



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:52 PM UTC

PDB ID : 3U6N / pdb_00003u6n
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

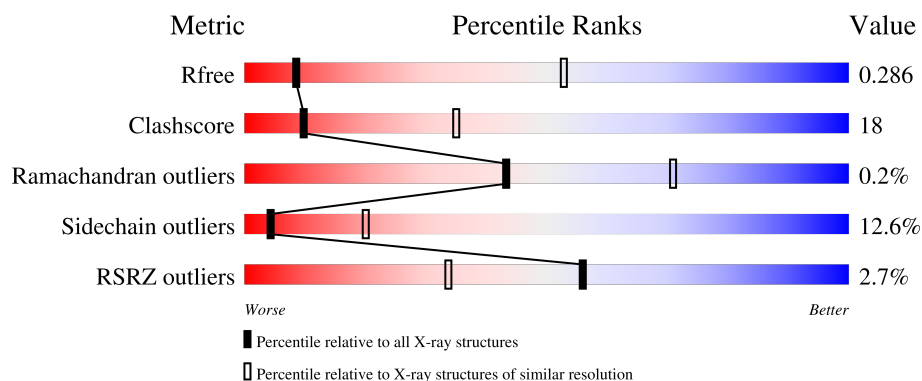
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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}	180053	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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 $\leq 5\%$. 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	
1	B	696	
1	C	696	
1	D	696	
1	E	696	

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Mol	Chain	Length	Quality of chain
1	F	696	4% 56% 25% • 16%
1	G	696	2% 55% 26% • 16%
1	H	696	2% 55% 25% • 16%

2 Entry composition

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
1	A	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	B	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	C	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	D	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	E	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	F	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	G	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	H	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			

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

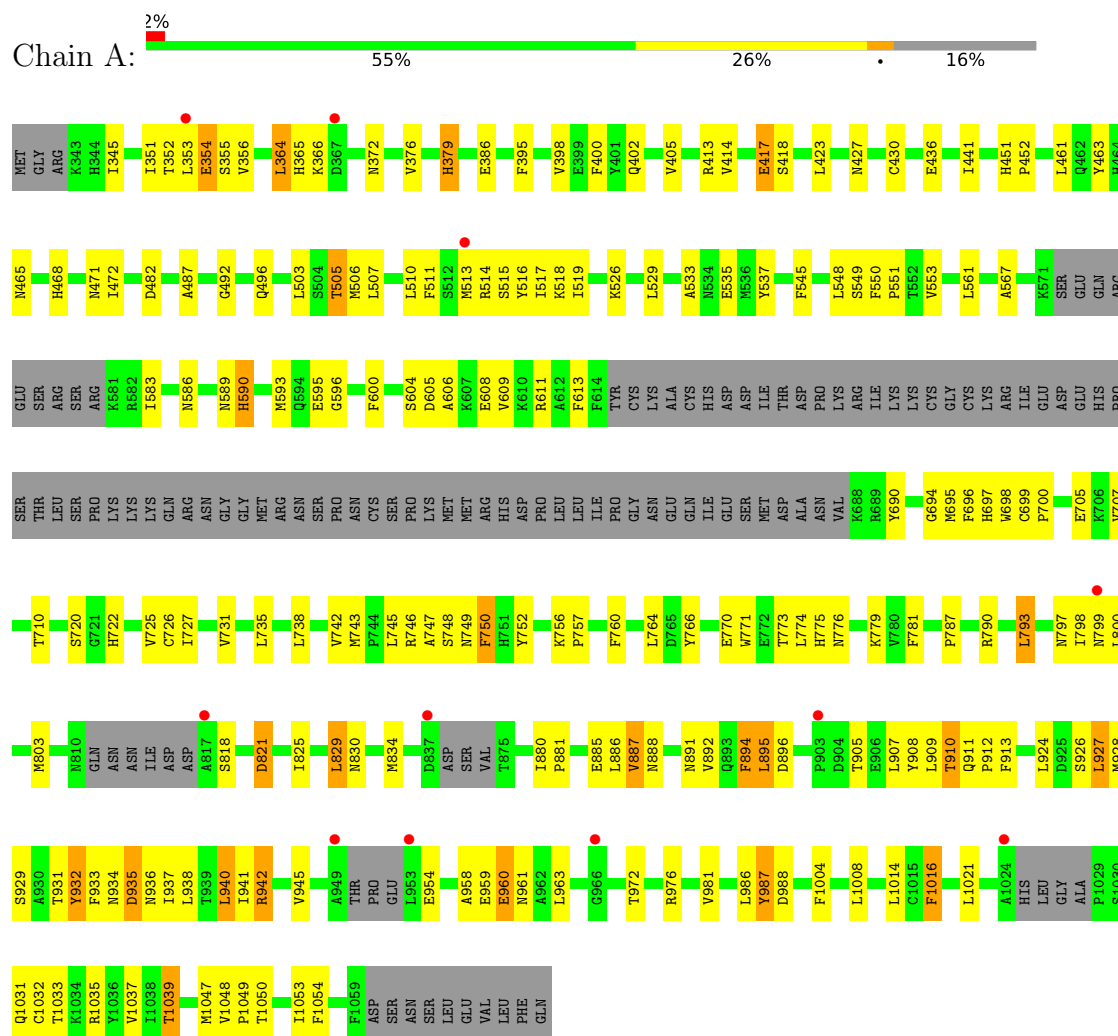
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

