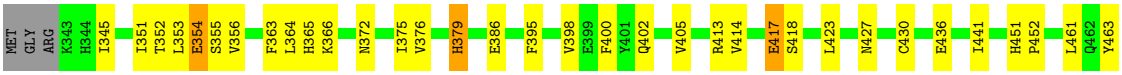
• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

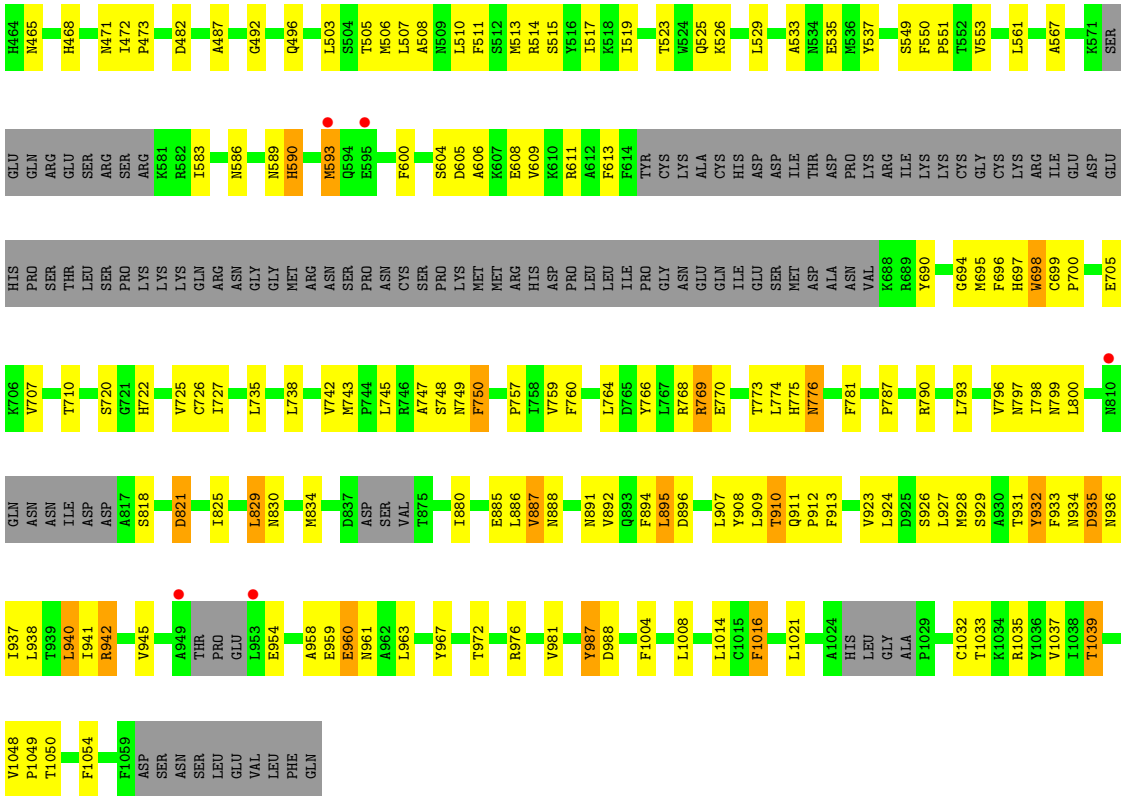
Chain A:



• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

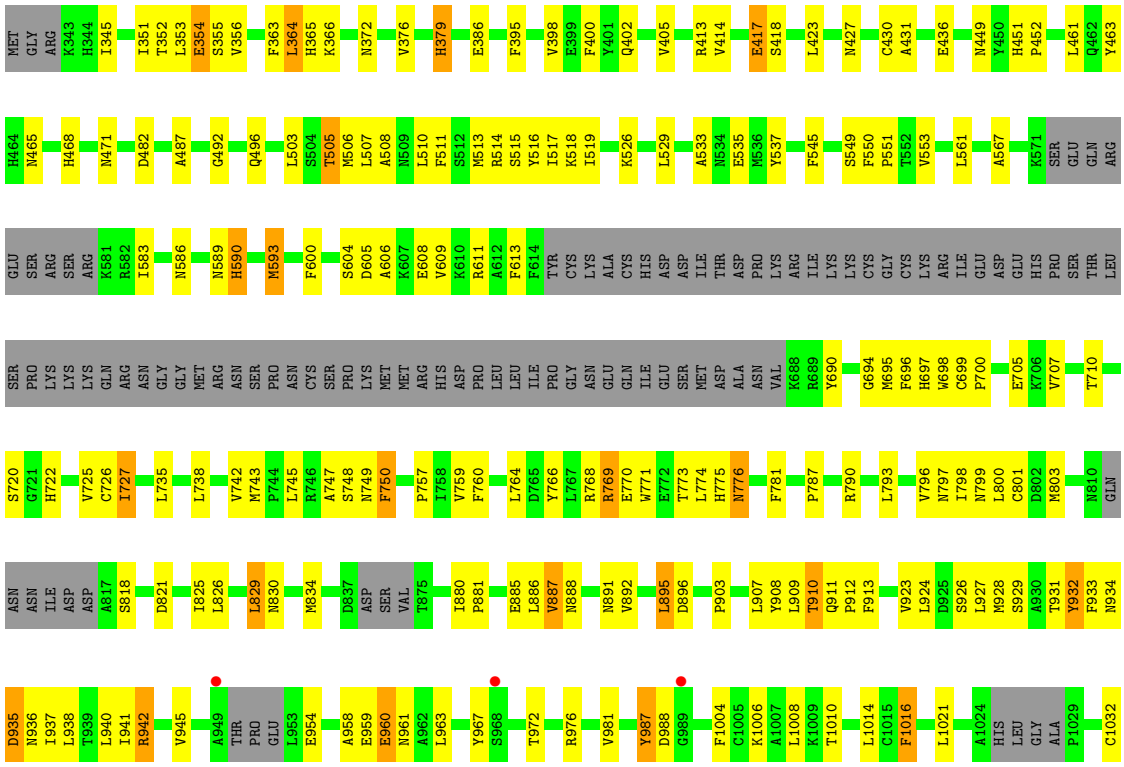
Chain B:

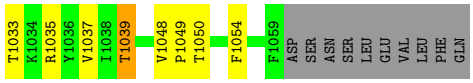




• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

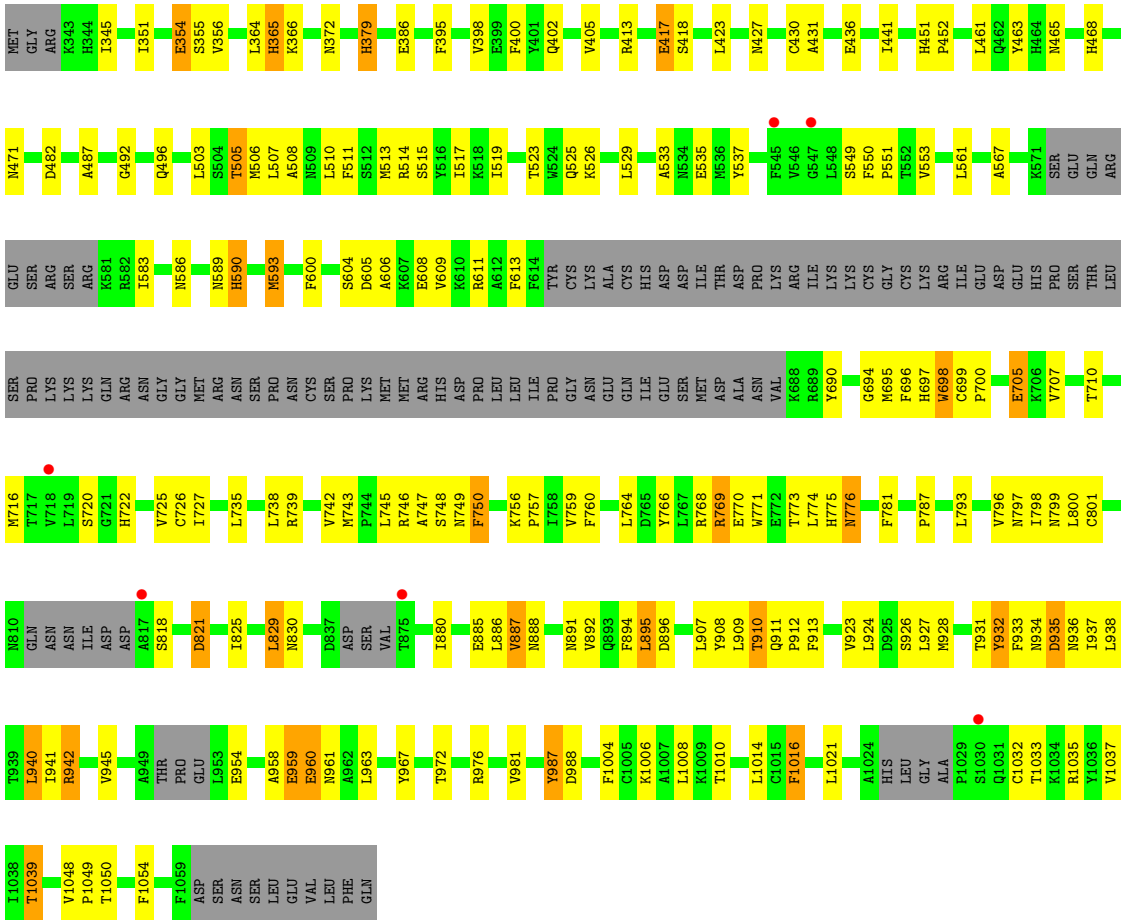
Chain C: 55% 26% • 16%





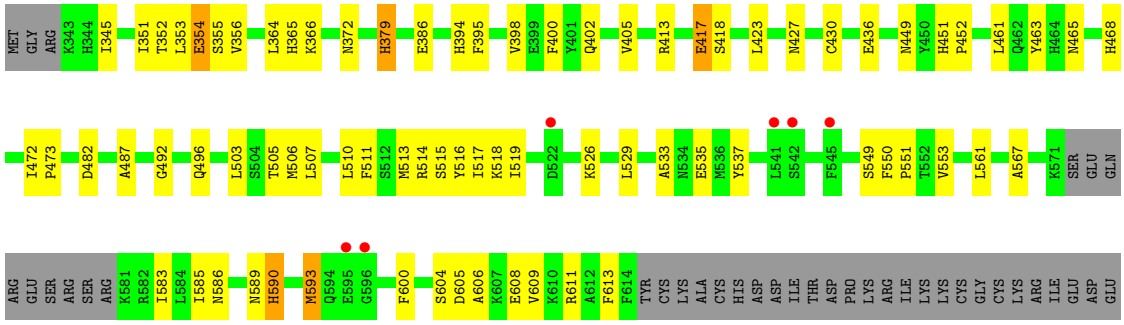
• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

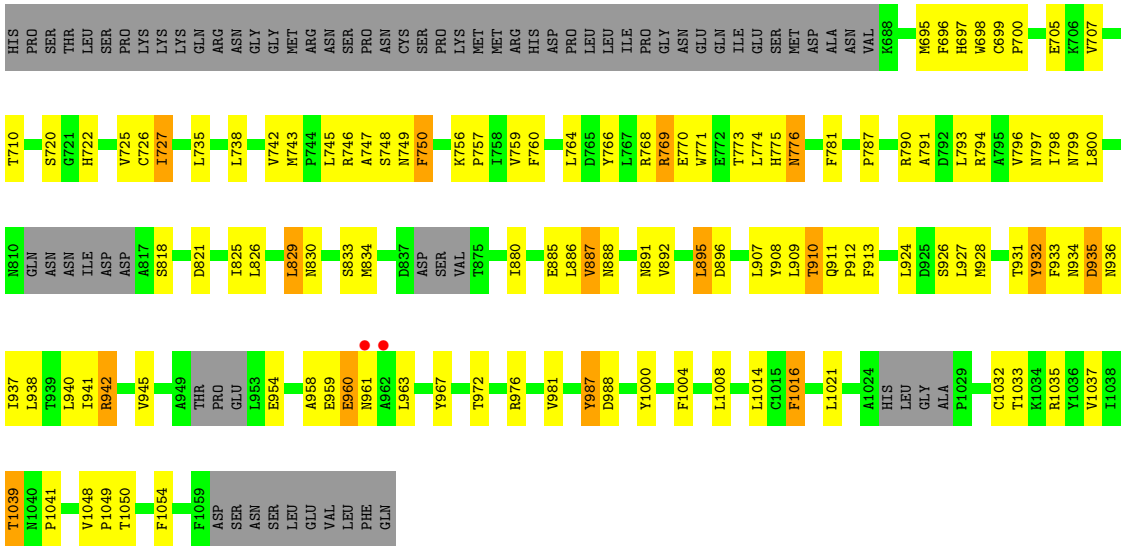
Chain D:



• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

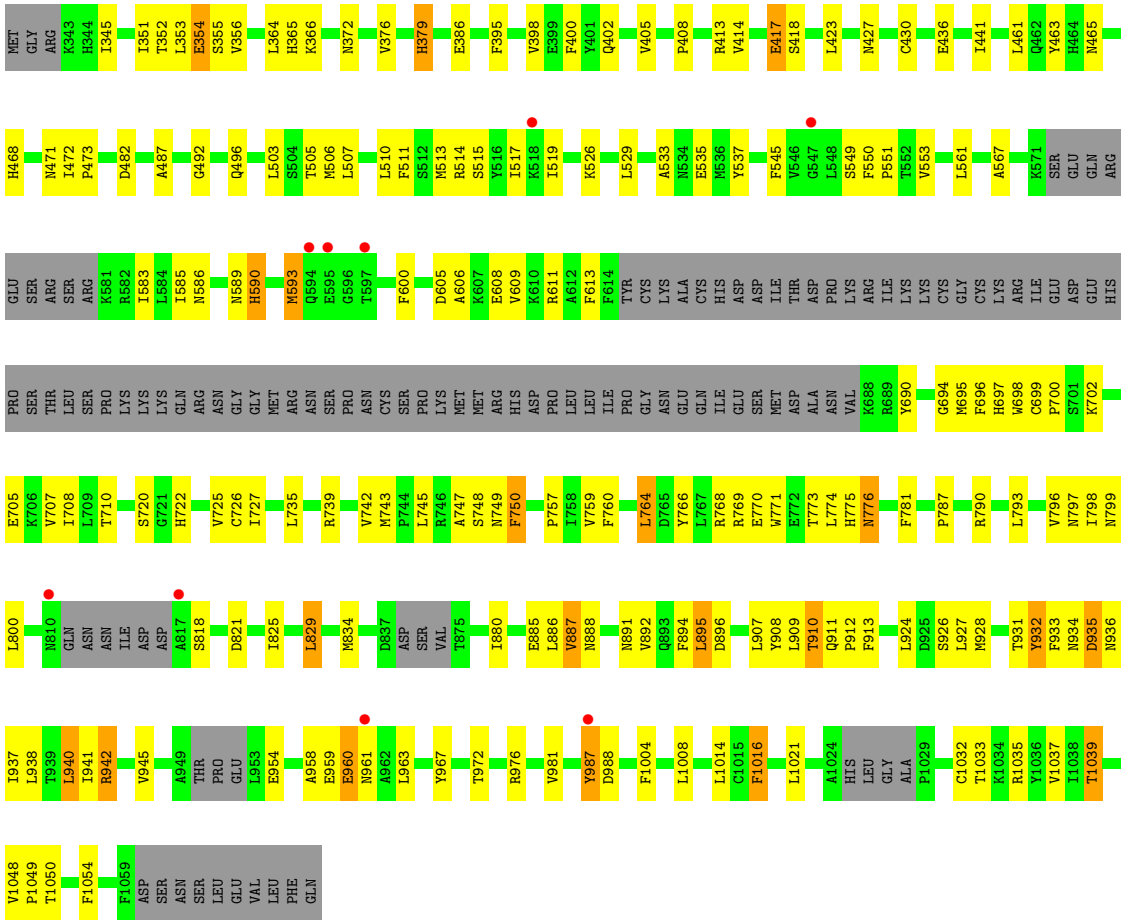
Chain E:





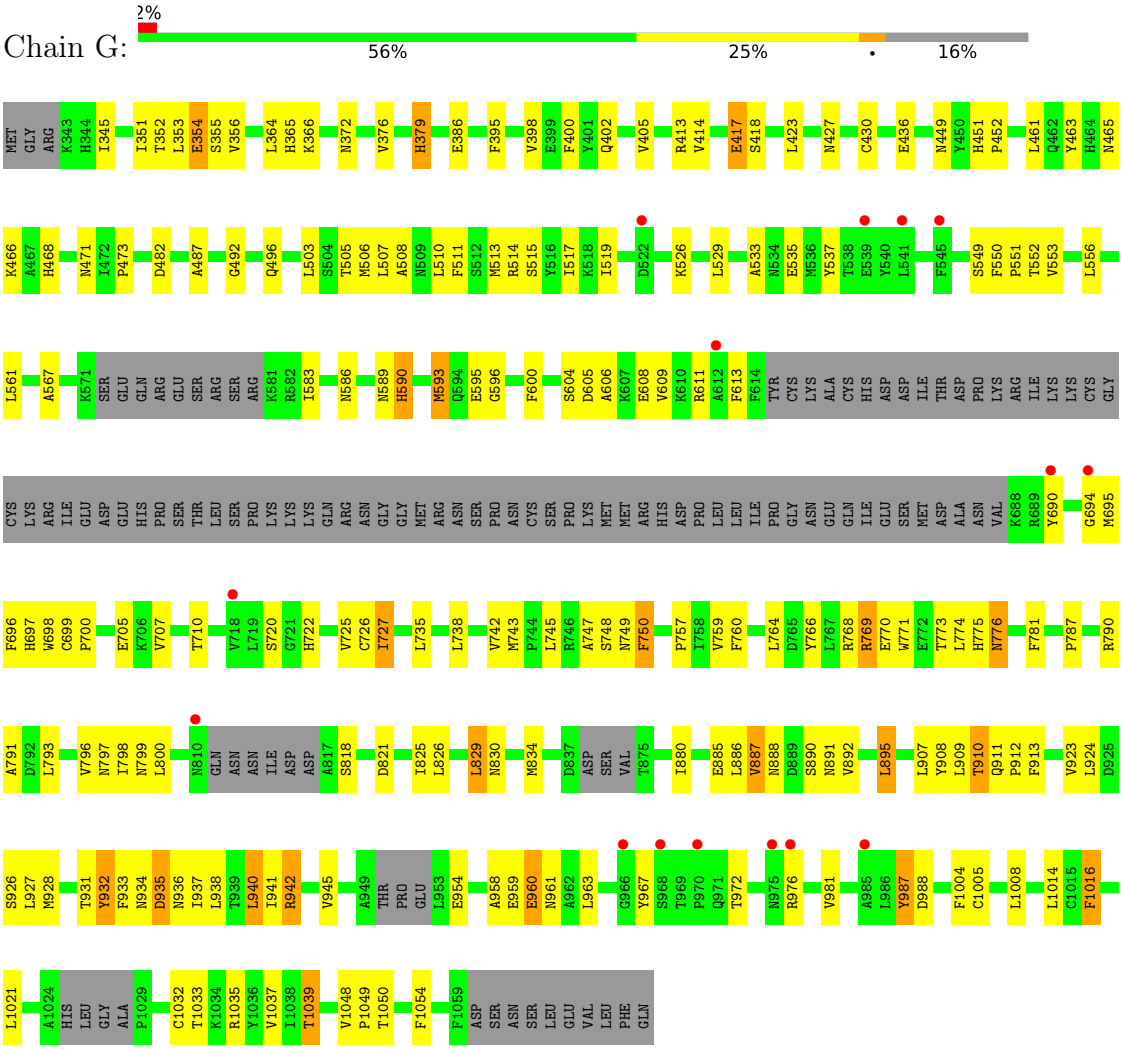
• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

Chain F:



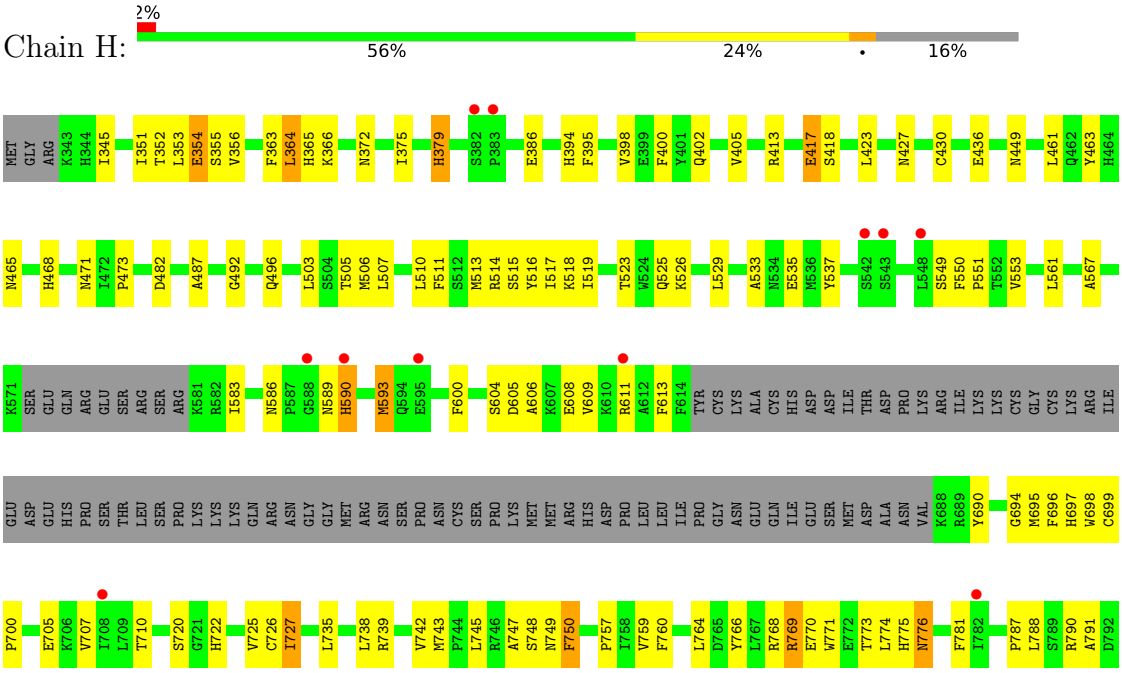
• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

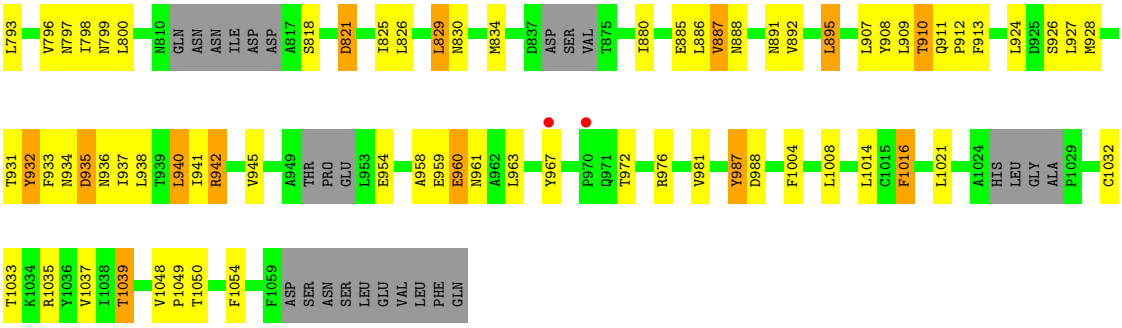
Chain G:



• Molecule 1: High-Conductance Ca2+-Activated K+ Channel protein

Chain H:




L793
V796
N797
I798
N799
L800
N810
GLN
ASN
ASN
ILE
ASP
ASP
A817
S818
D821
I825
L826
L829
N830
M834
D837
ASP
SER
VAL
T875
I880
E885
L886
V887
N888
N891
V892
L895
L907
Y908
L909
T910
Q911
P912
F913
L924
D925
S926
L927
M928
T931
Y932
F933
N934
D935
N936
I937
L938
T939
L940
I941
R942
V945
A949
THR
PRO
GLU
L953
E954
A958
E959
E960
N961
A962
L963
Y967
P970
Q971
T972
R976
V981
Y987
D988
F1004
L1008
L1014
C1015
F1016
L1021
A1024
HIS
LEU
GLY
ALA
P1029
C1032
T1033
K1034
R1035
Y1036
V1037
I1038
T1039
V1048
P1049
T1050
F1054
F1059
ASP
SER
ASN
SER
LEU
GLU
VAL
LEU
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.65Å 210.82Å 238.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 3.61 48.21 – 3.61	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.22-3.61) 89.1 (48.21-3.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 3.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.289 0.258 , 0.286	Depositor DCC
R_{free} test set	3620 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	91.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	34504	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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	A	0.42	0/4398	0.56	0/6001
1	B	0.42	1/4398 (0.0%)	0.56	0/6001
1	C	0.43	0/4398	0.56	0/6001
1	D	0.42	1/4398 (0.0%)	0.56	0/6001
1	E	0.43	0/4398	0.57	0/6001
1	F	0.43	0/4398	0.57	0/6001
1	G	0.42	0/4398	0.56	0/6001
1	H	0.41	0/4398	0.56	0/6001
All	All	0.42	2/35184 (0.0%)	0.56	0/48008

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	698	TRP	CD2-CE2	5.27	1.47	1.41
1	D	698	TRP	CD2-CE2	5.12	1.47	1.41

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	4312	0	4016	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4312	0	4016	144	0
1	C	4312	0	4017	145	0
1	D	4312	0	4016	148	1
1	E	4312	0	4017	147	1
1	F	4312	0	4017	147	1
1	G	4312	0	4017	155	1
1	H	4312	0	4017	145	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
All	All	34504	0	32133	1117	2

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 17.