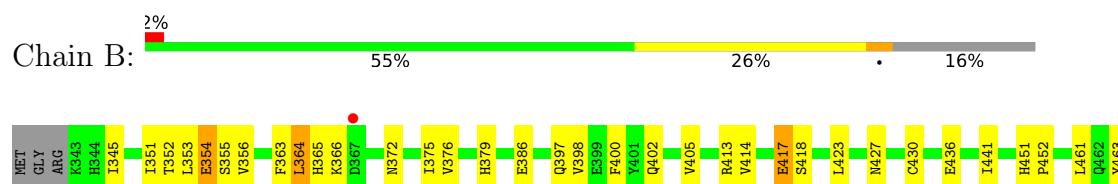
3 Residue-property plots

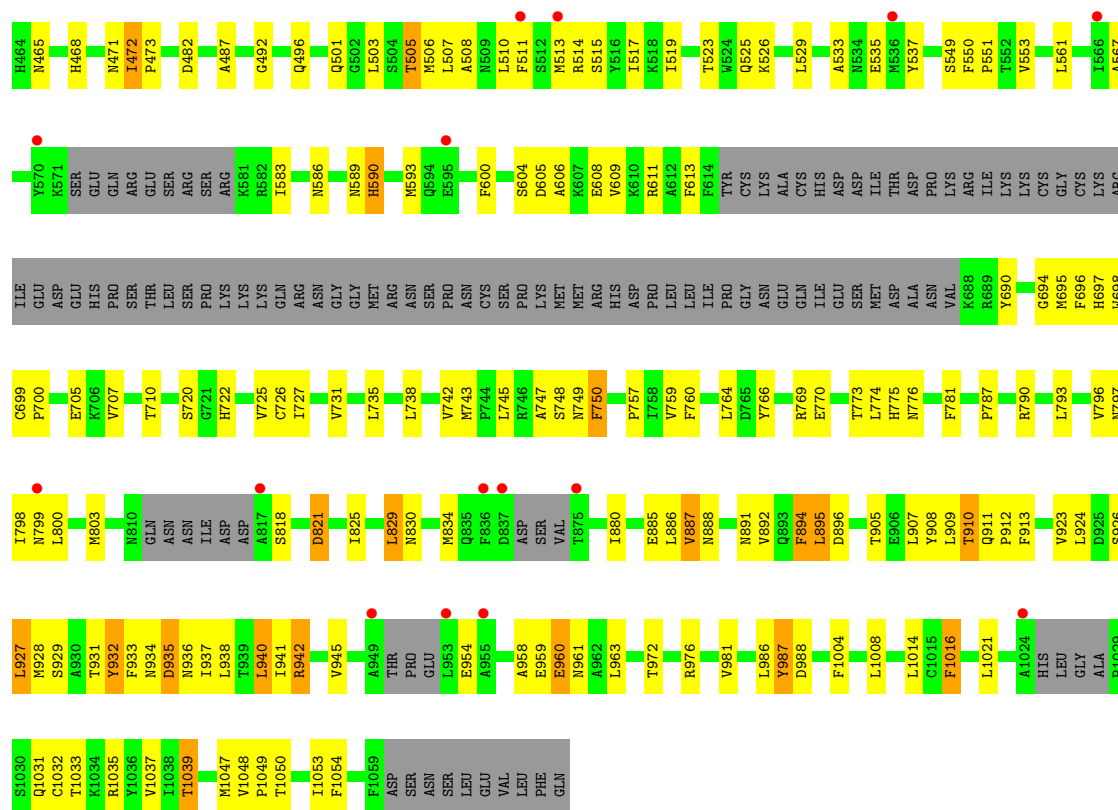
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: High-Conductance Ca^{2+} -Activated K^{+} Channel protein

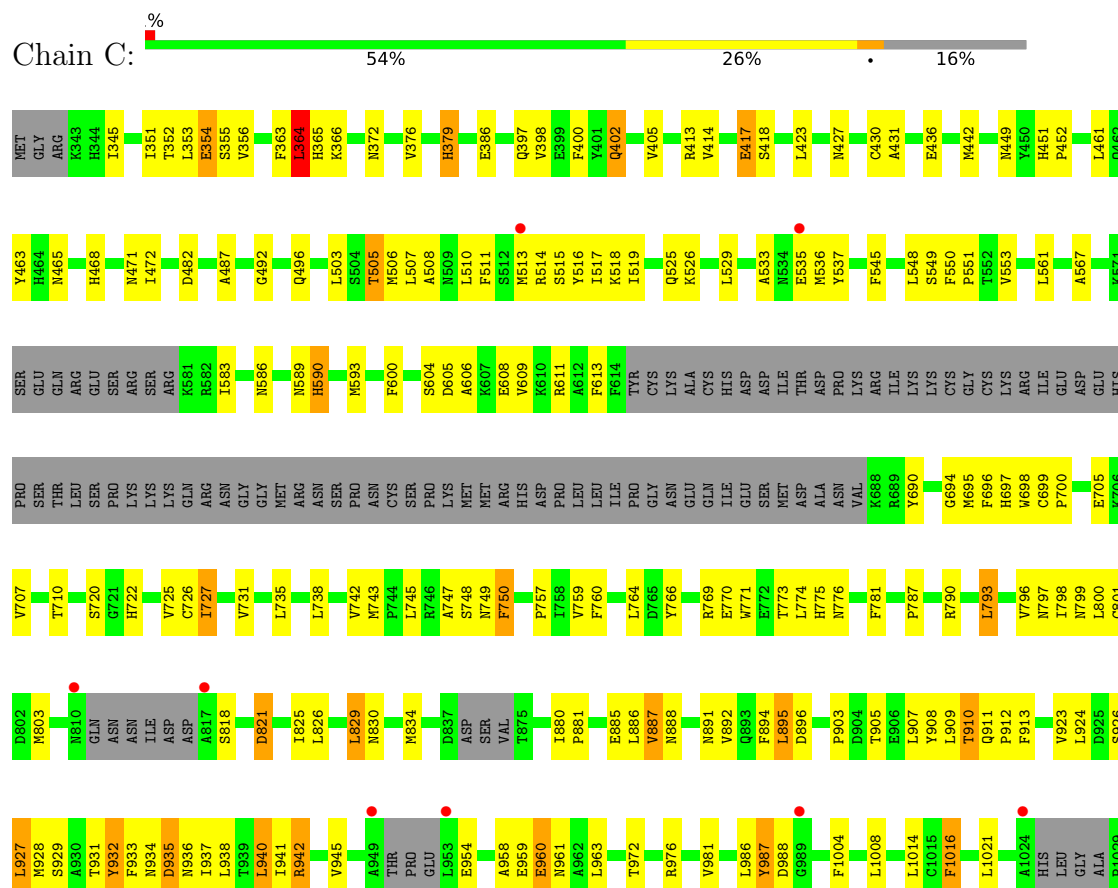


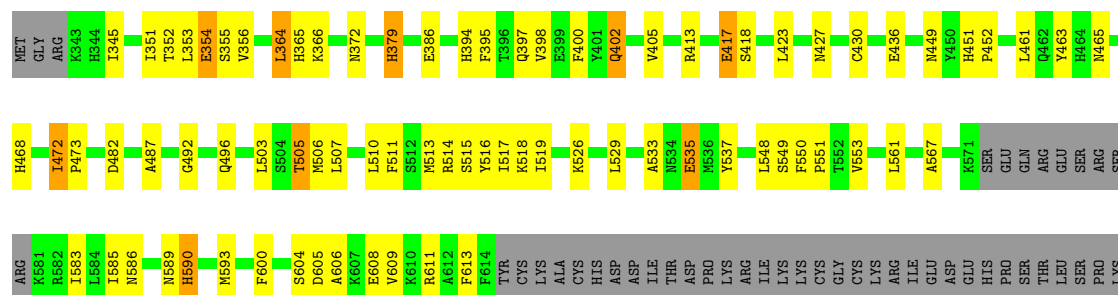
• Molecule 1: High-Conductance Ca^{2+} -Activated K^{+} Channel protein