All (1117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:PHE:CZ	1:B:941:ILE:CG2	2.27	1.17
1:G:511:PHE:CZ	1:G:941:ILE:CG2	2.28	1.17
1:H:511:PHE:CZ	1:H:941:ILE:CG2	2.28	1.16
1:C:511:PHE:CZ	1:C:941:ILE:CG2	2.29	1.15
1:E:511:PHE:CZ	1:E:941:ILE:CG2	2.29	1.15
1:D:511:PHE:CZ	1:D:941:ILE:CG2	2.30	1.15
1:F:511:PHE:CZ	1:F:941:ILE:CG2	2.30	1.14
1:A:511:PHE:CZ	1:A:941:ILE:CG2	2.30	1.13
1:B:413:ARG:HD2	1:E:413:ARG:HD2	1.29	1.11
1:F:413:ARG:HD2	1:G:413:ARG:HD2	1.27	1.08
1:B:511:PHE:CZ	1:B:941:ILE:HG21	1.88	1.08
1:G:511:PHE:CE1	1:G:941:ILE:HG21	1.89	1.07
1:H:511:PHE:CE1	1:H:941:ILE:HG21	1.90	1.07
1:B:511:PHE:CE1	1:B:941:ILE:HG21	1.92	1.05
1:D:511:PHE:CZ	1:D:941:ILE:HG21	1.90	1.05
1:H:511:PHE:CZ	1:H:941:ILE:HG21	1.90	1.05
1:G:511:PHE:CZ	1:G:941:ILE:HG21	1.89	1.05
1:A:511:PHE:CZ	1:A:941:ILE:HG21	1.92	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:PHE:CE1	1:C:941:ILE:HG21	1.90	1.04
1:D:413:ARG:HD2	1:H:413:ARG:HD2	1.36	1.04
1:D:511:PHE:CE1	1:D:941:ILE:HG21	1.92	1.04
1:E:511:PHE:CE1	1:E:941:ILE:HG21	1.92	1.04
1:A:511:PHE:CE1	1:A:941:ILE:HG21	1.93	1.04
1:C:511:PHE:CZ	1:C:941:ILE:HG21	1.93	1.03
1:F:511:PHE:CE1	1:F:941:ILE:HG21	1.92	1.03
1:E:511:PHE:CZ	1:E:941:ILE:HG21	1.92	1.02
1:F:496:GLN:HB3	1:F:503:LEU:HD23	1.42	1.01
1:B:496:GLN:HB3	1:B:503:LEU:HD23	1.42	1.01
1:D:496:GLN:HB3	1:D:503:LEU:HD23	1.41	1.01
1:C:496:GLN:HB3	1:C:503:LEU:HD23	1.40	1.00
1:F:511:PHE:CZ	1:F:941:ILE:HG21	1.93	1.00
1:H:496:GLN:HB3	1:H:503:LEU:HD23	1.45	0.99
1:D:960:GLU:OE1	1:E:791:ALA:HB2	1.63	0.99
1:E:496:GLN:HB3	1:E:503:LEU:HD23	1.41	0.99
1:A:496:GLN:HB3	1:A:503:LEU:HD23	1.44	0.99
1:G:496:GLN:HB3	1:G:503:LEU:HD23	1.42	0.98
1:G:511:PHE:HZ	1:G:941:ILE:CG2	1.71	0.97
1:C:511:PHE:HZ	1:C:941:ILE:CG2	1.73	0.96
1:B:511:PHE:HZ	1:B:941:ILE:CG2	1.70	0.96
1:E:793:LEU:HG	1:E:798:ILE:HD11	1.46	0.94
1:A:413:ARG:HD2	1:C:413:ARG:HD2	1.48	0.94
1:H:511:PHE:HZ	1:H:941:ILE:CG2	1.72	0.94
1:D:471:ASN:OD1	1:E:790:ARG:NH2	2.01	0.94
1:F:511:PHE:HZ	1:F:941:ILE:CG2	1.74	0.94
1:H:793:LEU:HG	1:H:798:ILE:HD11	1.50	0.94
1:E:511:PHE:HZ	1:E:941:ILE:CG2	1.74	0.94
1:F:793:LEU:HG	1:F:798:ILE:HD11	1.50	0.93
1:G:793:LEU:HG	1:G:798:ILE:HD11	1.49	0.93
1:A:793:LEU:HG	1:A:798:ILE:HD11	1.50	0.93
1:D:511:PHE:HZ	1:D:941:ILE:CG2	1.74	0.93
1:A:511:PHE:HZ	1:A:941:ILE:CG2	1.75	0.91
1:D:793:LEU:HG	1:D:798:ILE:HD11	1.52	0.91
1:C:793:LEU:HG	1:C:798:ILE:HD11	1.50	0.91
1:B:793:LEU:HG	1:B:798:ILE:HD11	1.52	0.88
1:E:473:PRO:HD2	1:F:829:LEU:HD12	1.58	0.86
1:B:345:ILE:HG21	1:B:932:TYR:HE1	1.41	0.85
1:F:345:ILE:HG21	1:F:932:TYR:HE1	1.42	0.84
1:G:511:PHE:CZ	1:G:941:ILE:HG22	2.11	0.84
1:C:511:PHE:CZ	1:C:941:ILE:HG22	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ILE:HG21	1:D:932:TYR:HE1	1.43	0.84
1:E:345:ILE:HG21	1:E:932:TYR:HE1	1.43	0.84
1:H:511:PHE:CZ	1:H:941:ILE:HG22	2.13	0.83
1:C:345:ILE:HG21	1:C:932:TYR:HE1	1.43	0.83
1:G:345:ILE:HG21	1:G:932:TYR:HE1	1.45	0.82
1:D:511:PHE:CZ	1:D:941:ILE:HG22	2.15	0.81
1:H:747:ALA:HB3	1:H:750:PHE:HE2	1.43	0.81
1:B:747:ALA:HB3	1:B:750:PHE:HE2	1.44	0.81
1:H:345:ILE:HG21	1:H:932:TYR:HE1	1.46	0.81
1:A:511:PHE:CZ	1:A:941:ILE:HG22	2.15	0.81
1:E:511:PHE:CZ	1:E:941:ILE:HG22	2.14	0.81
1:F:511:PHE:CZ	1:F:941:ILE:HG22	2.13	0.81
1:A:345:ILE:HG21	1:A:932:TYR:HE1	1.45	0.81
1:D:747:ALA:HB3	1:D:750:PHE:HE2	1.44	0.80
1:C:747:ALA:HB3	1:C:750:PHE:HE2	1.47	0.79
1:F:413:ARG:HD2	1:G:413:ARG:CD	2.11	0.79
1:B:511:PHE:CZ	1:B:941:ILE:HG22	2.15	0.79
1:D:503:LEU:HD22	1:D:981:VAL:HG11	1.65	0.79
1:A:747:ALA:HB3	1:A:750:PHE:HE2	1.48	0.79
1:G:747:ALA:HB3	1:G:750:PHE:HE2	1.47	0.79
1:B:503:LEU:HD22	1:B:981:VAL:HG11	1.65	0.78
1:C:503:LEU:HD22	1:C:981:VAL:HG11	1.64	0.78
1:F:503:LEU:HD22	1:F:981:VAL:HG11	1.65	0.78
1:E:473:PRO:CD	1:F:829:LEU:HD12	2.14	0.78
1:E:747:ALA:HB3	1:E:750:PHE:HE2	1.48	0.78
1:A:503:LEU:HD22	1:A:981:VAL:HG11	1.64	0.78
1:F:747:ALA:HB3	1:F:750:PHE:HE2	1.46	0.78
1:B:960:GLU:OE2	1:B:960:GLU:HA	1.84	0.77
1:E:503:LEU:HD22	1:E:981:VAL:HG11	1.66	0.77
1:H:503:LEU:HD22	1:H:981:VAL:HG11	1.64	0.77
1:D:960:GLU:HA	1:D:960:GLU:OE2	1.84	0.77
1:F:960:GLU:HA	1:F:960:GLU:OE2	1.84	0.76
1:E:793:LEU:HG	1:E:798:ILE:CD1	2.15	0.76
1:F:413:ARG:HD2	1:G:413:ARG:HH11	1.51	0.76
1:G:960:GLU:OE2	1:G:960:GLU:HA	1.87	0.75
1:G:503:LEU:HD22	1:G:981:VAL:HG11	1.66	0.75
1:C:366:LYS:NZ	1:C:533:ALA:O	2.18	0.74
1:B:471:ASN:OD1	1:H:790:ARG:NH2	2.18	0.74
1:H:960:GLU:OE2	1:H:960:GLU:HA	1.86	0.74
1:A:960:GLU:OE1	1:G:791:ALA:HB2	1.87	0.74
1:A:960:GLU:CD	1:G:791:ALA:HB2	2.09	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:NZ	1:A:533:ALA:O	2.18	0.73
1:C:960:GLU:OE2	1:C:960:GLU:HA	1.87	0.73
1:A:960:GLU:OE2	1:A:960:GLU:HA	1.87	0.73
1:B:441:ILE:HG21	1:H:826:LEU:HD21	1.71	0.73
1:F:413:ARG:CD	1:G:413:ARG:HD2	2.13	0.73
1:B:511:PHE:HZ	1:B:941:ILE:HG22	1.53	0.72
1:G:818:SER:HB2	1:G:887:VAL:HG11	1.72	0.72
1:C:511:PHE:HZ	1:C:941:ILE:HG22	1.50	0.72
1:C:790:ARG:NH2	1:F:471:ASN:OD1	2.23	0.72
1:B:366:LYS:NZ	1:B:533:ALA:O	2.20	0.72
1:E:707:VAL:HG13	1:E:781:PHE:HA	1.72	0.71
1:E:366:LYS:NZ	1:E:533:ALA:O	2.20	0.71
1:F:413:ARG:HD2	1:G:413:ARG:NH1	2.04	0.71
1:A:793:LEU:HG	1:A:798:ILE:CD1	2.20	0.71
1:E:960:GLU:OE2	1:E:960:GLU:HA	1.89	0.71
1:H:793:LEU:HG	1:H:798:ILE:CD1	2.20	0.71
1:B:726:CYS:HB2	1:B:787:PRO:HG3	1.73	0.71
1:D:932:TYR:C	1:D:932:TYR:CD2	2.64	0.71
1:A:818:SER:HB2	1:A:887:VAL:HG11	1.73	0.71
1:E:506:MET:CG	1:E:1039:THR:HG23	2.21	0.71
1:F:793:LEU:HG	1:F:798:ILE:CD1	2.20	0.71
1:F:413:ARG:HH11	1:G:413:ARG:CD	2.04	0.70
1:F:735:LEU:HD22	1:F:770:GLU:HG3	1.73	0.70
1:E:818:SER:HB2	1:E:887:VAL:HG11	1.73	0.70
1:H:726:CYS:HB2	1:H:787:PRO:HG3	1.73	0.70
1:H:818:SER:HB2	1:H:887:VAL:HG11	1.73	0.70
1:B:707:VAL:HG13	1:B:781:PHE:HA	1.74	0.70
1:A:932:TYR:C	1:A:932:TYR:CD2	2.64	0.70
1:G:793:LEU:HG	1:G:798:ILE:CD1	2.20	0.70
1:C:793:LEU:HG	1:C:798:ILE:CD1	2.22	0.70
1:D:726:CYS:HB2	1:D:787:PRO:HG3	1.73	0.70
1:G:932:TYR:C	1:G:932:TYR:CD2	2.65	0.70
1:D:793:LEU:HG	1:D:798:ILE:CD1	2.21	0.69
1:B:932:TYR:C	1:B:932:TYR:CD2	2.65	0.69
1:B:793:LEU:HG	1:B:798:ILE:CD1	2.22	0.69
1:G:735:LEU:HD22	1:G:770:GLU:HG3	1.74	0.69
1:A:471:ASN:OD1	1:G:790:ARG:NH2	2.25	0.69
1:F:511:PHE:HZ	1:F:941:ILE:HG22	1.52	0.69
1:H:735:LEU:HD22	1:H:770:GLU:HG3	1.74	0.69
1:B:735:LEU:HD22	1:B:770:GLU:HG3	1.75	0.69
1:E:449:ASN:ND2	1:F:894:PHE:HA	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:932:TYR:C	1:F:932:TYR:CD2	2.66	0.69
1:H:366:LYS:NZ	1:H:533:ALA:O	2.21	0.69
1:C:818:SER:HB2	1:C:887:VAL:HG11	1.73	0.69
1:E:932:TYR:C	1:E:932:TYR:CD2	2.66	0.69
1:F:707:VAL:HG13	1:F:781:PHE:HA	1.74	0.69
1:C:932:TYR:C	1:C:932:TYR:CD2	2.66	0.68
1:G:511:PHE:HZ	1:G:941:ILE:HG22	1.48	0.68
1:C:726:CYS:HB2	1:C:787:PRO:HG3	1.74	0.68
1:A:511:PHE:HZ	1:A:941:ILE:HG22	1.55	0.68
1:A:735:LEU:HD22	1:A:770:GLU:HG3	1.74	0.68
1:D:506:MET:CG	1:D:1039:THR:HG23	2.24	0.68
1:E:735:LEU:HD22	1:E:770:GLU:HG3	1.74	0.68
1:C:707:VAL:HG13	1:C:781:PHE:HA	1.76	0.68
1:G:707:VAL:HG13	1:G:781:PHE:HA	1.75	0.68
1:H:707:VAL:HG13	1:H:781:PHE:HA	1.75	0.68
1:A:726:CYS:HB2	1:A:787:PRO:HG3	1.74	0.67
1:E:726:CYS:HB2	1:E:787:PRO:HG3	1.74	0.67
1:F:413:ARG:CD	1:G:413:ARG:NH1	2.57	0.67
1:H:932:TYR:C	1:H:932:TYR:CD2	2.66	0.67
1:D:707:VAL:HG13	1:D:781:PHE:HA	1.74	0.67
1:B:506:MET:CG	1:B:1039:THR:HG23	2.24	0.67
1:C:549:SER:HB2	1:C:589:ASN:O	1.93	0.67
1:B:818:SER:HB2	1:B:887:VAL:HG11	1.75	0.67
1:A:707:VAL:HG13	1:A:781:PHE:HA	1.76	0.67
1:G:726:CYS:HB2	1:G:787:PRO:HG3	1.74	0.67
1:A:892:VAL:HG21	1:A:907:LEU:CD1	2.25	0.67
1:D:366:LYS:NZ	1:D:533:ALA:O	2.24	0.67
1:D:549:SER:HB2	1:D:589:ASN:O	1.95	0.67
1:C:735:LEU:HD22	1:C:770:GLU:HG3	1.75	0.67
1:F:549:SER:HB2	1:F:589:ASN:O	1.95	0.67
1:C:345:ILE:HG21	1:C:932:TYR:CE1	2.30	0.66
1:G:366:LYS:NZ	1:G:514:ARG:O	2.28	0.66
1:D:818:SER:HB2	1:D:887:VAL:HG11	1.76	0.66
1:G:506:MET:CG	1:G:1039:THR:HG23	2.26	0.66
1:E:345:ILE:HG21	1:E:932:TYR:CE1	2.30	0.66
1:F:413:ARG:CD	1:G:413:ARG:HH11	2.08	0.66
1:B:549:SER:HB2	1:B:589:ASN:O	1.95	0.66
1:A:492:GLY:HA3	1:A:945:VAL:CG1	2.26	0.66
1:D:735:LEU:HD22	1:D:770:GLU:HG3	1.76	0.66
1:F:818:SER:HB2	1:F:887:VAL:HG11	1.76	0.66
1:E:549:SER:HB2	1:E:589:ASN:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:549:SER:HB2	1:H:589:ASN:O	1.96	0.66
1:B:605:ASP:HB3	1:B:608:GLU:HG2	1.78	0.66
1:H:892:VAL:HG21	1:H:907:LEU:CD1	2.26	0.66
1:B:960:GLU:CD	1:H:791:ALA:HB2	2.16	0.65
1:A:892:VAL:HG21	1:A:907:LEU:HD13	1.78	0.65
1:D:505:THR:HG21	1:D:913:PHE:O	1.94	0.65
1:E:511:PHE:HZ	1:E:941:ILE:HG22	1.53	0.65
1:F:505:THR:HG21	1:F:913:PHE:O	1.96	0.65
1:B:492:GLY:HA3	1:B:945:VAL:CG1	2.27	0.65
1:F:366:LYS:NZ	1:F:514:ARG:O	2.29	0.65
1:F:726:CYS:HB2	1:F:787:PRO:HG3	1.78	0.65
1:G:892:VAL:HG21	1:G:907:LEU:HD13	1.79	0.65
1:E:394:HIS:HE1	1:H:394:HIS:HE1	1.44	0.65
1:G:505:THR:HG21	1:G:913:PHE:O	1.96	0.65
1:B:471:ASN:HB3	1:H:830:ASN:HA	1.79	0.65
1:H:505:THR:HG21	1:H:913:PHE:O	1.97	0.65
1:D:366:LYS:NZ	1:D:514:ARG:O	2.30	0.65
1:F:492:GLY:HA3	1:F:945:VAL:CG1	2.27	0.65
1:F:892:VAL:HG21	1:F:907:LEU:HD13	1.79	0.65
1:A:345:ILE:HG21	1:A:932:TYR:CE1	2.31	0.65
1:A:825:ILE:O	1:A:829:LEU:HD23	1.96	0.65
1:C:492:GLY:HA3	1:C:945:VAL:CG1	2.26	0.65
1:E:366:LYS:NZ	1:E:514:ARG:O	2.30	0.64
1:H:892:VAL:HG21	1:H:907:LEU:HD13	1.80	0.64
1:C:892:VAL:HG21	1:C:907:LEU:HD13	1.79	0.64
1:G:549:SER:HB2	1:G:589:ASN:O	1.97	0.64
1:B:829:LEU:HD12	1:G:473:PRO:HD2	1.80	0.64
1:F:506:MET:CG	1:F:1039:THR:HG23	2.27	0.64
1:B:960:GLU:OE1	1:H:791:ALA:HB2	1.98	0.64
1:C:605:ASP:HB3	1:C:608:GLU:HG2	1.80	0.64
1:D:492:GLY:HA3	1:D:945:VAL:CG1	2.28	0.64
1:E:720:SER:HB2	1:E:800:LEU:HB3	1.80	0.64
1:G:605:ASP:HB3	1:G:608:GLU:HG2	1.80	0.64
1:F:413:ARG:HH11	1:G:413:ARG:HD2	1.62	0.64
1:H:605:ASP:HB3	1:H:608:GLU:HG2	1.78	0.64
1:H:825:ILE:O	1:H:829:LEU:HD23	1.98	0.64
1:A:549:SER:HB2	1:A:589:ASN:O	1.98	0.64
1:D:1016:PHE:HE1	1:D:1054:PHE:HB3	1.63	0.64
1:F:825:ILE:O	1:F:829:LEU:HD23	1.98	0.64
1:G:366:LYS:NZ	1:G:533:ALA:O	2.25	0.64
1:H:492:GLY:HA3	1:H:945:VAL:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:492:GLY:HA3	1:E:945:VAL:CG1	2.28	0.63
1:E:892:VAL:HG21	1:E:907:LEU:CD1	2.28	0.63
1:F:892:VAL:HG21	1:F:907:LEU:CD1	2.29	0.63
1:G:492:GLY:HA3	1:G:945:VAL:CG1	2.28	0.63
1:A:506:MET:CG	1:A:1039:THR:HG23	2.28	0.63
1:D:908:TYR:HA	1:D:913:PHE:CD2	2.33	0.63
1:E:394:HIS:CE1	1:H:394:HIS:HE1	2.16	0.63
1:H:506:MET:CG	1:H:1039:THR:HG23	2.27	0.63
1:B:825:ILE:O	1:B:829:LEU:HD23	1.99	0.63
1:C:517:ILE:HD12	1:C:529:LEU:HD22	1.81	0.63
1:C:892:VAL:HG21	1:C:907:LEU:CD1	2.28	0.63
1:D:605:ASP:HB3	1:D:608:GLU:HG2	1.81	0.63
1:C:366:LYS:NZ	1:C:514:ARG:O	2.32	0.63
1:F:366:LYS:NZ	1:F:533:ALA:O	2.25	0.63
1:F:345:ILE:HG21	1:F:932:TYR:CE1	2.29	0.63
1:F:908:TYR:HA	1:F:913:PHE:CD2	2.34	0.63
1:E:892:VAL:HG21	1:E:907:LEU:HD13	1.81	0.62
1:B:505:THR:HG21	1:B:913:PHE:O	1.99	0.62
1:C:506:MET:CG	1:C:1039:THR:HG23	2.29	0.62
1:A:366:LYS:NZ	1:A:514:ARG:O	2.31	0.62
1:A:932:TYR:C	1:A:932:TYR:HD2	2.03	0.62
1:A:605:ASP:HB3	1:A:608:GLU:HG2	1.80	0.62
1:D:932:TYR:C	1:D:932:TYR:HD2	2.01	0.62
1:G:1016:PHE:CE1	1:G:1054:PHE:HB3	2.35	0.62
1:C:505:THR:HG21	1:C:913:PHE:O	1.99	0.62
1:D:345:ILE:HG21	1:D:932:TYR:CE1	2.31	0.62
1:D:1016:PHE:CE1	1:D:1054:PHE:HB3	2.34	0.62
1:A:505:THR:HG21	1:A:913:PHE:O	2.00	0.62
1:F:605:ASP:HB3	1:F:608:GLU:HG2	1.81	0.61
1:F:941:ILE:HG13	1:F:942:ARG:N	2.15	0.61
1:C:511:PHE:CE1	1:C:941:ILE:CG2	2.68	0.61
1:D:941:ILE:HG13	1:D:942:ARG:N	2.16	0.61
1:E:537:TYR:HB2	1:E:609:VAL:HG21	1.82	0.61
1:B:830:ASN:HA	1:G:471:ASN:HB3	1.82	0.61
1:B:932:TYR:C	1:B:932:TYR:HD2	2.04	0.61
1:E:605:ASP:HB3	1:E:608:GLU:HG2	1.82	0.61
1:H:345:ILE:HG21	1:H:932:TYR:CE1	2.32	0.61
1:B:366:LYS:NZ	1:B:514:ARG:O	2.33	0.61
1:G:908:TYR:HA	1:G:913:PHE:CD2	2.36	0.61
1:G:892:VAL:HG21	1:G:907:LEU:CD1	2.30	0.61
1:G:932:TYR:C	1:G:932:TYR:HD2	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:ILE:HD12	1:E:529:LEU:HD22	1.82	0.61
1:F:1016:PHE:CE1	1:F:1054:PHE:HB3	2.35	0.61
1:E:506:MET:HB2	1:E:1037:VAL:HG11	1.82	0.61
1:G:1016:PHE:HE1	1:G:1054:PHE:HB3	1.64	0.61
1:E:505:THR:HG21	1:E:913:PHE:O	1.99	0.61
1:E:932:TYR:C	1:E:932:TYR:HD2	2.04	0.61
1:F:1016:PHE:HE1	1:F:1054:PHE:HB3	1.64	0.61
1:H:366:LYS:NZ	1:H:514:ARG:O	2.34	0.61
1:B:908:TYR:HA	1:B:913:PHE:CD2	2.36	0.60
1:G:941:ILE:HG13	1:G:942:ARG:N	2.16	0.60
1:F:506:MET:HB2	1:F:1037:VAL:HG11	1.82	0.60
1:A:1016:PHE:CE1	1:A:1054:PHE:HB3	2.36	0.60
1:H:517:ILE:HD12	1:H:529:LEU:HD22	1.84	0.60
1:E:1016:PHE:CE1	1:E:1054:PHE:HB3	2.37	0.60
1:F:517:ILE:HD12	1:F:529:LEU:HD22	1.82	0.60
1:B:892:VAL:HG21	1:B:907:LEU:HD13	1.84	0.60
1:G:517:ILE:HD12	1:G:529:LEU:HD22	1.84	0.60
1:A:1016:PHE:HE1	1:A:1054:PHE:HB3	1.66	0.60
1:C:908:TYR:HA	1:C:913:PHE:CD2	2.36	0.60
1:E:1016:PHE:HE1	1:E:1054:PHE:HB3	1.65	0.60
1:G:345:ILE:HG21	1:G:932:TYR:CE1	2.31	0.60
1:G:720:SER:HB2	1:G:800:LEU:HB3	1.84	0.60
1:C:903:PRO:HD3	1:F:408:PRO:HG2	1.84	0.60
1:C:1016:PHE:HE1	1:C:1054:PHE:HB3	1.67	0.60
1:B:941:ILE:HG13	1:B:942:ARG:N	2.17	0.60
1:D:517:ILE:HD12	1:D:529:LEU:HD22	1.82	0.60
1:D:825:ILE:O	1:D:829:LEU:HD23	2.02	0.60
1:H:379:HIS:HD2	1:H:402:GLN:HA	1.67	0.60
1:D:553:VAL:HG21	1:D:593:MET:HE3	1.84	0.59
1:A:941:ILE:HG13	1:A:942:ARG:N	2.17	0.59
1:C:1016:PHE:CE1	1:C:1054:PHE:HB3	2.37	0.59
1:E:1048:VAL:HG13	1:E:1049:PRO:HD2	1.84	0.59
1:H:1016:PHE:CE1	1:H:1054:PHE:HB3	2.37	0.59
1:H:1016:PHE:HE1	1:H:1054:PHE:HB3	1.68	0.59
1:H:932:TYR:C	1:H:932:TYR:HD2	2.05	0.59
1:H:941:ILE:HG13	1:H:942:ARG:N	2.16	0.59
1:A:960:GLU:OE1	1:G:791:ALA:CB	2.50	0.59
1:E:908:TYR:HA	1:E:913:PHE:CD2	2.38	0.59
1:C:932:TYR:C	1:C:932:TYR:HD2	2.06	0.59
1:D:379:HIS:HD2	1:D:402:GLN:HA	1.67	0.59
1:A:1048:VAL:HG12	1:A:1050:THR:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:HIS:HD2	1:A:402:GLN:HA	1.67	0.59
1:A:506:MET:HB2	1:A:1037:VAL:HG11	1.85	0.59
1:B:345:ILE:HG21	1:B:932:TYR:CE1	2.30	0.59
1:F:932:TYR:C	1:F:932:TYR:HD2	2.05	0.59
1:E:506:MET:HG3	1:E:1039:THR:HG23	1.84	0.58
1:G:379:HIS:HD2	1:G:402:GLN:HA	1.68	0.58
1:A:720:SER:HB2	1:A:800:LEU:HB3	1.85	0.58
1:B:1048:VAL:HG13	1:B:1049:PRO:HD2	1.84	0.58
1:B:892:VAL:HG21	1:B:907:LEU:CD1	2.33	0.58
1:D:1048:VAL:HG12	1:D:1050:THR:H	1.68	0.58
1:D:561:LEU:O	1:D:611:ARG:NH2	2.36	0.58
1:F:379:HIS:HD2	1:F:402:GLN:HA	1.69	0.58
1:B:517:ILE:HD12	1:B:529:LEU:HD22	1.84	0.58
1:E:379:HIS:HD2	1:E:402:GLN:HA	1.68	0.58
1:H:908:TYR:HA	1:H:913:PHE:CD2	2.39	0.58
1:B:750:PHE:N	1:B:750:PHE:CD2	2.71	0.58
1:D:720:SER:HB2	1:D:800:LEU:HB3	1.86	0.58
1:E:511:PHE:CE1	1:E:941:ILE:CG2	2.70	0.58
1:H:720:SER:HB2	1:H:800:LEU:HB3	1.85	0.58
1:D:511:PHE:CE1	1:D:941:ILE:CG2	2.72	0.58
1:E:941:ILE:HG13	1:E:942:ARG:N	2.18	0.58
1:F:553:VAL:HG21	1:F:593:MET:HE3	1.86	0.58
1:G:561:LEU:O	1:G:611:ARG:NH2	2.37	0.58
1:A:517:ILE:HD12	1:A:529:LEU:HD22	1.85	0.58
1:B:1016:PHE:CE1	1:B:1054:PHE:HB3	2.38	0.58
1:C:941:ILE:HG13	1:C:942:ARG:N	2.18	0.58
1:C:379:HIS:HD2	1:C:402:GLN:HA	1.68	0.57
1:E:561:LEU:O	1:E:611:ARG:NH2	2.37	0.57
1:G:818:SER:HB2	1:G:887:VAL:CG1	2.33	0.57
1:G:825:ILE:O	1:G:829:LEU:HD23	2.03	0.57
1:F:720:SER:HB2	1:F:800:LEU:HB3	1.86	0.57
1:G:1048:VAL:HG12	1:G:1050:THR:H	1.69	0.57
1:C:825:ILE:O	1:C:829:LEU:HD23	2.04	0.57
1:F:561:LEU:O	1:F:611:ARG:NH2	2.37	0.57
1:H:561:LEU:O	1:H:611:ARG:NH2	2.38	0.57
1:A:830:ASN:HA	1:H:471:ASN:HB3	1.87	0.57
1:C:398:VAL:CG1	1:C:400:PHE:HE2	2.17	0.57
1:C:449:ASN:ND2	1:D:894:PHE:HA	2.20	0.57
1:C:506:MET:HB2	1:C:1037:VAL:HG11	1.86	0.57
1:A:695:MET:C	1:A:696:PHE:HD2	2.08	0.57
1:B:379:HIS:HD2	1:B:402:GLN:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:892:VAL:HG21	1:D:907:LEU:HD13	1.86	0.57
1:E:825:ILE:O	1:E:829:LEU:HD23	2.03	0.57
1:A:553:VAL:HG21	1:A:593:MET:HE3	1.87	0.57
1:D:506:MET:HB2	1:D:1037:VAL:HG11	1.87	0.57
1:G:938:LEU:HD12	1:G:941:ILE:HD11	1.87	0.57
1:H:465:ASN:HA	1:H:468:HIS:HD2	1.70	0.57
1:C:553:VAL:HG21	1:C:593:MET:HE3	1.87	0.57
1:D:1048:VAL:HG13	1:D:1049:PRO:HD2	1.86	0.57
1:B:695:MET:C	1:B:696:PHE:HD2	2.08	0.57
1:C:818:SER:HB2	1:C:887:VAL:CG1	2.35	0.57
1:G:750:PHE:N	1:G:750:PHE:CD2	2.73	0.57
1:F:1048:VAL:HG12	1:F:1050:THR:H	1.69	0.57
1:B:561:LEU:O	1:B:611:ARG:NH2	2.38	0.56
1:C:561:LEU:O	1:C:611:ARG:NH2	2.38	0.56
1:A:818:SER:HB2	1:A:887:VAL:CG1	2.35	0.56
1:B:1016:PHE:HE1	1:B:1054:PHE:HB3	1.70	0.56
1:F:537:TYR:HB2	1:F:609:VAL:HG21	1.87	0.56
1:C:1048:VAL:HG13	1:C:1049:PRO:HD2	1.88	0.56
1:D:465:ASN:HA	1:D:468:HIS:HD2	1.70	0.56
1:D:695:MET:C	1:D:696:PHE:HD2	2.09	0.56
1:E:398:VAL:CG1	1:E:400:PHE:HE2	2.18	0.56
1:F:398:VAL:CG1	1:F:400:PHE:HE2	2.18	0.56
1:F:465:ASN:HA	1:F:468:HIS:HD2	1.70	0.56