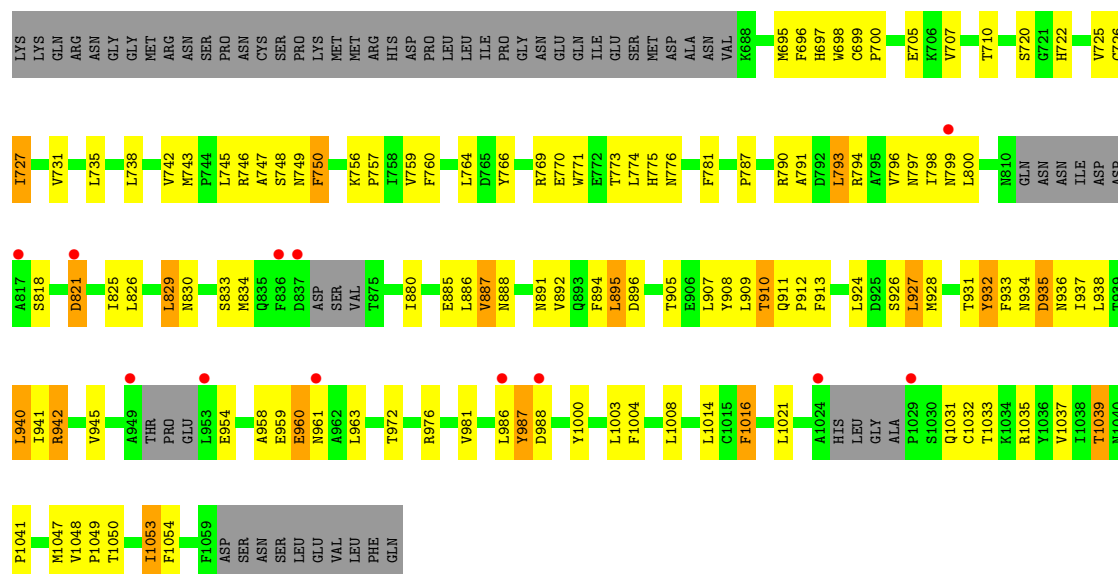




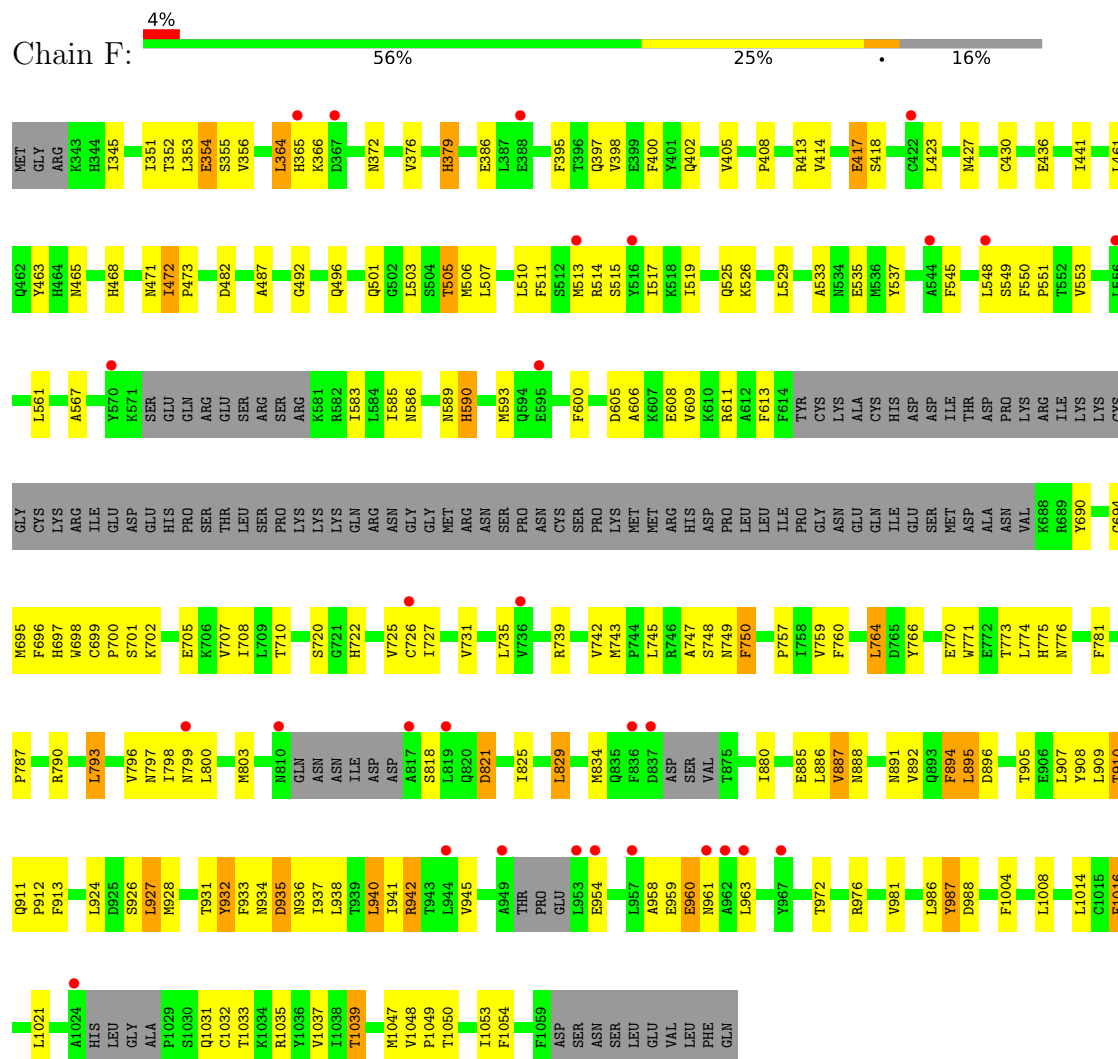
• Molecule 1: High-Conductance Ca²⁺-Activated K⁺ Channel protein



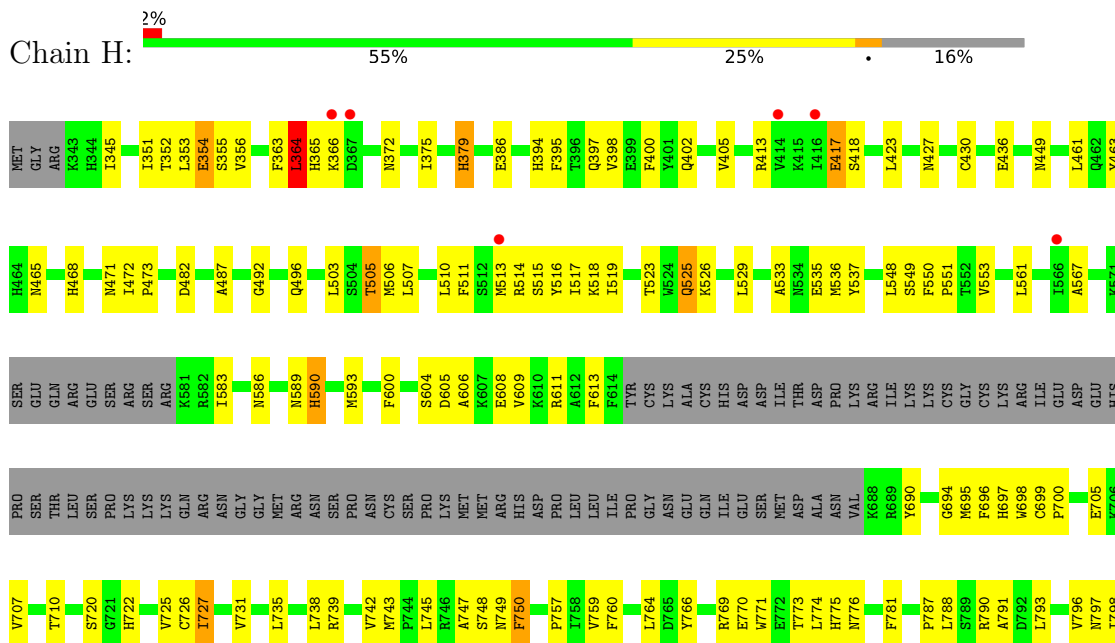
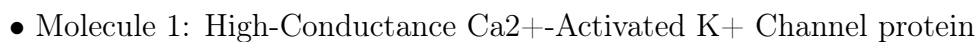


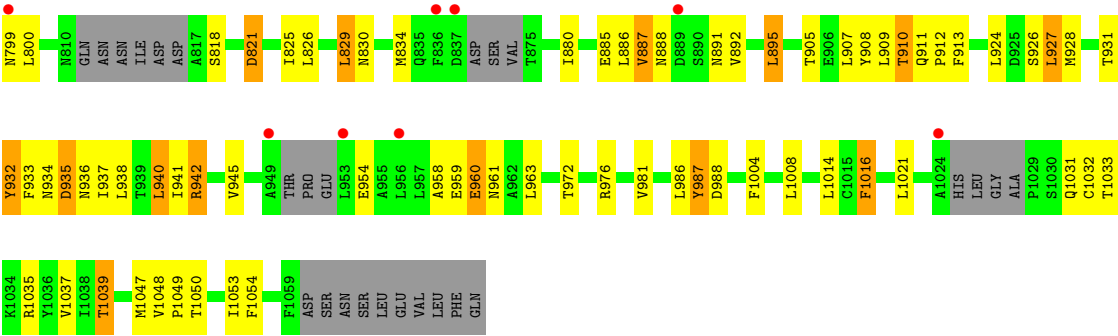


• Molecule 1: High-Conductance Ca^{2+} -Activated K^{+} Channel protein



• Molecule 1: High-Conductance Ca^{2+} -Activated K^{+} Channel protein





4 Data and refinement statistics

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 48.22 – 3.61	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.22-3.61) 89.3 (48.22-3.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.29 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.58	0/4398	0.89	4/6001 (0.1%)
1	B	0.59	0/4398	0.89	4/6001 (0.1%)
1	C	0.60	0/4398	0.90	4/6001 (0.1%)
1	D	0.59	0/4398	0.89	5/6001 (0.1%)
1	E	0.61	0/4398	0.90	6/6001 (0.1%)
1	F	0.60	0/4398	0.90	4/6001 (0.1%)
1	G	0.59	0/4398	0.89	4/6001 (0.1%)
1	H	0.59	0/4398	0.89	3/6001 (0.0%)
All	All	0.60	0/35184	0.90	34/48008 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	894	PHE	N-CA-C	6.29	118.21	111.36
1	A	894	PHE	N-CA-C	6.10	118.01	111.36
1	G	364	LEU	N-CA-C	6.01	117.78	109.54
1	G	472	ILE	CA-C-N	5.99	125.47	119.24
1	G	472	ILE	C-N-CA	5.99	125.47	119.24
1	C	894	PHE	N-CA-C	5.98	117.87	111.36
1	B	472	ILE	CA-C-N	5.95	125.43	119.24
1	B	472	ILE	C-N-CA	5.95	125.43	119.24
1	B	364	LEU	N-CA-C	5.92	117.65	109.54
1	D	472	ILE	CA-C-N	5.88	125.36	119.24
1	D	472	ILE	C-N-CA	5.88	125.36	119.24
1	H	472	ILE	CA-C-N	5.85	125.32	119.24
1	H	472	ILE	C-N-CA	5.85	125.32	119.24
1	E	472	ILE	CA-C-N	5.84	125.31	119.24
1	E	472	ILE	C-N-CA	5.84	125.31	119.24
1	C	472	ILE	CA-C-N	5.82	125.29	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	472	ILE	C-N-CA	5.82	125.29	119.24
1	F	364	LEU	N-CA-C	5.74	117.40	109.54
1	E	894	PHE	N-CA-C	5.70	117.57	111.36
1	E	364	LEU	N-CA-C	5.70	117.34	109.54
1	A	364	LEU	N-CA-C	5.67	117.31	109.54
1	F	472	ILE	CA-C-N	5.66	125.12	119.24
1	F	472	ILE	C-N-CA	5.66	125.12	119.24
1	C	364	LEU	N-CA-C	5.64	117.27	109.54
1	B	894	PHE	N-CA-C	5.63	117.50	111.36
1	F	894	PHE	N-CA-C	5.61	117.48	111.36
1	H	364	LEU	N-CA-C	5.61	117.22	109.54
1	D	364	LEU	N-CA-C	5.47	117.03	109.54
1	A	472	ILE	CA-C-N	5.43	124.89	119.24
1	A	472	ILE	C-N-CA	5.43	124.89	119.24
1	D	372	ASN	N-CA-C	5.15	116.97	111.36
1	E	535	GLU	N-CA-C	-5.13	100.23	108.55
1	E	1053	ILE	N-CA-C	5.11	115.20	107.75
1	G	372	ASN	N-CA-C	5.09	116.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	148	0
1	B	4312	0	4016	148	0
1	C	4312	0	4017	154	0
1	D	4312	0	4016	154	1
1	E	4312	0	4017	154	1
1	F	4312	0	4017	155	1
1	G	4312	0	4017	164	1
1	H	4312	0	4017	152	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1171	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 18.