1:F:910:THR:HB	1:F:912:PRO:HD2	1.86	0.56
1:D:892:VAL:HG21	1:D:907:LEU:CD1	2.34	0.56
1:A:465:ASN:HA	1:A:468:HIS:HD2	1.69	0.56
1:B:886:LEU:HD11	1:B:895:LEU:HD21	1.88	0.56
1:E:818:SER:HB2	1:E:887:VAL:CG1	2.36	0.56
1:G:398:VAL:CG1	1:G:400:PHE:HE2	2.18	0.56
1:H:398:VAL:CG1	1:H:400:PHE:HE2	2.19	0.56
1:B:818:SER:HB2	1:B:887:VAL:CG1	2.36	0.56
1:B:1048:VAL:HG12	1:B:1050:THR:H	1.71	0.56
1:E:935:ASP:OD1	1:E:935:ASP:N	2.38	0.56
1:H:506:MET:HB2	1:H:1037:VAL:HG11	1.87	0.56
1:C:935:ASP:OD1	1:C:935:ASP:N	2.39	0.56
1:F:818:SER:HB2	1:F:887:VAL:CG1	2.36	0.56
1:H:818:SER:HB2	1:H:887:VAL:CG1	2.35	0.56
1:B:398:VAL:CG1	1:B:400:PHE:HE2	2.18	0.56
1:B:720:SER:HB2	1:B:800:LEU:HB3	1.86	0.56
1:D:511:PHE:HZ	1:D:941:ILE:HG22	1.53	0.56
1:D:935:ASP:N	1:D:935:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:TYR:HB2	1:A:609:VAL:HG21	1.87	0.56
1:A:750:PHE:N	1:A:750:PHE:CD2	2.74	0.56
1:B:506:MET:HB2	1:B:1037:VAL:HG11	1.86	0.56
1:F:553:VAL:HG21	1:F:593:MET:CE	2.36	0.56
1:G:910:THR:HB	1:G:912:PRO:HD2	1.88	0.56
1:B:894:PHE:HA	1:G:449:ASN:ND2	2.20	0.56
1:D:1021:LEU:HD23	1:D:1035:ARG:HG2	1.88	0.56
1:F:1048:VAL:HG13	1:F:1049:PRO:HD2	1.87	0.56
1:H:537:TYR:HB2	1:H:609:VAL:HG21	1.87	0.56
1:A:935:ASP:OD1	1:A:935:ASP:N	2.39	0.55
1:C:750:PHE:N	1:C:750:PHE:CD2	2.74	0.55
1:G:695:MET:C	1:G:696:PHE:HD2	2.09	0.55
1:C:553:VAL:HG21	1:C:593:MET:CE	2.36	0.55
1:A:398:VAL:CG1	1:A:400:PHE:HE2	2.19	0.55
1:C:1048:VAL:HG12	1:C:1050:THR:H	1.71	0.55
1:E:938:LEU:HD12	1:E:941:ILE:HD11	1.88	0.55
1:C:465:ASN:HA	1:C:468:HIS:HD2	1.71	0.55
1:C:695:MET:C	1:C:696:PHE:HD2	2.10	0.55
1:E:695:MET:C	1:E:696:PHE:HD2	2.09	0.55
1:E:750:PHE:N	1:E:750:PHE:CD2	2.73	0.55
1:E:1048:VAL:HG12	1:E:1050:THR:H	1.71	0.55
1:H:1048:VAL:HG12	1:H:1050:THR:H	1.71	0.55
1:D:750:PHE:N	1:D:750:PHE:CD2	2.74	0.55
1:E:590:HIS:ND1	1:E:590:HIS:N	2.54	0.55
1:G:1048:VAL:HG13	1:G:1049:PRO:HD2	1.87	0.55
1:H:935:ASP:OD1	1:H:935:ASP:N	2.40	0.55
1:A:441:ILE:HG21	1:G:826:LEU:HD21	1.89	0.55
1:F:750:PHE:N	1:F:750:PHE:CD2	2.74	0.55
1:G:506:MET:HB2	1:G:1037:VAL:HG11	1.86	0.55
1:G:463:TYR:C	1:G:463:TYR:CD2	2.80	0.55
1:G:465:ASN:HA	1:G:468:HIS:HD2	1.71	0.55
1:H:910:THR:HB	1:H:912:PRO:HD2	1.89	0.55
1:H:1021:LEU:HD23	1:H:1035:ARG:HG2	1.89	0.55
1:A:553:VAL:HG21	1:A:593:MET:CE	2.37	0.55
1:A:825:ILE:HD12	1:A:825:ILE:H	1.70	0.55
1:B:463:TYR:C	1:B:463:TYR:CD2	2.80	0.55
1:C:537:TYR:HB2	1:C:609:VAL:HG21	1.88	0.55
1:D:398:VAL:CG1	1:D:400:PHE:HE2	2.19	0.55
1:H:553:VAL:HG21	1:H:593:MET:CE	2.37	0.55
1:A:908:TYR:HA	1:A:913:PHE:CD2	2.41	0.55
1:C:720:SER:HB2	1:C:800:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:537:TYR:HB2	1:D:609:VAL:HG21	1.88	0.55
1:G:1021:LEU:HD23	1:G:1035:ARG:HG2	1.89	0.55
1:H:511:PHE:HZ	1:H:941:ILE:HG22	1.52	0.55
1:H:1048:VAL:HG13	1:H:1049:PRO:HD2	1.87	0.55
1:D:960:GLU:CD	1:E:791:ALA:HB2	2.28	0.55
1:A:561:LEU:O	1:A:611:ARG:NH2	2.40	0.54
1:C:1021:LEU:HD23	1:C:1035:ARG:HG2	1.89	0.54
1:H:695:MET:C	1:H:696:PHE:HD2	2.10	0.54
1:A:463:TYR:C	1:A:463:TYR:CD2	2.81	0.54
1:A:888:ASN:HB3	1:A:891:ASN:ND2	2.23	0.54
1:F:695:MET:C	1:F:696:PHE:HD2	2.11	0.54
1:D:553:VAL:HG21	1:D:593:MET:CE	2.38	0.54
1:G:553:VAL:HG21	1:G:593:MET:HE3	1.89	0.54
1:H:750:PHE:N	1:H:750:PHE:CD2	2.75	0.54
1:A:938:LEU:HD12	1:A:941:ILE:HD11	1.90	0.54
1:F:825:ILE:HD12	1:F:825:ILE:H	1.72	0.54
1:E:463:TYR:C	1:E:463:TYR:CD2	2.82	0.54
1:E:888:ASN:HB3	1:E:891:ASN:ND2	2.23	0.54
1:B:537:TYR:HB2	1:B:609:VAL:HG21	1.89	0.54
1:D:818:SER:HB2	1:D:887:VAL:CG1	2.37	0.54
1:D:910:THR:HB	1:D:912:PRO:HD2	1.89	0.54
1:E:519:ILE:HG22	1:E:526:LYS:HA	1.90	0.54
1:C:463:TYR:C	1:C:463:TYR:CD2	2.81	0.53
1:G:553:VAL:HG21	1:G:593:MET:CE	2.38	0.53
1:A:1048:VAL:HG13	1:A:1049:PRO:HD2	1.88	0.53
1:D:441:ILE:HG21	1:E:826:LEU:HD21	1.90	0.53
1:E:1021:LEU:HD23	1:E:1035:ARG:HG2	1.89	0.53
1:F:1021:LEU:HD23	1:F:1035:ARG:HG2	1.90	0.53
1:B:697:HIS:CE1	1:B:748:SER:HA	2.43	0.53
1:B:465:ASN:HA	1:B:468:HIS:HD2	1.72	0.53
1:B:590:HIS:ND1	1:B:590:HIS:N	2.56	0.53
1:B:825:ILE:H	1:B:825:ILE:HD12	1.72	0.53
1:C:605:ASP:OD1	1:C:606:ALA:N	2.41	0.53
1:E:825:ILE:HD12	1:E:825:ILE:H	1.72	0.53
1:F:935:ASP:OD1	1:F:935:ASP:N	2.41	0.53
1:C:461:LEU:O	1:C:487:ALA:HB2	2.09	0.53
1:F:590:HIS:ND1	1:F:590:HIS:N	2.57	0.53
1:D:605:ASP:OD1	1:D:606:ALA:N	2.41	0.53
1:D:825:ILE:HD12	1:D:825:ILE:H	1.73	0.53
1:G:886:LEU:HD11	1:G:895:LEU:HD21	1.90	0.53
1:D:697:HIS:CE1	1:D:748:SER:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:TYR:C	1:F:463:TYR:CD2	2.81	0.53
1:G:537:TYR:HB2	1:G:609:VAL:HG21	1.89	0.53
1:G:935:ASP:N	1:G:935:ASP:OD1	2.38	0.53
1:B:511:PHE:CE1	1:B:941:ILE:CG2	2.71	0.53
1:A:1021:LEU:HD23	1:A:1035:ARG:HG2	1.90	0.53
1:E:605:ASP:OD1	1:E:606:ALA:N	2.41	0.53
1:G:461:LEU:O	1:G:487:ALA:HB2	2.08	0.53
1:G:825:ILE:HD12	1:G:825:ILE:H	1.74	0.53
1:A:511:PHE:CE1	1:A:941:ILE:CG2	2.71	0.53
1:A:590:HIS:ND1	1:A:590:HIS:N	2.56	0.53
1:B:506:MET:HG3	1:B:1039:THR:HG23	1.90	0.53
1:B:553:VAL:HG21	1:B:593:MET:HE3	1.91	0.53
1:B:1021:LEU:HD23	1:B:1035:ARG:HG2	1.90	0.53
1:E:550:PHE:HB3	1:E:551:PRO:HD3	1.90	0.53
1:H:825:ILE:HD12	1:H:825:ILE:H	1.74	0.53
1:B:938:LEU:HD12	1:B:941:ILE:HD11	1.90	0.52
1:C:590:HIS:ND1	1:C:590:HIS:N	2.57	0.52
1:F:938:LEU:HD12	1:F:941:ILE:HD11	1.91	0.52
1:G:590:HIS:ND1	1:G:590:HIS:N	2.56	0.52
1:G:427:ASN:O	1:G:430:CYS:HB2	2.09	0.52
1:H:463:TYR:C	1:H:463:TYR:CD2	2.82	0.52
1:F:550:PHE:HB3	1:F:551:PRO:HD3	1.92	0.52
1:F:605:ASP:OD1	1:F:606:ALA:N	2.43	0.52
1:H:605:ASP:OD1	1:H:606:ALA:N	2.43	0.52
1:E:427:ASN:O	1:E:430:CYS:HB2	2.10	0.52
1:E:465:ASN:HA	1:E:468:HIS:HD2	1.72	0.52
1:E:720:SER:CB	1:E:800:LEU:HB3	2.39	0.52
1:G:605:ASP:OD1	1:G:606:ALA:N	2.42	0.52
1:A:605:ASP:OD1	1:A:606:ALA:N	2.42	0.52
1:B:550:PHE:HB3	1:B:551:PRO:HD3	1.90	0.52
1:C:910:THR:HB	1:C:912:PRO:HD2	1.91	0.52
1:B:722:HIS:HB3	1:B:757:PRO:HG2	1.90	0.52
1:H:427:ASN:O	1:H:430:CYS:HB2	2.10	0.52
1:H:590:HIS:ND1	1:H:590:HIS:N	2.57	0.52
1:A:427:ASN:O	1:A:430:CYS:HB2	2.09	0.52
1:B:519:ILE:HG22	1:B:526:LYS:HA	1.92	0.52
1:C:423:LEU:HD23	1:C:928:MET:HG3	1.91	0.52
1:G:934:ASN:HB2	1:G:937:ILE:HG12	1.92	0.52
1:D:550:PHE:HB3	1:D:551:PRO:HD3	1.92	0.52
1:F:722:HIS:HB3	1:F:757:PRO:HG2	1.91	0.52
1:F:797:ASN:HB3	1:F:800:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:722:HIS:HB3	1:H:757:PRO:HG2	1.92	0.52
1:B:935:ASP:N	1:B:935:ASP:OD1	2.38	0.52
1:H:461:LEU:O	1:H:487:ALA:HB2	2.10	0.52
1:B:605:ASP:OD1	1:B:606:ALA:N	2.43	0.51
1:B:910:THR:HB	1:B:912:PRO:HD2	1.91	0.51
1:E:797:ASN:HB3	1:E:800:LEU:HD12	1.91	0.51
1:F:720:SER:CB	1:F:800:LEU:HB3	2.41	0.51
1:B:366:LYS:HE3	1:B:515:SER:HA	1.93	0.51
1:B:553:VAL:HG21	1:B:593:MET:CE	2.40	0.51
1:D:590:HIS:ND1	1:D:590:HIS:N	2.57	0.51
1:E:553:VAL:HG21	1:E:593:MET:CE	2.39	0.51
1:B:423:LEU:HD23	1:B:928:MET:HG3	1.93	0.51
1:C:611:ARG:C	1:C:613:PHE:H	2.14	0.51
1:C:797:ASN:HB3	1:C:800:LEU:HD12	1.93	0.51
1:D:934:ASN:HB2	1:D:937:ILE:HG12	1.92	0.51
1:H:423:LEU:HD23	1:H:928:MET:HG3	1.93	0.51
1:H:553:VAL:HG21	1:H:593:MET:HE3	1.93	0.51
1:B:720:SER:CB	1:B:800:LEU:HB3	2.41	0.51
1:C:550:PHE:HB3	1:C:551:PRO:HD3	1.92	0.51
1:D:938:LEU:HD12	1:D:941:ILE:HD11	1.92	0.51
1:D:959:GLU:OE1	1:E:794:ARG:NH2	2.43	0.51
1:E:697:HIS:CE1	1:E:748:SER:HA	2.45	0.51
1:F:461:LEU:O	1:F:487:ALA:HB2	2.11	0.51
1:H:511:PHE:CE1	1:H:941:ILE:CG2	2.69	0.51
1:D:423:LEU:HD23	1:D:928:MET:HG3	1.92	0.51
1:D:463:TYR:C	1:D:463:TYR:CD2	2.83	0.51
1:D:506:MET:HG3	1:D:1039:THR:HG23	1.92	0.51
1:F:427:ASN:O	1:F:430:CYS:HB2	2.10	0.51
1:G:506:MET:HG3	1:G:1039:THR:HG23	1.92	0.51
1:A:697:HIS:CE1	1:A:748:SER:HA	2.46	0.51
1:F:423:LEU:HD23	1:F:928:MET:HG3	1.92	0.51
1:H:611:ARG:C	1:H:613:PHE:H	2.14	0.51
1:A:550:PHE:HB3	1:A:551:PRO:HD3	1.92	0.51
1:A:720:SER:CB	1:A:800:LEU:HB3	2.41	0.51
1:B:427:ASN:O	1:B:430:CYS:HB2	2.10	0.51
1:C:825:ILE:HD12	1:C:825:ILE:H	1.75	0.51
1:D:886:LEU:HD11	1:D:895:LEU:HD21	1.93	0.51
1:E:910:THR:HB	1:E:912:PRO:HD2	1.93	0.51
1:F:886:LEU:HD12	1:F:892:VAL:HG22	1.93	0.51
1:C:720:SER:CB	1:C:800:LEU:HB3	2.41	0.51
1:E:553:VAL:HG21	1:E:593:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:586:ASN:HB2	1:E:1014:LEU:HD12	1.93	0.51
1:F:698:TRP:CH2	1:F:700:PRO:HA	2.46	0.51
1:F:747:ALA:HB3	1:F:750:PHE:CE2	2.37	0.51
1:H:519:ILE:HG22	1:H:526:LYS:HA	1.93	0.51
1:D:954:GLU:O	1:D:958:ALA:N	2.44	0.50
1:E:934:ASN:HB2	1:E:937:ILE:HG12	1.92	0.50
1:G:550:PHE:HB3	1:G:551:PRO:HD3	1.92	0.50
1:C:725:VAL:O	1:C:760:PHE:HA	2.12	0.50
1:H:511:PHE:CD1	1:H:927:LEU:HD11	2.46	0.50
1:E:423:LEU:HD23	1:E:928:MET:HG3	1.93	0.50
1:G:423:LEU:HD23	1:G:928:MET:HG3	1.92	0.50
1:H:550:PHE:HB3	1:H:551:PRO:HD3	1.91	0.50
1:A:910:THR:HB	1:A:912:PRO:HD2	1.92	0.50
1:C:938:LEU:HD12	1:C:941:ILE:HD11	1.93	0.50
1:F:934:ASN:HB2	1:F:937:ILE:HG12	1.92	0.50
1:G:511:PHE:CD1	1:G:927:LEU:HD11	2.46	0.50
1:B:886:LEU:HD12	1:B:892:VAL:HG22	1.93	0.50
1:A:423:LEU:HD23	1:A:928:MET:HG3	1.93	0.50
1:B:934:ASN:HB2	1:B:937:ILE:HG12	1.92	0.50
1:E:698:TRP:CH2	1:E:700:PRO:HA	2.47	0.50
1:E:722:HIS:HB3	1:E:757:PRO:HG2	1.93	0.50
1:E:748:SER:HB2	1:E:976:ARG:HG2	1.94	0.50
1:E:1048:VAL:CG1	1:E:1049:PRO:HD2	2.42	0.50
1:F:549:SER:O	1:F:553:VAL:HG23	2.11	0.50
1:D:427:ASN:O	1:D:430:CYS:HB2	2.12	0.50
1:E:366:LYS:HE3	1:E:515:SER:HA	1.93	0.50
1:G:611:ARG:C	1:G:613:PHE:H	2.15	0.50
1:G:722:HIS:HB3	1:G:757:PRO:HG2	1.94	0.50
1:G:747:ALA:HB3	1:G:750:PHE:CE2	2.38	0.50
1:A:511:PHE:CD1	1:A:927:LEU:HD11	2.47	0.50
1:A:894:PHE:HA	1:H:449:ASN:ND2	2.27	0.50
1:C:722:HIS:HB3	1:C:757:PRO:HG2	1.93	0.50
1:E:886:LEU:HD12	1:E:892:VAL:HG22	1.93	0.50
1:H:954:GLU:O	1:H:958:ALA:N	2.45	0.50
1:A:461:LEU:O	1:A:487:ALA:HB2	2.12	0.49
1:A:611:ARG:C	1:A:613:PHE:H	2.15	0.49
1:B:611:ARG:C	1:B:613:PHE:H	2.14	0.49
1:A:354:GLU:HG2	1:A:355:SER:N	2.27	0.49
1:F:888:ASN:HB3	1:F:891:ASN:ND2	2.27	0.49
1:G:366:LYS:HE3	1:G:515:SER:HA	1.94	0.49
1:G:519:ILE:HG22	1:G:526:LYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:697:HIS:CE1	1:G:748:SER:HA	2.46	0.49
1:A:519:ILE:HG22	1:A:526:LYS:HA	1.94	0.49
1:A:698:TRP:CH2	1:A:700:PRO:HA	2.47	0.49
1:B:725:VAL:O	1:B:760:PHE:HA	2.12	0.49
1:D:506:MET:HG2	1:D:1039:THR:HG23	1.94	0.49
1:D:519:ILE:HG22	1:D:526:LYS:HA	1.94	0.49
1:H:698:TRP:CH2	1:H:700:PRO:HA	2.47	0.49
1:H:934:ASN:HB2	1:H:937:ILE:HG12	1.94	0.49
1:B:1048:VAL:CG1	1:B:1049:PRO:HD2	2.42	0.49
1:C:510:LEU:O	1:C:535:GLU:HA	2.13	0.49
1:D:960:GLU:OE1	1:E:791:ALA:CB	2.50	0.49
1:E:775:HIS:ND1	1:E:776:ASN:ND2	2.61	0.49
1:F:954:GLU:O	1:F:958:ALA:N	2.45	0.49
1:A:417:GLU:OE2	1:A:418:SER:N	2.45	0.49
1:A:829:LEU:HD12	1:H:473:PRO:HD2	1.95	0.49
1:B:888:ASN:HB3	1:B:891:ASN:ND2	2.28	0.49
1:D:471:ASN:ND2	1:E:830:ASN:HA	2.27	0.49
1:D:698:TRP:CH2	1:D:700:PRO:HA	2.47	0.49
1:F:351:ILE:HG23	1:F:356:VAL:CG2	2.43	0.49
1:G:888:ASN:HB3	1:G:891:ASN:ND2	2.27	0.49
1:H:697:HIS:CE1	1:H:748:SER:HA	2.47	0.49
1:A:722:HIS:HB3	1:A:757:PRO:HG2	1.94	0.49
1:B:748:SER:HB2	1:B:976:ARG:HG2	1.94	0.49
1:B:797:ASN:HB3	1:B:800:LEU:HD12	1.94	0.49
1:D:725:VAL:O	1:D:760:PHE:HA	2.12	0.49
1:C:427:ASN:O	1:C:430:CYS:HB2	2.13	0.49
1:C:506:MET:HG3	1:C:1039:THR:HG23	1.95	0.49
1:F:506:MET:HG2	1:F:1039:THR:HG23	1.95	0.49
1:F:697:HIS:CE1	1:F:748:SER:HA	2.47	0.49
1:H:492:GLY:HA3	1:H:945:VAL:HG12	1.94	0.49
1:H:938:LEU:HD12	1:H:941:ILE:HD11	1.92	0.49
1:A:934:ASN:HB2	1:A:937:ILE:HG12	1.94	0.49
1:F:506:MET:HG3	1:F:1039:THR:HG23	1.94	0.49
1:F:586:ASN:HB2	1:F:1014:LEU:HD12	1.94	0.49
1:A:797:ASN:HB3	1:A:800:LEU:HD12	1.93	0.49
1:B:461:LEU:O	1:B:487:ALA:HB2	2.13	0.49
1:C:417:GLU:OE2	1:C:418:SER:N	2.44	0.49
1:C:697:HIS:CE1	1:C:748:SER:HA	2.48	0.49
1:D:720:SER:CB	1:D:800:LEU:HB3	2.43	0.49
1:D:722:HIS:HB3	1:D:757:PRO:HG2	1.94	0.49
1:E:725:VAL:O	1:E:760:PHE:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ILE:HG22	1:C:526:LYS:HA	1.94	0.48
1:E:394:HIS:HE1	1:H:394:HIS:CE1	2.27	0.48
1:E:461:LEU:O	1:E:487:ALA:HB2	2.13	0.48
1:G:720:SER:CB	1:G:800:LEU:HB3	2.42	0.48
1:B:417:GLU:OE2	1:B:418:SER:N	2.45	0.48
1:B:954:GLU:O	1:B:958:ALA:N	2.46	0.48
1:C:775:HIS:ND1	1:C:776:ASN:ND2	2.61	0.48
1:D:888:ASN:HB3	1:D:891:ASN:ND2	2.28	0.48
1:E:366:LYS:CE	1:E:514:ARG:O	2.61	0.48
1:F:611:ARG:C	1:F:613:PHE:H	2.17	0.48
1:A:492:GLY:HA3	1:A:945:VAL:HG12	1.95	0.48
1:E:611:ARG:C	1:E:613:PHE:H	2.16	0.48
1:F:725:VAL:O	1:F:760:PHE:HA	2.12	0.48
1:G:698:TRP:CH2	1:G:700:PRO:HA	2.48	0.48
1:C:698:TRP:CH2	1:C:700:PRO:HA	2.48	0.48
1:D:797:ASN:HB3	1:D:800:LEU:HD12	1.95	0.48
1:E:510:LEU:O	1:E:535:GLU:HA	2.13	0.48
1:F:886:LEU:HD11	1:F:895:LEU:HD21	1.96	0.48
1:H:586:ASN:HB2	1:H:1014:LEU:HD12	1.96	0.48
1:H:720:SER:CB	1:H:800:LEU:HB3	2.42	0.48
1:A:506:MET:HG3	1:A:1039:THR:HG23	1.94	0.48
1:G:567:ALA:HB3	1:G:600:PHE:HD2	1.79	0.48
1:H:725:VAL:O	1:H:760:PHE:HA	2.13	0.48
1:C:934:ASN:HB2	1:C:937:ILE:HG12	1.96	0.48
1:D:611:ARG:C	1:D:613:PHE:H	2.15	0.48
1:F:511:PHE:CE1	1:F:941:ILE:CG2	2.70	0.48
1:H:747:ALA:HB3	1:H:750:PHE:CE2	2.34	0.48
1:C:511:PHE:CD1	1:C:927:LEU:HD11	2.49	0.48
1:C:954:GLU:O	1:C:958:ALA:N	2.47	0.48
1:E:924:LEU:O	1:E:927:LEU:HB2	2.14	0.48
1:H:886:LEU:HD11	1:H:895:LEU:HD21	1.96	0.48
1:A:954:GLU:O	1:A:958:ALA:N	2.47	0.48
1:B:747:ALA:HB3	1:B:750:PHE:CE2	2.35	0.48
1:C:932:TYR:HD2	1:C:933:PHE:N	2.11	0.48
1:G:354:GLU:HG2	1:G:355:SER:N	2.28	0.48
1:A:747:ALA:HB3	1:A:750:PHE:CE2	2.39	0.48
1:A:775:HIS:ND1	1:A:776:ASN:ND2	2.61	0.48
1:F:748:SER:HB2	1:F:976:ARG:HG2	1.94	0.48
1:G:954:GLU:O	1:G:958:ALA:N	2.46	0.48
1:A:911:GLN:HB3	1:A:912:PRO:HD3	1.96	0.48
1:B:506:MET:HG2	1:B:1039:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:775:HIS:ND1	1:G:776:ASN:ND2	2.62	0.48
1:H:775:HIS:ND1	1:H:776:ASN:ND2	2.62	0.48
1:B:698:TRP:CH2	1:B:700:PRO:HA	2.49	0.47
1:C:748:SER:HB2	1:C:976:ARG:HG2	1.96	0.47
1:D:510:LEU:O	1:D:535:GLU:HA	2.13	0.47
1:E:366:LYS:HE3	1:E:514:ARG:O	2.14	0.47
1:E:954:GLU:O	1:E:958:ALA:N	2.47	0.47
1:H:506:MET:HG3	1:H:1039:THR:HG23	1.95	0.47
1:A:506:MET:HG2	1:A:1039:THR:HG23	1.97	0.47
1:B:775:HIS:ND1	1:B:776:ASN:ND2	2.62	0.47
1:C:366:LYS:HE3	1:C:515:SER:HA	1.96	0.47
1:D:366:LYS:HE3	1:D:515:SER:HA	1.96	0.47
1:E:449:ASN:HD22	1:F:894:PHE:HA	1.78	0.47
1:E:551:PRO:HG2	1:E:589:ASN:HA	1.96	0.47
1:F:519:ILE:HG22	1:F:526:LYS:HA	1.94	0.47
1:G:907:LEU:O	1:G:910:THR:OG1	2.31	0.47
1:A:471:ASN:HB3	1:G:830:ASN:HA	1.95	0.47
1:B:511:PHE:HZ	1:B:941:ILE:HG23	1.72	0.47
1:C:888:ASN:HB3	1:C:891:ASN:ND2	2.29	0.47
1:D:775:HIS:ND1	1:D:776:ASN:ND2	2.62	0.47
1:G:351:ILE:HG23	1:G:356:VAL:CG2	2.44	0.47
1:E:907:LEU:O	1:E:910:THR:OG1	2.32	0.47
1:F:366:LYS:HE3	1:F:515:SER:HA	1.96	0.47
1:F:510:LEU:O	1:F:535:GLU:HA	2.13	0.47
1:G:1004:PHE:CD1	1:G:1004:PHE:C	2.87	0.47
1:H:798:ILE:HG22	1:H:880:ILE:HG21	1.96	0.47
1:H:907:LEU:O	1:H:910:THR:OG1	2.31	0.47
1:A:586:ASN:HB2	1:A:1014:LEU:HD12	1.96	0.47
1:B:351:ILE:HG23	1:B:356:VAL:CG2	2.45	0.47
1:B:511:PHE:CD1	1:B:927:LEU:HD11	2.50	0.47
1:C:354:GLU:HG2	1:C:355:SER:N	2.29	0.47
1:F:707:VAL:CG1	1:F:781:PHE:HA	2.44	0.47
1:H:551:PRO:HG2	1:H:589:ASN:HA	1.96	0.47
1:A:932:TYR:HD2	1:A:933:PHE:N	2.12	0.47
1:C:492:GLY:HA3	1:C:945:VAL:HG12	1.97	0.47
1:C:826:LEU:HD21	1:F:441:ILE:HG21	1.97	0.47
1:C:886:LEU:HD12	1:C:892:VAL:HG22	1.97	0.47
1:D:551:PRO:HG2	1:D:589:ASN:HA	1.97	0.47
1:D:932:TYR:HD2	1:D:933:PHE:N	2.13	0.47
1:G:506:MET:HG2	1:G:1039:THR:HG23	1.97	0.47
1:G:511:PHE:CE1	1:G:941:ILE:CG2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:748:SER:HB2	1:G:976:ARG:HG2	1.96	0.47
1:B:551:PRO:HG2	1:B:589:ASN:HA	1.95	0.47
1:E:354:GLU:HG2	1:E:355:SER:N	2.30	0.47
1:F:696:PHE:HE1	1:F:743:MET:SD	2.37	0.47
1:H:354:GLU:HG2	1:H:355:SER:N	2.29	0.47
1:H:797:ASN:HB3	1:H:800:LEU:HD12	1.97	0.47
1:H:366:LYS:HE3	1:H:515:SER:HA	1.96	0.47
1:H:748:SER:HB2	1:H:976:ARG:HG2	1.97	0.47
1:B:696:PHE:HE1	1:B:743:MET:SD	2.38	0.46
1:B:707:VAL:CG1	1:B:781:PHE:HA	2.43	0.46
1:B:829:LEU:HD12	1:G:473:PRO:CD	2.45	0.46
1:C:567:ALA:HB3	1:C:600:PHE:HD2	1.80	0.46
1:D:492:GLY:HA3	1:D:945:VAL:HG12	1.97	0.46
1:G:931:THR:HG21	1:G:938:LEU:HD13	1.98	0.46
1:G:1048:VAL:CG1	1:G:1049:PRO:HD2	2.45	0.46
1:A:907:LEU:O	1:A:910:THR:OG1	2.33	0.46
1:C:931:THR:HG21	1:C:938:LEU:HD13	1.96	0.46
1:D:461:LEU:O	1:D:487:ALA:HB2	2.15	0.46
1:D:471:ASN:O	1:E:833:SER:OG	2.15	0.46
1:E:911:GLN:HB3	1:E:912:PRO:HD3	1.97	0.46
1:F:1048:VAL:CG1	1:F:1049:PRO:HD2	2.46	0.46
1:H:506:MET:HG2	1:H:1039:THR:HG23	1.95	0.46
1:D:1048:VAL:CG1	1:D:1049:PRO:HD2	2.46	0.46
1:E:506:MET:HG2	1:E:1039:THR:HG23	1.95	0.46
1:F:551:PRO:HG2	1:F:589:ASN:HA	1.97	0.46
1:G:797:ASN:HB3	1:G:800:LEU:HD12	1.96	0.46
1:H:888:ASN:HB3	1:H:891:ASN:ND2	2.30	0.46
1:A:366:LYS:CE	1:A:514:ARG:O	2.64	0.46
1:E:759:VAL:HG11	1:E:796:VAL:HG11	1.97	0.46