All (1171) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:553:VAL:HG21	1:F:593:MET:HE3	1.46	0.98
1:G:511:PHE:HZ	1:G:941:ILE:CG2	1.71	0.97
1:H:553:VAL:HG21	1:H:593:MET:HE3	1.47	0.96
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:A:553:VAL:HG21	1:A:593:MET:HE3	1.46	0.95
1:G:553:VAL:HG21	1:G:593:MET:HE3	1.47	0.95
1:C:553:VAL:HG21	1:C:593:MET:HE3	1.46	0.94
1:D:553:VAL:HG21	1:D:593:MET:HE3	1.48	0.94
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:B:553:VAL:HG21	1:B:593:MET:HE3	1.50	0.93
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:E:553:VAL:HG21	1:E:593:MET:HE3	1.51	0.90
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:960:GLU:CD	1:G:791:ALA:HB2	2.09	0.77
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:D:932:TYR:C	1:D:932:TYR:CD2	2.64	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:A:932:TYR:C	1:A:932:TYR:CD2	2.64	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:G:932:TYR:C	1:G:932:TYR:CD2	2.65	0.74
1:B:932:TYR:C	1:B:932:TYR:CD2	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:932:TYR:C	1:F:932:TYR:CD2	2.66	0.73
1:A:366:LYS:NZ	1:A:533:ALA:O	2.18	0.73
1:E:932:TYR:C	1:E:932:TYR:CD2	2.66	0.73
1:C:960:GLU:OE2	1:C:960:GLU:HA	1.87	0.73
1:C:932:TYR:C	1:C:932:TYR:CD2	2.66	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:H:932:TYR:C	1:H:932:TYR:CD2	2.66	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: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:G:793:LEU:HG	1:G:798:ILE:CD1	2.20	0.70
1:B:960:GLU:CD	1:H:791:ALA:HB2	2.16	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:D:793:LEU:HG	1:D:798:ILE:CD1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:707:VAL:HG13	1:F:781:PHE:HA	1.74	0.69
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: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:A:932:TYR:C	1:A:932:TYR:HD2	2.03	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:D:932:TYR:C	1:D:932:TYR:HD2	2.01	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:G:932:TYR:C	1:G:932:TYR:HD2	2.03	0.66
1:B:549:SER:HB2	1:B:589:ASN:O	1.95	0.66
1:B:932:TYR:C	1:B:932:TYR:HD2	2.04	0.66
1:A:492:GLY:HA3	1:A:945:VAL:CG1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:932:TYR:C	1:E:932:TYR:HD2	2.04	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:F:932:TYR:C	1:F:932:TYR:HD2	2.05	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:H:932:TYR:C	1:H:932:TYR:HD2	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:932:TYR:C	1:C:932:TYR:HD2	2.06	0.63
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:605:ASP:HB3	1:A:608:GLU:HG2	1.80	0.62
1:G:1016:PHE:CE1	1:G:1054:PHE:HB3	2.35	0.62
1:A:695:MET:C	1:A:696:PHE:HD2	2.08	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:B:695:MET:C	1:B:696:PHE:HD2	2.08	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: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:D:695:MET:C	1:D:696:PHE:HD2	2.09	0.61
1:E:605:ASP:HB3	1:E:608:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:695:MET:C	1:C:696:PHE:HD2	2.10	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:E:695:MET:C	1:E:696:PHE:HD2	2.09	0.60
1:G:695:MET:C	1:G:696:PHE:HD2	2.09	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:A:941:ILE:HG13	1:A:942:ARG:N	2.17	0.59
1:B:463:TYR:C	1:B:463:TYR:CD2	2.80	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:D:960:GLU:CD	1:E:791:ALA:HB2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:941:ILE:HG13	1:H:942:ARG:N	2.16	0.59
1:H:695:MET:C	1:H:696:PHE:HD2	2.10	0.59
1:A:463:TYR:C	1:A:463:TYR:CD2	2.81	0.59
1:A:960:GLU:OE1	1:G:791:ALA:CB	2.50	0.59
1:D:941:ILE:HG13	1:D:942:ARG:N	2.16	0.59
1:E:908:TYR:HA	1:E:913:PHE:CD2	2.38	0.59
1:D:379:HIS:HD2	1:D:402:GLN:HA	1.67	0.59
1:F:695:MET:C	1:F:696:PHE:HD2	2.11	0.59
1:A:1048:VAL:HG12	1:A:1050:THR:H	1.68	0.59
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:G:463:TYR:C	1:G:463:TYR:CD2	2.80	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:E:463:TYR:C	1:E:463:TYR:CD2	2.82	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:C:463:TYR:C	1:C:463:TYR:CD2	2.81	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: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:E:986:LEU:HD11	1:E:1047:MET:HE3	1.86	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:F:463:TYR:C	1:F:463:TYR:CD2	2.81	0.57
1:G:818:SER:HB2	1:G:887:VAL:CG1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:986:LEU:HD11	1:D:1047:MET:HE3	1.86	0.57
1:B:379:HIS:HD2	1:B:402:GLN:HA	1.69	0.57
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:H:463:TYR:C	1:H:463:TYR:CD2	2.82	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:D:1048:VAL:HG13	1:D:1049:PRO:HD2	1.86	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:F:986:LEU:HD11	1:F:1047:MET:HE3	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:611:ARG:C	1:C:613:PHE:H	2.14	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
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:D:463:TYR:C	1:D:463:TYR:CD2	2.83	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:H:611:ARG:C	1:H:613:PHE:H	2.14	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: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: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:825:ILE:HD12	1:A:825:ILE:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:537:TYR:HB2	1:D:609:VAL:HG21	1.88	0.55
1:G:611:ARG:C	1:G:613:PHE:H	2.15	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:A:561:LEU:O	1:A:611:ARG:NH2	2.40	0.54
1:A:611:ARG:C	1:A:613:PHE:H	2.15	0.54
1:C:1021:LEU:HD23	1:C:1035:ARG:HG2	1.89	0.54
1:A:888:ASN:HB3	1:A:891:ASN:ND2	2.23	0.54
1:B:611:ARG:C	1:B:613:PHE:H	2.14	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:D:471:ASN:O	1:E:833:SER:OG	2.15	0.54
1:F:825:ILE:HD12	1:F:825:ILE:H	1.72	0.54
1:C:986:LEU:HD11	1:C:1047:MET:HE3	1.90	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: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:611:ARG:C	1:F:613:PHE:H	2.17	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:E:611:ARG:C	1:E:613:PHE:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:886:LEU:HD11	1:G:895:LEU:HD21	1.90	0.53
1:C:553:VAL:CG2	1:C:593:MET:HE3	2.31	0.53
1:D:697:HIS:CE1	1:D:748:SER:HA	2.44	0.53
1:G:537:TYR:HB2	1:G:609:VAL:HG21	1.89	0.53
1:G:935:ASP:OD1	1:G:935:ASP:N	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:H:986:LEU:HD11	1:H:1047:MET:HE3	1.91	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: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:D:611:ARG:C	1:D:613:PHE:H	2.15	0.52
1:G:427:ASN:O	1:G:430:CYS:HB2	2.09	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:G:986:LEU:HD11	1:G:1047:MET:HE3	1.90	0.52
1:B:722:HIS:HB3	1:B:757:PRO:HG2	1.90	0.52
1:G:1004:PHE:CD1	1:G:1004:PHE:C	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:590:HIS:ND1	1:D:590:HIS:N	2.57	0.51
1:B:423:LEU:HD23	1:B:928:MET:HG3	1.93	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:1004:PHE:CD1	1:H:1004:PHE:C	2.90	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:E:1004:PHE:CD1	1:E:1004:PHE:C	2.88	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:821:ASP:OD2	1:A:821:ASP:C	2.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1004:PHE:CD1	1:D:1004:PHE:C	2.89	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:F:1004:PHE:CD1	1:F:1004:PHE:C	2.89	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:B:986:LEU:HD11	1:B:1047:MET:HE3	1.94	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:A:492:GLY:HA3	1:A:945:VAL:HG12	1.95	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:A:986:LEU:HD11	1:A:1047:MET:HE3	1.94	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:A:940:LEU:C	1:A:940:LEU:HD12	2.38	0.48
1:C:1004:PHE:CD1	1:C:1004:PHE:C	2.89	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: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:553:VAL:CG2	1:A:593:MET:HE3	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:MET:HG2	1:B:1039:THR:HG23	1.94	0.48
1:B:940:LEU:C	1:B:940:LEU:HD12	2.39	0.48
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:B:1004:PHE:CD1	1:B:1004:PHE:C	2.91	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:G:940:LEU:C	1:G:940:LEU:HD12	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:TYR:HD2	1:D:933:PHE:N	2.13	0.47
1:F:553:VAL:CG2	1:F:593:MET:HE3	2.31	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
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:D:766:TYR:C	1:D:766:TYR:CD2	2.93	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:766:TYR:C	1:B:766:TYR:CD2	2.93	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:593:MET:HE2	1:D:593:MET:H	1.81	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:H:940:LEU:HD12	1:H:940:LEU:C	2.41	0.46
1:D:940:LEU:C	1:D:940:LEU:HD12	2.40	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:A:1004:PHE:CD1	1:A:1004:PHE:C	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:766:TYR:C	1:E:766:TYR:CD2	2.92	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
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:F:766:TYR:C	1:F:766:TYR:CD2	2.93	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:H:821:ASP:OD2	1:H:821:ASP:C	2.58	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:821:ASP:OD2	1:D:821:ASP:C	2.59	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:C:766:TYR:C	1:C:766:TYR:CD2	2.94	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:H:553:VAL:CG2	1:H:593:MET:HE3	2.33	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:1047:MET:HE1	1:H:1053:ILE:HD11	1.98	0.45
1:A:549:SER:O	1:A:553:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:442:MET:HE3	1:D:822:LYS:CB	2.46	0.45
1:F:798:ILE:HG22	1:F:880:ILE:HG21	1.98	0.45
1:F:940:LEU:C	1:F:940:LEU:HD12	2.41	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: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
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:821:ASP:OD2	1:B:821:ASP:C	2.59	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: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:A:766:TYR:CD2	1:A:766:TYR:C	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:821:ASP:C	1:G:821:ASP:OD2	2.60	0.45
1:H:567:ALA:HB3	1:H:600:PHE:HD2	1.82	0.45
1:E:940:LEU:HD12	1:E:940:LEU:C	2.42	0.45
1:E:1047:MET:HE1	1:E:1053:ILE:HD11	1.99	0.45
1:F:354:GLU:HG2	1:F:355:SER:N	2.31	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:695:MET:C	1:A:696:PHE:CD2	2.93	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:553:VAL:CG2	1:E:593:MET:HE3	2.36	0.44
1:E:567:ALA:HB2	1:E:585:ILE:HA	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:695:MET:C	1:B:696:PHE:CD2	2.94	0.44
1:C:548:LEU:O	1:C:593:MET:HE2	2.18	0.44
1:C:940:LEU:HD12	1:C:940:LEU:C	2.42	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:D:1047:MET:HE1	1:D:1053:ILE:HD11	1.99	0.44
1:E:821:ASP:OD2	1:E:821:ASP:C	2.60	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
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:H:536:MET:HE3	1:H:937:ILE:HD12	2.00	0.44
1:E:707:VAL:HG21	1:E:771:TRP:CH2	2.53	0.43
1:F:821:ASP:OD2	1:F:821:ASP:C	2.60	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: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:766:TYR:CD2	1:H:766:TYR:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:593:MET:HE2	1:E:593:MET:H	1.84	0.43
1:G:417:GLU:OE2	1:G:418:SER:N	2.47	0.43
1:G:766:TYR:C	1:G:766:TYR:CD2	2.96	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:C:536:MET:HE3	1:C:937:ILE:HD12	2.00	0.43
1:C:821:ASP:OD2	1:C:821:ASP:C	2.62	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:F:700:PRO:O	1:F:701:SER:C	2.62	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
1:F:695:MET:C	1:F:696:PHE:CD2	2.95	0.43
1:H:695:MET:C	1:H:696:PHE:CD2	2.95	0.43
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:C:1047:MET:HE1	1:C:1053:ILE:HD11	2.01	0.43
1:D:451:HIS:HA	1:D:452:PRO:HD3	1.83	0.43
1:G:695:MET:C	1:G:696:PHE:CD2	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:593:MET:HE2	1:H:593:MET:H	1.84	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:C:536:MET:HE3	1:C:937:ILE:CD1	2.49	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:G:548:LEU:O	1:G:593:MET:HE2	2.19	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:553:VAL:CG2	1:G:593:MET:HE3	2.32	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:B:1047:MET:HE1	1:B:1053:ILE:HD11	2.02	0.42
1:D:501:GLN:HG3	1:D:803:MET:HE1	2.00	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
1:G:366:LYS:CE	1:G:515:SER:HA	2.50	0.42
1:G:593:MET:HE2	1:G:593:MET:H	1.85	0.42
1:G:987:TYR:CD2	1:G:988:ASP:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:593:MET:HE2	1:C:593:MET:H	1.85	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:B:501:GLN:HG3	1:B:803:MET:HE1	2.01	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:G:536:MET:HE3	1:G:937:ILE:HD12	2.02	0.42
1:H:366:LYS:HE3	1:H:514:ARG:O	2.20	0.42
1:A:1047:MET:HE1	1:A:1053:ILE:HD11	2.02	0.42
1:B:376:VAL:HG11	1:B:414:VAL:HG13	2.01	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:C:830:ASN:HA	1:F:471:ASN:HB3	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:695:MET:C	1:C:696:PHE:CD2	2.95	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:G:1047:MET:HE1	1:G:1053:ILE:HD11	2.01	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: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:593:MET:H	1:B:593:MET:HE2	1.84	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:536:MET:HE3	1:D:937:ILE:HD12	2.01	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: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: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:F:907:LEU:O	1:F:910:THR:OG1	2.37	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
1:B:468:HIS:HE1	1:H:788:LEU:HB3	1.86	0.41
1:D:430:CYS:SG	1:D:431:ALA:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:501:GLN:HG3	1:F:803:MET:HE1	2.02	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:553:VAL:CG2	1:D:593:MET:HE3	2.34	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:1047:MET:HE1	1:F:1053:ILE:HD11	2.03	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:548:LEU:O	1:A:593:MET:HE2	2.20	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:593:MET:H	1:F:593:MET:HE2	1.85	0.41
1:F:695:MET:O	1:F:696:PHE:HD2	2.04	0.41
1:H:548:LEU:O	1:H:593:MET:HE2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:PHE:HD2	1:C:364:LEU:CD2	2.34	0.40
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: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:E:695:MET:C	1:E:696:PHE:CD2	2.95	0.40
1:F:548:LEU:O	1:F:593:MET:HE2	2.21	0.40
1:G:506:MET:CB	1:G:1037:VAL:HG11	2.51	0.40
1:G:536:MET:HE3	1:G:937:ILE:CD1	2.52	0.40
1:A:463:TYR:C	1:A:463:TYR:HD2	2.28	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: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:E:548:LEU:O	1:E:593:MET:HE2	2.21	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%)	43	71
1	B	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	43	71
1	C	571/696 (82%)	538 (94%)	32 (6%)	1 (0%)	43	71
1	D	571/696 (82%)	540 (95%)	30 (5%)	1 (0%)	43	71
1	E	571/696 (82%)	538 (94%)	32 (6%)	1 (0%)	43	71
1	F	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	43	71
1	G	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	43	71
1	H	571/696 (82%)	537 (94%)	33 (6%)	1 (0%)	43	71
All	All	4568/5568 (82%)	4310 (94%)	250 (6%)	8 (0%)	43	71