1:A:748:SER:HB2	1:A:976:ARG:HG2	1.97	0.46
1:D:366:LYS:CE	1:D:514:ARG:O	2.63	0.46
1:D:417:GLU:OE2	1:D:418:SER:N	2.45	0.46
1:D:886:LEU:HD12	1:D:892:VAL:HG22	1.97	0.46
1:H:510:LEU:O	1:H:535:GLU:HA	2.14	0.46
1:C:471:ASN:HB3	1:D:830:ASN:HA	1.98	0.46
1:C:1048:VAL:CG1	1:C:1049:PRO:HD2	2.46	0.46
1:D:511:PHE:CD1	1:D:927:LEU:HD11	2.50	0.46
1:E:417:GLU:OE2	1:E:418:SER:N	2.45	0.46
1:G:366:LYS:CE	1:G:514:ARG:O	2.64	0.46
1:B:354:GLU:HG2	1:B:355:SER:N	2.31	0.46
1:B:510:LEU:O	1:B:535:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:THR:HG21	1:B:938:LEU:HD13	1.98	0.46
1:B:960:GLU:OE1	1:H:791:ALA:CB	2.62	0.46
1:H:1048:VAL:CG1	1:H:1049:PRO:HD2	2.45	0.46
1:A:886:LEU:HD12	1:A:892:VAL:HG22	1.98	0.46
1:B:529:LEU:HD21	1:B:909:LEU:HD21	1.98	0.46
1:C:586:ASN:HB2	1:C:1014:LEU:HD12	1.97	0.46
1:C:798:ILE:HG22	1:C:880:ILE:HG21	1.97	0.46
1:C:886:LEU:HD11	1:C:895:LEU:HD21	1.97	0.46
1:H:436:GLU:HA	1:H:436:GLU:OE1	2.16	0.46
1:C:436:GLU:HA	1:C:436:GLU:OE1	2.16	0.46
1:C:506:MET:HG2	1:C:1039:THR:HG23	1.97	0.46
1:D:748:SER:HB2	1:D:976:ARG:HG2	1.98	0.46
1:D:931:THR:HG21	1:D:938:LEU:HD13	1.97	0.46
1:E:511:PHE:CD1	1:E:927:LEU:HD11	2.51	0.46
1:H:886:LEU:HD12	1:H:892:VAL:HG22	1.98	0.46
1:A:510:LEU:O	1:A:535:GLU:HA	2.16	0.46
1:B:492:GLY:HA3	1:B:945:VAL:HG12	1.97	0.46
1:C:690:TYR:HB3	1:C:694:GLY:HA2	1.97	0.46
1:E:707:VAL:CG1	1:E:781:PHE:HA	2.44	0.46
1:E:798:ILE:HG22	1:E:880:ILE:HG21	1.98	0.46
1:F:376:VAL:HG11	1:F:414:VAL:HG13	1.98	0.46
1:A:352:THR:HG22	1:A:353:LEU:N	2.30	0.45
1:C:907:LEU:O	1:C:910:THR:OG1	2.32	0.45
1:G:551:PRO:HG2	1:G:589:ASN:HA	1.98	0.45
1:H:1004:PHE:CD1	1:H:1004:PHE:C	2.90	0.45
1:A:549:SER:O	1:A:553:VAL:HG23	2.17	0.45
1:E:696:PHE:HE1	1:E:743:MET:SD	2.39	0.45
1:F:413:ARG:HD3	1:G:413:ARG:NH1	2.30	0.45
1:F:567:ALA:HB3	1:F:600:PHE:HD2	1.81	0.45
1:G:924:LEU:O	1:G:927:LEU:HB2	2.16	0.45
1:H:690:TYR:HB3	1:H:694:GLY:HA2	1.98	0.45
1:A:551:PRO:HG2	1:A:589:ASN:HA	1.98	0.45
1:F:798:ILE:HG22	1:F:880:ILE:HG21	1.98	0.45
1:G:696:PHE:HE1	1:G:743:MET:SD	2.40	0.45
1:G:725:VAL:O	1:G:760:PHE:HA	2.16	0.45
1:H:351:ILE:HG23	1:H:356:VAL:CG2	2.46	0.45
1:D:567:ALA:HB3	1:D:600:PHE:HD2	1.82	0.45
1:E:1004:PHE:CD1	1:E:1004:PHE:C	2.88	0.45
1:F:366:LYS:CE	1:F:514:ARG:O	2.65	0.45
1:G:510:LEU:O	1:G:535:GLU:HA	2.16	0.45
1:B:366:LYS:CE	1:B:514:ARG:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:747:ALA:HB3	1:C:750:PHE:CE2	2.38	0.45
1:C:911:GLN:HB3	1:C:912:PRO:HD3	1.98	0.45
1:D:907:LEU:O	1:D:910:THR:OG1	2.34	0.45
1:E:492:GLY:HA3	1:E:945:VAL:HG12	1.98	0.45
1:F:413:ARG:NH1	1:G:413:ARG:CD	2.76	0.45
1:G:932:TYR:HD2	1:G:933:PHE:N	2.13	0.45
1:B:932:TYR:HD2	1:B:933:PHE:N	2.14	0.45
1:D:529:LEU:HD21	1:D:909:LEU:HD21	1.99	0.45
1:F:352:THR:HG22	1:F:353:LEU:N	2.32	0.45
1:F:924:LEU:O	1:F:927:LEU:HB2	2.17	0.45
1:G:586:ASN:HB2	1:G:1014:LEU:HD12	1.98	0.45
1:H:549:SER:CB	1:H:589:ASN:O	2.65	0.45
1:A:351:ILE:HG23	1:A:356:VAL:CG2	2.47	0.45
1:A:529:LEU:HD21	1:A:909:LEU:HD21	1.98	0.45
1:A:725:VAL:O	1:A:760:PHE:HA	2.16	0.45
1:A:821:ASP:OD2	1:A:821:ASP:C	2.55	0.45
1:C:551:PRO:HG2	1:C:589:ASN:HA	1.98	0.45
1:D:351:ILE:HG23	1:D:356:VAL:CG2	2.46	0.45
1:D:586:ASN:HB2	1:D:1014:LEU:HD12	1.98	0.45
1:H:417:GLU:OE2	1:H:418:SER:N	2.48	0.45
1:H:766:TYR:O	1:H:769:ARG:HG2	2.17	0.45
1:B:907:LEU:O	1:B:910:THR:OG1	2.35	0.45
1:C:707:VAL:CG1	1:C:781:PHE:HA	2.47	0.45
1:D:549:SER:CB	1:D:589:ASN:O	2.64	0.45
1:D:924:LEU:O	1:D:927:LEU:HB2	2.16	0.45
1:F:417:GLU:OE2	1:F:418:SER:N	2.48	0.45
1:H:696:PHE:HE1	1:H:743:MET:SD	2.40	0.45
1:A:366:LYS:HE3	1:A:514:ARG:O	2.17	0.45
1:D:1004:PHE:CD1	1:D:1004:PHE:C	2.89	0.45
1:E:987:TYR:CD2	1:E:988:ASP:N	2.85	0.45
1:F:549:SER:CB	1:F:589:ASN:O	2.64	0.45
1:G:376:VAL:HG11	1:G:414:VAL:HG13	1.99	0.45
1:H:567:ALA:HB3	1:H:600:PHE:HD2	1.82	0.45
1:F:354:GLU:HG2	1:F:355:SER:N	2.31	0.45
1:F:1004:PHE:CD1	1:F:1004:PHE:C	2.89	0.45
1:H:366:LYS:NZ	1:H:604:SER:O	2.50	0.45
1:A:690:TYR:HB3	1:A:694:GLY:HA2	1.99	0.44
1:A:707:VAL:CG1	1:A:781:PHE:HA	2.44	0.44
1:A:886:LEU:HD11	1:A:895:LEU:HD21	1.98	0.44
1:C:766:TYR:O	1:C:769:ARG:HG2	2.17	0.44
1:E:567:ALA:HB2	1:E:585:ILE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:908:TYR:CZ	1:E:909:LEU:HG	2.52	0.44
1:G:549:SER:CB	1:G:589:ASN:O	2.65	0.44
1:B:549:SER:O	1:B:553:VAL:HG23	2.16	0.44
1:B:690:TYR:HB3	1:B:694:GLY:HA2	2.00	0.44
1:D:354:GLU:HG2	1:D:355:SER:N	2.31	0.44
1:F:932:TYR:HD2	1:F:933:PHE:N	2.16	0.44
1:G:738:LEU:HG	1:G:770:GLU:OE2	2.17	0.44
1:B:366:LYS:NZ	1:B:604:SER:O	2.50	0.44
1:C:351:ILE:HG23	1:C:356:VAL:CG2	2.47	0.44
1:C:366:LYS:CE	1:C:514:ARG:O	2.66	0.44
1:D:366:LYS:HE3	1:D:514:ARG:O	2.18	0.44
1:F:690:TYR:HB3	1:F:694:GLY:HA2	2.00	0.44
1:G:798:ILE:HG22	1:G:880:ILE:HG21	2.00	0.44
1:B:567:ALA:HB3	1:B:600:PHE:HD2	1.82	0.44
1:B:451:HIS:HA	1:B:452:PRO:HD3	1.83	0.44
1:C:529:LEU:HD21	1:C:909:LEU:HD21	1.99	0.44
1:C:696:PHE:HE1	1:C:743:MET:SD	2.41	0.44
1:D:707:VAL:CG1	1:D:781:PHE:HA	2.43	0.44
1:D:908:TYR:CZ	1:D:909:LEU:HG	2.53	0.44
1:D:911:GLN:HB3	1:D:912:PRO:HD3	1.99	0.44
1:E:726:CYS:HB2	1:E:787:PRO:CG	2.47	0.44
1:F:511:PHE:CD1	1:F:927:LEU:HD11	2.52	0.44
1:A:696:PHE:HE1	1:A:743:MET:SD	2.41	0.44
1:A:908:TYR:CZ	1:A:909:LEU:HG	2.53	0.44
1:B:366:LYS:HE3	1:B:514:ARG:O	2.18	0.44
1:E:766:TYR:O	1:E:769:ARG:HG2	2.17	0.44
1:E:931:THR:HG21	1:E:938:LEU:HD13	1.99	0.44
1:F:492:GLY:HA3	1:F:945:VAL:HG12	1.99	0.44
1:G:690:TYR:HB3	1:G:694:GLY:HA2	2.00	0.44
1:H:529:LEU:HD21	1:H:909:LEU:HD21	2.00	0.44
1:A:366:LYS:NZ	1:A:604:SER:O	2.50	0.44
1:C:376:VAL:HG11	1:C:414:VAL:HG13	1.99	0.44
1:H:352:THR:HG22	1:H:353:LEU:N	2.33	0.44
1:A:798:ILE:HG22	1:A:880:ILE:HG21	1.99	0.44
1:A:931:THR:HG21	1:A:938:LEU:HD13	2.00	0.44
1:C:908:TYR:CZ	1:C:909:LEU:HG	2.53	0.44
1:A:366:LYS:HE3	1:A:515:SER:HA	1.99	0.44
1:C:759:VAL:HG11	1:C:796:VAL:HG11	1.99	0.44
1:C:924:LEU:O	1:C:927:LEU:HB2	2.18	0.44
1:C:987:TYR:CD2	1:C:988:ASP:N	2.85	0.44
1:E:790:ARG:HD3	1:E:834:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:775:HIS:ND1	1:F:776:ASN:ND2	2.66	0.44
1:F:931:THR:HG21	1:F:938:LEU:HD13	1.98	0.44
1:E:707:VAL:HG21	1:E:771:TRP:CH2	2.53	0.43
1:G:707:VAL:HG21	1:G:771:TRP:CH2	2.53	0.43
1:G:766:TYR:O	1:G:769:ARG:HG2	2.18	0.43
1:H:911:GLN:HB3	1:H:912:PRO:HD3	1.99	0.43
1:A:940:LEU:C	1:A:940:LEU:HD12	2.38	0.43
1:C:1004:PHE:CD1	1:C:1004:PHE:C	2.89	0.43
1:D:747:ALA:HB3	1:D:750:PHE:CE2	2.35	0.43
1:E:727:ILE:HD11	1:E:738:LEU:HD11	2.00	0.43
1:G:549:SER:O	1:G:553:VAL:HG23	2.19	0.43
1:H:931:THR:HG21	1:H:938:LEU:HD13	2.00	0.43
1:A:567:ALA:HB3	1:A:600:PHE:HD2	1.83	0.43
1:D:690:TYR:HB3	1:D:694:GLY:HA2	1.98	0.43
1:D:766:TYR:O	1:D:769:ARG:HG2	2.18	0.43
1:G:417:GLU:OE2	1:G:418:SER:N	2.47	0.43
1:G:886:LEU:HD12	1:G:892:VAL:HG22	2.00	0.43
1:A:436:GLU:HA	1:A:436:GLU:OE1	2.17	0.43
1:A:896:ASP:HB2	1:A:912:PRO:HG3	1.99	0.43
1:B:436:GLU:OE1	1:B:436:GLU:HA	2.18	0.43
1:E:886:LEU:HD11	1:E:895:LEU:HD21	1.99	0.43
1:F:759:VAL:HG11	1:F:796:VAL:HG11	2.00	0.43
1:H:366:LYS:CE	1:H:514:ARG:O	2.67	0.43
1:H:430:CYS:SG	1:H:436:GLU:HB2	2.58	0.43
1:B:798:ILE:HG22	1:B:880:ILE:HG21	2.00	0.43
1:D:549:SER:O	1:D:553:VAL:HG23	2.18	0.43
1:F:436:GLU:HA	1:F:436:GLU:OE1	2.19	0.43
1:A:1048:VAL:CG1	1:A:1049:PRO:HD2	2.47	0.43
1:B:924:LEU:O	1:B:927:LEU:HB2	2.17	0.43
1:C:516:TYR:CE2	1:C:518:LYS:CB	3.02	0.43
1:D:798:ILE:HG22	1:D:880:ILE:HG21	2.01	0.43
1:F:790:ARG:HD3	1:F:834:MET:HG2	2.01	0.43
1:G:529:LEU:HD21	1:G:909:LEU:HD21	1.99	0.43
1:G:707:VAL:HG21	1:G:771:TRP:HH2	1.83	0.43
1:A:987:TYR:CD2	1:A:988:ASP:N	2.87	0.43
1:D:739:ARG:O	1:D:743:MET:HG3	2.18	0.43
1:D:759:VAL:HG11	1:D:796:VAL:HG11	2.00	0.43
1:G:508:ALA:HB1	1:G:923:VAL:HG11	2.01	0.43
1:H:987:TYR:CD2	1:H:988:ASP:N	2.87	0.43
1:C:363:PHE:HB3	1:C:364:LEU:CD2	2.49	0.43
1:E:567:ALA:HB3	1:E:600:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:932:TYR:HD2	1:H:933:PHE:N	2.15	0.43
1:A:376:VAL:HG11	1:A:414:VAL:HG13	2.00	0.43
1:B:766:TYR:O	1:B:769:ARG:HG2	2.18	0.43
1:B:940:LEU:C	1:B:940:LEU:HD12	2.39	0.43
1:B:1004:PHE:CD1	1:B:1004:PHE:C	2.91	0.43
1:D:451:HIS:HA	1:D:452:PRO:HD3	1.83	0.43
1:B:987:TYR:CD2	1:B:988:ASP:N	2.86	0.43
1:C:790:ARG:HD3	1:C:834:MET:HG2	1.99	0.43
1:F:911:GLN:HB3	1:F:912:PRO:HD3	2.00	0.43
1:C:366:LYS:HE3	1:C:514:ARG:O	2.19	0.42
1:E:776:ASN:N	1:E:776:ASN:HD22	2.17	0.42
1:E:932:TYR:HD2	1:E:933:PHE:N	2.17	0.42
1:F:472:ILE:HA	1:F:473:PRO:HD2	1.86	0.42
1:G:940:LEU:C	1:G:940:LEU:HD12	2.39	0.42
1:H:707:VAL:CG1	1:H:781:PHE:HA	2.44	0.42
1:A:738:LEU:HG	1:A:770:GLU:OE2	2.18	0.42
1:G:451:HIS:HA	1:G:452:PRO:HD3	1.82	0.42
1:H:496:GLN:HB3	1:H:503:LEU:CD2	2.33	0.42
1:H:790:ARG:HD3	1:H:834:MET:HG2	2.00	0.42
1:B:586:ASN:HB2	1:B:1014:LEU:HD12	2.01	0.42
1:B:759:VAL:HG11	1:B:796:VAL:HG11	2.01	0.42
1:B:1016:PHE:CD1	1:B:1016:PHE:N	2.86	0.42
1:C:549:SER:O	1:C:553:VAL:HG23	2.18	0.42
1:E:746:ARG:NH1	1:E:756:LYS:O	2.45	0.42
1:F:896:ASP:HB2	1:F:912:PRO:HG3	2.01	0.42
1:H:549:SER:O	1:H:553:VAL:HG23	2.20	0.42
1:D:707:VAL:HG21	1:D:771:TRP:CH2	2.55	0.42
1:E:436:GLU:OE1	1:E:436:GLU:HA	2.19	0.42
1:G:759:VAL:HG11	1:G:796:VAL:HG11	2.02	0.42
1:B:726:CYS:HB2	1:B:787:PRO:CG	2.47	0.42
1:C:896:ASP:HB2	1:C:912:PRO:HG3	2.01	0.42
1:E:472:ILE:HA	1:E:473:PRO:HD2	1.83	0.42
1:G:492:GLY:HA3	1:G:945:VAL:HG12	1.98	0.42
1:G:938:LEU:O	1:G:941:ILE:HG12	2.20	0.42
1:H:600:PHE:CD2	1:H:940:LEU:HD22	2.54	0.42
1:H:776:ASN:N	1:H:776:ASN:HD22	2.16	0.42
1:A:430:CYS:SG	1:A:436:GLU:HB2	2.60	0.42
1:A:595:GLU:HB3	1:A:596:GLY:H	1.68	0.42
1:B:472:ILE:HA	1:B:473:PRO:HD2	1.85	0.42
1:D:896:ASP:HB2	1:D:912:PRO:HG3	2.01	0.42
1:G:366:LYS:HE3	1:G:514:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:LYS:CE	1:G:515:SER:HA	2.50	0.42
1:G:987:TYR:CD2	1:G:988:ASP:N	2.88	0.42
1:H:363:PHE:CD2	1:H:375:ILE:HD11	2.54	0.42
1:H:924:LEU:O	1:H:927:LEU:HB2	2.19	0.42
1:A:752:TYR:CE2	1:A:779:LYS:HE3	2.54	0.42
1:F:908:TYR:CZ	1:F:909:LEU:HG	2.55	0.42
1:G:707:VAL:CG1	1:G:781:PHE:HA	2.46	0.42
1:C:508:ALA:HB1	1:C:923:VAL:HG11	2.01	0.42
1:D:695:MET:O	1:D:748:SER:N	2.52	0.42
1:D:766:TYR:C	1:D:766:TYR:CD2	2.93	0.42
1:H:366:LYS:HE3	1:H:514:ARG:O	2.20	0.42
1:B:376:VAL:HG11	1:B:414:VAL:HG13	2.01	0.42
1:B:766:TYR:CD2	1:B:766:TYR:C	2.93	0.42
1:B:896:ASP:HB2	1:B:912:PRO:HG3	2.02	0.42
1:C:496:GLN:HB3	1:C:503:LEU:CD2	2.30	0.42
1:C:549:SER:CB	1:C:589:ASN:O	2.63	0.42
1:E:516:TYR:CE2	1:E:518:LYS:CB	3.03	0.42
1:E:896:ASP:HB2	1:E:912:PRO:HG3	2.01	0.42
1:F:529:LEU:HD21	1:F:909:LEU:HD21	2.01	0.42
1:G:436:GLU:OE1	1:G:436:GLU:HA	2.19	0.42
1:H:707:VAL:HG21	1:H:771:TRP:HH2	1.85	0.42
1:A:790:ARG:HD3	1:A:834:MET:HG2	2.01	0.42
1:C:366:LYS:NZ	1:C:604:SER:O	2.52	0.42
1:C:727:ILE:HD11	1:C:738:LEU:HD11	2.02	0.42
1:H:940:LEU:HD12	1:H:940:LEU:C	2.41	0.42
1:C:830:ASN:HA	1:F:471:ASN:HB3	2.02	0.41
1:C:1006:LYS:O	1:C:1010:THR:OG1	2.28	0.41
1:D:940:LEU:C	1:D:940:LEU:HD12	2.40	0.41
1:D:941:ILE:CG1	1:D:942:ARG:N	2.83	0.41
1:D:1006:LYS:O	1:D:1010:THR:OG1	2.31	0.41
1:E:351:ILE:HG23	1:E:356:VAL:CG2	2.50	0.41
1:E:529:LEU:HD21	1:E:909:LEU:HD21	2.02	0.41
1:E:549:SER:O	1:E:553:VAL:HG23	2.20	0.41
1:G:908:TYR:CZ	1:G:909:LEU:HG	2.55	0.41
1:H:363:PHE:HB3	1:H:364:LEU:CD2	2.50	0.41
1:A:924:LEU:O	1:A:927:LEU:HB2	2.19	0.41
1:A:929:SER:O	1:A:932:TYR:HB3	2.20	0.41
1:B:908:TYR:CZ	1:B:909:LEU:HG	2.55	0.41
1:C:451:HIS:HA	1:C:452:PRO:HD3	1.84	0.41
1:D:726:CYS:HB2	1:D:787:PRO:CG	2.47	0.41
1:D:987:TYR:CD2	1:D:988:ASP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:927:LEU:O	1:E:931:THR:HG23	2.20	0.41
1:F:366:LYS:HE3	1:F:514:ARG:O	2.20	0.41
1:F:987:TYR:CD2	1:F:988:ASP:N	2.88	0.41
1:H:516:TYR:CE2	1:H:518:LYS:CB	3.04	0.41
1:H:707:VAL:HG21	1:H:771:TRP:CH2	2.55	0.41
1:D:707:VAL:HG21	1:D:771:TRP:HH2	1.84	0.41
1:E:727:ILE:CD1	1:E:738:LEU:HD11	2.50	0.41
1:F:708:ILE:HD11	1:F:764:LEU:HD21	2.03	0.41
1:G:595:GLU:HB3	1:G:596:GLY:H	1.69	0.41
1:B:430:CYS:SG	1:B:436:GLU:HB2	2.60	0.41
1:B:929:SER:O	1:B:932:TYR:HB3	2.21	0.41
1:E:430:CYS:SG	1:E:436:GLU:HB2	2.61	0.41
1:E:766:TYR:CD2	1:E:766:TYR:C	2.92	0.41
1:F:545:PHE:CD1	1:F:553:VAL:HG13	2.55	0.41
1:G:600:PHE:CD2	1:G:940:LEU:HD22	2.56	0.41
1:G:776:ASN:HD22	1:G:776:ASN:N	2.16	0.41
1:A:366:LYS:HD3	1:A:605:ASP:HA	2.02	0.41
1:B:790:ARG:HD3	1:B:834:MET:HG2	2.01	0.41
1:C:430:CYS:SG	1:C:431:ALA:N	2.93	0.41
1:C:1021:LEU:HD23	1:C:1035:ARG:CG	2.50	0.41
1:D:738:LEU:HG	1:D:770:GLU:OE2	2.20	0.41
1:A:451:HIS:HA	1:A:452:PRO:HD3	1.82	0.41
1:B:549:SER:CB	1:B:589:ASN:O	2.65	0.41
1:B:695:MET:O	1:B:696:PHE:HD2	2.03	0.41
1:C:352:THR:HG22	1:C:353:LEU:N	2.35	0.41
1:C:929:SER:O	1:C:932:TYR:HB3	2.21	0.41
1:E:549:SER:CB	1:E:589:ASN:O	2.65	0.41
1:E:707:VAL:HG21	1:E:771:TRP:HH2	1.85	0.41
1:F:766:TYR:CD2	1:F:766:TYR:C	2.93	0.41
1:H:821:ASP:OD2	1:H:821:ASP:C	2.58	0.41
1:H:908:TYR:CZ	1:H:909:LEU:HG	2.55	0.41
1:C:366:LYS:HD3	1:C:605:ASP:HA	2.02	0.41
1:C:545:PHE:CD1	1:C:553:VAL:HG13	2.56	0.41
1:C:1016:PHE:CD1	1:C:1016:PHE:N	2.87	0.41
1:D:821:ASP:OD2	1:D:821:ASP:C	2.59	0.41
1:E:738:LEU:HG	1:E:770:GLU:OE2	2.21	0.41
1:E:1000:TYR:CE2	1:E:1041:PRO:HD2	2.56	0.41
1:F:739:ARG:O	1:F:743:MET:HG3	2.21	0.41
1:H:366:LYS:HD3	1:H:605:ASP:HA	2.02	0.41
1:A:549:SER:CB	1:A:589:ASN:O	2.67	0.41
1:B:352:THR:HG22	1:B:353:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:HIS:HE1	1:H:788:LEU:HB3	1.86	0.41
1:C:766:TYR:CD2	1:C:766:TYR:C	2.94	0.41
1:D:430:CYS:SG	1:D:431:ALA:N	2.94	0.41
1:D:523:THR:OG1	1:D:525:GLN:HG2	2.20	0.41
1:D:722:HIS:O	1:D:801:CYS:HB2	2.20	0.41
1:E:1016:PHE:CD1	1:E:1016:PHE:N	2.87	0.41
1:F:413:ARG:HH11	1:G:413:ARG:HD3	1.80	0.41
1:F:600:PHE:CD2	1:F:940:LEU:HD22	2.56	0.41
1:G:366:LYS:NZ	1:G:604:SER:O	2.53	0.41
1:G:911:GLN:HB3	1:G:912:PRO:HD3	2.02	0.41
1:H:759:VAL:HG11	1:H:796:VAL:HG11	2.02	0.41
1:A:803:MET:HA	1:A:881:PRO:HB2	2.03	0.41
1:B:523:THR:OG1	1:B:525:GLN:HG2	2.21	0.41
1:B:738:LEU:HG	1:B:770:GLU:OE2	2.20	0.41
1:C:707:VAL:HG21	1:C:771:TRP:CH2	2.56	0.41
1:C:722:HIS:O	1:C:801:CYS:HB2	2.21	0.41
1:D:366:LYS:NZ	1:D:604:SER:O	2.54	0.41
1:D:931:THR:CG2	1:D:938:LEU:HB2	2.51	0.41
1:E:366:LYS:CE	1:E:515:SER:HA	2.50	0.41
1:F:567:ALA:HB2	1:F:585:ILE:HA	2.03	0.41
1:F:707:VAL:HG21	1:F:771:TRP:CH2	2.56	0.41
1:F:940:LEU:C	1:F:940:LEU:HD12	2.41	0.41
1:G:352:THR:HG22	1:G:353:LEU:N	2.36	0.41
1:G:508:ALA:HB1	1:G:923:VAL:CG1	2.51	0.41
1:G:727:ILE:CD1	1:G:738:LEU:HD11	2.51	0.41
1:H:523:THR:OG1	1:H:525:GLN:HG2	2.21	0.41
1:H:727:ILE:CD1	1:H:738:LEU:HD11	2.51	0.41
1:A:941:ILE:CG1	1:A:942:ARG:N	2.84	0.41
1:B:366:LYS:CE	1:B:515:SER:HA	2.51	0.41
1:C:727:ILE:CD1	1:C:738:LEU:HD11	2.51	0.41
1:C:903:PRO:CG	1:F:408:PRO:HD2	2.51	0.41
1:D:379:HIS:CD2	1:D:402:GLN:HA	2.53	0.41
1:E:366:LYS:NZ	1:E:604:SER:O	2.50	0.41
1:F:366:LYS:HD3	1:F:605:ASP:HA	2.03	0.41
1:F:695:MET:O	1:F:696:PHE:HD2	2.04	0.41
1:F:907:LEU:O	1:F:910:THR:OG1	2.37	0.41
1:B:508:ALA:HB1	1:B:923:VAL:HG11	2.04	0.40
1:D:705:GLU:H	1:D:705:GLU:HG2	1.65	0.40
1:G:496:GLN:HB3	1:G:503:LEU:CD2	2.31	0.40
1:B:363:PHE:CD2	1:B:375:ILE:HD11	2.56	0.40
1:C:363:PHE:HD2	1:C:364:LEU:CD2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:HIS:HB3	1:D:366:LYS:H	1.75	0.40
1:D:430:CYS:SG	1:D:436:GLU:HB2	2.61	0.40
1:D:776:ASN:N	1:D:776:ASN:HD22	2.19	0.40
1:E:352:THR:HG22	1:E:353:LEU:N	2.36	0.40
1:E:451:HIS:HA	1:E:452:PRO:HD3	1.81	0.40
1:F:941:ILE:CG1	1:F:942:ARG:N	2.83	0.40
1:G:463:TYR:O	1:G:466:LYS:HB3	2.21	0.40
1:G:552:THR:O	1:G:556:LEU:HG	2.21	0.40
1:A:545:PHE:CD1	1:A:553:VAL:HG13	2.55	0.40
1:A:1004:PHE:C	1:A:1004:PHE:CD1	2.92	0.40
1:B:821:ASP:OD2	1:B:821:ASP:C	2.59	0.40
1:D:508:ALA:HB1	1:D:923:VAL:HG11	2.04	0.40
1:D:1021:LEU:HD23	1:D:1035:ARG:CG	2.51	0.40
1:H:738:LEU:HG	1:H:770:GLU:OE2	2.20	0.40
1:H:739:ARG:O	1:H:743:MET:HG3	2.21	0.40
1:A:516:TYR:CE2	1:A:518:LYS:CB	3.05	0.40
1:A:707:VAL:HG21	1:A:771:TRP:CH2	2.57	0.40
1:A:746:ARG:NH1	1:A:756:LYS:O	2.46	0.40
1:C:738:LEU:HG	1:C:770:GLU:OE2	2.21	0.40
1:C:803:MET:HA	1:C:881:PRO:HB2	2.04	0.40
1:D:436:GLU:OE1	1:D:436:GLU:HA	2.21	0.40
1:D:696:PHE:HE1	1:D:743:MET:SD	2.44	0.40
1:G:506:MET:CB	1:G:1037:VAL:HG11	2.51	0.40
1:A:695:MET:O	1:A:748:SER:N	2.52	0.40
1:A:695:MET:O	1:A:696:PHE:HD2	2.04	0.40
1:A:766:TYR:CD2	1:A:766:TYR:C	2.94	0.40
1:A:938:LEU:O	1:A:941:ILE:HG12	2.22	0.40
1:B:911:GLN:HB3	1:B:912:PRO:HD3	2.03	0.40
1:C:776:ASN:HD22	1:C:776:ASN:N	2.20	0.40
1:D:746:ARG:NH1	1:D:756:LYS:O	2.46	0.40
1:G:790:ARG:HD3	1:G:834:MET:HG2	2.02	0.40
1:G:1014:LEU:HD23	1:G:1014:LEU:HA	1.95	0.40
1:H:941:ILE:CG1	1:H:942:ARG:N	2.84	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:716:MET:CE	1:G:1005:CYS:CB[3_454]	2.06	0.14
1:E:987:TYR:OH	1:F:702:LYS:C[4_555]	2.17	0.03

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	571/696 (82%)	540 (95%)	30 (5%)	1 (0%)	47	79
1	B	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	47	79
1	C	571/696 (82%)	538 (94%)	32 (6%)	1 (0%)	47	79
1	D	571/696 (82%)	540 (95%)	30 (5%)	1 (0%)	47	79
1	E	571/696 (82%)	538 (94%)	32 (6%)	1 (0%)	47	79
1	F	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	47	79
1	G	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	47	79
1	H	571/696 (82%)	537 (94%)	33 (6%)	1 (0%)	47	79
All	All	4568/5568 (82%)	4310 (94%)	250 (6%)	8 (0%)	47	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	799	ASN
1	D	799	ASN
1	F	799	ASN
1	G	799	ASN
1	H	799	ASN
1	A	799	ASN
1	B	799	ASN
1	E	799	ASN

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	432/616 (70%)	378 (88%)	54 (12%)	4 25
1	B	432/616 (70%)	379 (88%)	53 (12%)	4 26
1	C	432/616 (70%)	378 (88%)	54 (12%)	4 25
1	D	432/616 (70%)	378 (88%)	54 (12%)	4 25
1	E	432/616 (70%)	379 (88%)	53 (12%)	4 26
1	F	432/616 (70%)	379 (88%)	53 (12%)	4 26
1	G	432/616 (70%)	378 (88%)	54 (12%)	4 25
1	H	432/616 (70%)	379 (88%)	53 (12%)	4 26
All	All	3456/4928 (70%)	3028 (88%)	428 (12%)	4 25

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	GLU
1	A	364	LEU
1	A	365	HIS
1	A	372	ASN
1	A	379	HIS
1	A	386	GLU
1	A	395	PHE
1	A	405	VAL
1	A	417	GLU
1	A	482	ASP
1	A	507	LEU
1	A	513	MET
1	A	583	ILE
1	A	590	HIS
1	A	593	MET
1	A	699	CYS
1	A	705	GLU
1	A	710	THR
1	A	727	ILE
1	A	742	VAL
1	A	745	LEU
1	A	749	ASN
1	A	750	PHE
1	A	764	LEU
1	A	768	ARG
1	A	769	ARG
1	A	773	THR

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Mol	Chain	Res	Type
1	A	774	LEU
1	A	776	ASN
1	A	821	ASP
1	A	829	LEU
1	A	885	GLU
1	A	887	VAL
1	A	895	LEU
1	A	910	THR
1	A	926	SER
1	A	932	TYR
1	A	935	ASP
1	A	936	ASN
1	A	940	LEU
1	A	942	ARG
1	A	959	GLU
1	A	960	GLU
1	A	961	ASN
1	A	963	LEU
1	A	967	TYR
1	A	972	THR
1	A	980	ARG
1	A	987	TYR
1	A	1008	LEU
1	A	1016	PHE
1	A	1032	CYS
1	A	1033	THR
1	A	1039	THR
1	B	354	GLU
1	B	364	LEU
1	B	365	HIS
1	B	372	ASN
1	B	379	HIS
1	B	386	GLU
1	B	395	PHE
1	B	405	VAL
1	B	417	GLU
1	B	482	ASP
1	B	507	LEU
1	B	513	MET
1	B	583	ILE
1	B	590	HIS
1	B	593	MET

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Mol	Chain	Res	Type
1	B	699	CYS
1	B	705	GLU
1	B	710	THR
1	B	727	ILE
1	B	742	VAL
1	B	745	LEU
1	B	749	ASN
1	B	750	PHE
1	B	764	LEU
1	B	768	ARG
1	B	769	ARG
1	B	773	THR
1	B	774	LEU
1	B	776	ASN
1	B	821	ASP
1	B	829	LEU
1	B	885	GLU
1	B	887	VAL
1	B	895	LEU
1	B	910	THR
1	B	926	SER
1	B	932	TYR
1	B	935	ASP
1	B	936	ASN
1	B	940	LEU
1	B	942	ARG
1	B	959	GLU
1	B	960	GLU
1	B	961	ASN
1	B	963	LEU
1	B	967	TYR
1	B	972	THR
1	B	987	TYR
1	B	1008	LEU
1	B	1016	PHE
1	B	1032	CYS
1	B	1033	THR
1	B	1039	THR
1	C	354	GLU
1	C	364	LEU
1	C	365	HIS
1	C	372	ASN

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Mol	Chain	Res	Type
1	C	379	HIS
1	C	386	GLU
1	C	395	PHE
1	C	405	VAL
1	C	417	GLU
1	C	482	ASP
1	C	505	THR
1	C	507	LEU
1	C	513	MET
1	C	583	ILE
1	C	590	HIS
1	C	593	MET
1	C	699	CYS
1	C	705	GLU
1	C	710	THR
1	C	727	ILE
1	C	742	VAL
1	C	745	LEU
1	C	749	ASN
1	C	750	PHE
1	C	764	LEU
1	C	768	ARG
1	C	769	ARG
1	C	773	THR
1	C	774	LEU
1	C	776	ASN
1	C	821	ASP
1	C	829	LEU
1	C	885	GLU
1	C	887	VAL
1	C	895	LEU
1	C	910	THR
1	C	926	SER
1	C	932	TYR
1	C	935	ASP
1	C	936	ASN
1	C	940	LEU
1	C	942	ARG
1	C	959	GLU
1	C	960	GLU
1	C	961	ASN
1	C	963	LEU

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Mol	Chain	Res	Type
1	C	967	TYR
1	C	972	THR
1	C	987	TYR
1	C	1008	LEU
1	C	1016	PHE
1	C	1032	CYS
1	C	1033	THR
1	C	1039	THR
1	D	354	GLU
1	D	364	LEU
1	D	365	HIS
1	D	372	ASN
1	D	379	HIS
1	D	386	GLU
1	D	395	PHE
1	D	405	VAL
1	D	417	GLU
1	D	482	ASP
1	D	505	THR
1	D	507	LEU
1	D	513	MET
1	D	583	ILE
1	D	590	HIS
1	D	593	MET
1	D	699	CYS
1	D	705	GLU
1	D	710	THR
1	D	727	ILE
1	D	742	VAL
1	D	745	LEU
1	D	749	ASN
1	D	750	PHE
1	D	764	LEU
1	D	768	ARG
1	D	769	ARG
1	D	773	THR
1	D	774	LEU
1	D	776	ASN
1	D	821	ASP
1	D	829	LEU
1	D	885	GLU
1	D	887	VAL

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Mol	Chain	Res	Type
1	D	895	LEU
1	D	910	THR
1	D	926	SER
1	D	932	TYR
1	D	935	ASP
1	D	936	ASN
1	D	940	LEU
1	D	942	ARG
1	D	959	GLU
1	D	960	GLU
1	D	961	ASN
1	D	963	LEU
1	D	967	TYR
1	D	972	THR
1	D	987	TYR
1	D	1008	LEU
1	D	1016	PHE
1	D	1032	CYS
1	D	1033	THR
1	D	1039	THR
1	E	354	GLU
1	E	364	LEU
1	E	365	HIS
1	E	372	ASN
1	E	379	HIS
1	E	386	GLU
1	E	395	PHE
1	E	405	VAL
1	E	417	GLU
1	E	482	ASP
1	E	507	LEU
1	E	513	MET
1	E	583	ILE
1	E	590	HIS
1	E	593	MET
1	E	699	CYS
1	E	705	GLU
1	E	710	THR
1	E	727	ILE
1	E	742	VAL
1	E	745	LEU
1	E	749	ASN

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Mol	Chain	Res	Type
1	E	750	PHE
1	E	764	LEU
1	E	768	ARG
1	E	769	ARG
1	E	773	THR
1	E	774	LEU
1	E	776	ASN
1	E	821	ASP
1	E	829	LEU
1	E	885	GLU
1	E	887	VAL
1	E	895	LEU
1	E	910	THR
1	E	926	SER
1	E	932	TYR
1	E	935	ASP
1	E	936	ASN
1	E	940	LEU
1	E	942	ARG
1	E	959	GLU
1	E	960	GLU
1	E	961	ASN
1	E	963	LEU
1	E	967	TYR
1	E	972	THR
1	E	987	TYR
1	E	1008	LEU
1	E	1016	PHE
1	E	1032	CYS
1	E	1033	THR
1	E	1039	THR
1	F	354	GLU
1	F	364	LEU
1	F	365	HIS
1	F	372	ASN
1	F	379	HIS
1	F	386	GLU
1	F	395	PHE
1	F	405	VAL
1	F	417	GLU
1	F	482	ASP
1	F	507	LEU

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Mol	Chain	Res	Type
1	F	513	MET
1	F	583	ILE
1	F	590	HIS
1	F	593	MET
1	F	699	CYS
1	F	705	GLU
1	F	710	THR
1	F	727	ILE
1	F	742	VAL
1	F	745	LEU
1	F	749	ASN
1	F	750	PHE
1	F	764	LEU
1	F	768	ARG
1	F	769	ARG
1	F	773	THR
1	F	774	LEU
1	F	776	ASN
1	F	821	ASP
1	F	829	LEU
1	F	885	GLU
1	F	887	VAL
1	F	895	LEU
1	F	910	THR
1	F	926	SER
1	F	932	TYR
1	F	935	ASP
1	F	936	ASN
1	F	940	LEU
1	F	942	ARG
1	F	959	GLU
1	F	960	GLU
1	F	961	ASN
1	F	963	LEU
1	F	967	TYR
1	F	972	THR
1	F	987	TYR
1	F	1008	LEU
1	F	1016	PHE
1	F	1032	CYS
1	F	1033	THR
1	F	1039	THR

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Mol	Chain	Res	Type
1	G	354	GLU
1	G	364	LEU
1	G	365	HIS
1	G	372	ASN
1	G	379	HIS
1	G	386	GLU
1	G	395	PHE
1	G	405	VAL
1	G	417	GLU
1	G	482	ASP
1	G	507	LEU
1	G	513	MET
1	G	583	ILE
1	G	590	HIS
1	G	593	MET
1	G	699	CYS
1	G	705	GLU
1	G	710	THR
1	G	727	ILE
1	G	742	VAL
1	G	745	LEU
1	G	749	ASN
1	G	750	PHE
1	G	764	LEU
1	G	768	ARG
1	G	769	ARG
1	G	773	THR
1	G	774	LEU
1	G	776	ASN
1	G	821	ASP
1	G	829	LEU
1	G	885	GLU
1	G	887	VAL
1	G	890	SER
1	G	895	LEU
1	G	910	THR
1	G	926	SER
1	G	932	TYR
1	G	935	ASP
1	G	936	ASN
1	G	940	LEU
1	G	942	ARG

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Mol	Chain	Res	Type
1	G	959	GLU
1	G	960	GLU
1	G	961	ASN
1	G	963	LEU
1	G	967	TYR
1	G	972	THR
1	G	987	TYR
1	G	1008	LEU
1	G	1016	PHE
1	G	1032	CYS
1	G	1033	THR
1	G	1039	THR
1	H	354	GLU
1	H	364	LEU
1	H	365	HIS
1	H	372	ASN
1	H	379	HIS
1	H	386	GLU
1	H	395	PHE
1	H	405	VAL
1	H	417	GLU
1	H	482	ASP
1	H	507	LEU
1	H	513	MET
1	H	583	ILE
1	H	590	HIS
1	H	593	MET
1	H	699	CYS
1	H	705	GLU
1	H	710	THR
1	H	727	ILE
1	H	742	VAL
1	H	745	LEU
1	H	749	ASN
1	H	750	PHE
1	H	764	LEU
1	H	768	ARG
1	H	769	ARG
1	H	773	THR
1	H	774	LEU
1	H	776	ASN
1	H	821	ASP

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Mol	Chain	Res	Type
1	H	829	LEU
1	H	885	GLU
1	H	887	VAL
1	H	895	LEU
1	H	910	THR
1	H	926	SER
1	H	932	TYR
1	H	935	ASP
1	H	936	ASN
1	H	940	LEU
1	H	942	ARG
1	H	959	GLU
1	H	960	GLU
1	H	961	ASN
1	H	963	LEU
1	H	967	TYR
1	H	972	THR
1	H	987	TYR
1	H	1008	LEU
1	H	1016	PHE
1	H	1032	CYS
1	H	1033	THR
1	H	1039	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	HIS
1	A	394	HIS
1	A	468	HIS
1	A	697	HIS
1	A	776	ASN
1	A	891	ASN
1	B	379	HIS
1	B	394	HIS
1	B	465	ASN
1	B	468	HIS
1	B	697	HIS
1	B	776	ASN
1	B	891	ASN
1	C	379	HIS
1	C	394	HIS

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Mol	Chain	Res	Type
1	C	468	HIS
1	C	697	HIS
1	C	776	ASN
1	C	797	ASN
1	C	891	ASN
1	D	379	HIS
1	D	394	HIS
1	D	465	ASN
1	D	468	HIS
1	D	697	HIS
1	D	776	ASN
1	D	891	ASN
1	E	379	HIS
1	E	394	HIS
1	E	468	HIS
1	E	697	HIS
1	E	776	ASN
1	E	891	ASN
1	F	379	HIS
1	F	394	HIS
1	F	465	ASN
1	F	468	HIS
1	F	697	HIS
1	F	776	ASN
1	F	891	ASN
1	G	379	HIS
1	G	394	HIS
1	G	468	HIS
1	G	697	HIS
1	G	776	ASN
1	G	891	ASN
1	H	379	HIS
1	H	394	HIS
1	H	465	ASN
1	H	468	HIS
1	H	697	HIS
1	H	776	ASN
1	H	891	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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 (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	585/696 (84%)	-0.23	4 (0%)	87	78	58, 105, 158, 185	0
1	B	585/696 (84%)	-0.22	5 (0%)	84	73	67, 105, 151, 179	0
1	C	585/696 (84%)	-0.31	3 (0%)	91	83	55, 95, 141, 181	0
1	D	585/696 (84%)	-0.22	6 (1%)	82	70	57, 102, 155, 217	0
1	E	585/696 (84%)	-0.28	8 (1%)	75	61	50, 86, 134, 180	0
1	F	585/696 (84%)	-0.22	9 (1%)	73	60	59, 96, 149, 200	0
1	G	585/696 (84%)	-0.09	15 (2%)	56	40	68, 108, 160, 198	0
1	H	585/696 (84%)	-0.08	13 (2%)	62	46	75, 112, 161, 203	0
All	All	4680/5568 (84%)	-0.21	63 (1%)	77	64	50, 101, 154, 217	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	875	THR	4.5
1	F	595	GLU	4.3
1	D	718	VAL	4.1
1	A	966	GLY	3.8
1	G	970	PRO	3.7
1	E	595	GLU	3.5
1	B	595	GLU	3.4
1	F	961	ASN	3.2
1	G	539	GLU	3.1
1	G	541	LEU	3.1
1	E	596	GLY	2.9
1	H	611	ARG	2.9
1	D	545	PHE	2.9
1	H	590	HIS	2.8
1	F	817	ALA	2.8
1	G	968	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	542	SER	2.7
1	B	949	ALA	2.7
1	E	542	SER	2.7
1	H	595	GLU	2.6
1	C	968	SER	2.6
1	G	694	GLY	2.5
1	F	810	ASN	2.5
1	G	966	GLY	2.4
1	E	961	ASN	2.4
1	H	588	GLY	2.4
1	G	545	PHE	2.3
1	H	708	ILE	2.3
1	G	976	ARG	2.3
1	H	782	ILE	2.3
1	B	810	ASN	2.3
1	G	612	ALA	2.3
1	F	597	THR	2.3
1	D	817	ALA	2.3
1	F	594	GLN	2.3
1	H	967	TYR	2.3
1	G	985	ALA	2.2
1	A	589	ASN	2.2
1	F	987	TYR	2.2
1	D	547	GLY	2.2
1	G	522	ASP	2.2
1	C	989	GLY	2.2
1	G	690	TYR	2.2
1	H	548	LEU	2.2
1	H	970	PRO	2.2
1	E	522	ASP	2.2
1	H	543	SER	2.2
1	C	949	ALA	2.2
1	B	953	LEU	2.1
1	E	541	LEU	2.1
1	F	547	GLY	2.1
1	H	382	SER	2.1
1	A	545	PHE	2.1
1	G	975	ASN	2.1
1	H	383	PRO	2.1
1	E	962	ALA	2.0
1	E	545	PHE	2.0
1	B	593	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	1030	SER	2.0
1	A	542	SER	2.0
1	G	718	VAL	2.0
1	F	518	LYS	2.0
1	G	810	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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	F	2001	1/1	0.91	0.15	72,72,72,72	0
2	CA	H	2001	1/1	0.91	0.14	82,82,82,82	0
2	CA	C	2001	1/1	0.96	0.08	61,61,61,61	0
2	CA	D	2001	1/1	0.97	0.10	50,50,50,50	0
2	CA	E	2001	1/1	0.97	0.09	57,57,57,57	0
2	CA	B	2001	1/1	0.97	0.12	73,73,73,73	0
2	CA	A	2001	1/1	0.97	0.08	68,68,68,68	0
2	CA	G	2001	1/1	0.98	0.11	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.