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 ⓘ

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	20
1	B	432/616 (70%)	380 (88%)	52 (12%)	5	22
1	C	432/616 (70%)	376 (87%)	56 (13%)	4	19
1	D	432/616 (70%)	379 (88%)	53 (12%)	4	21
1	E	432/616 (70%)	375 (87%)	57 (13%)	4	19
1	F	432/616 (70%)	376 (87%)	56 (13%)	4	19
1	G	432/616 (70%)	378 (88%)	54 (12%)	4	20
1	H	432/616 (70%)	377 (87%)	55 (13%)	4	20
All	All	3456/4928 (70%)	3019 (87%)	437 (13%)	4	20

All (437) 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	505	THR
1	A	507	LEU
1	A	513	MET
1	A	583	ILE
1	A	590	HIS
1	A	699	CYS
1	A	705	GLU
1	A	710	THR
1	A	727	ILE

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Mol	Chain	Res	Type
1	A	731	VAL
1	A	742	VAL
1	A	745	LEU
1	A	749	ASN
1	A	750	PHE
1	A	764	LEU
1	A	773	THR
1	A	774	LEU
1	A	793	LEU
1	A	821	ASP
1	A	829	LEU
1	A	885	GLU
1	A	887	VAL
1	A	895	LEU
1	A	905	THR
1	A	910	THR
1	A	926	SER
1	A	927	LEU
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	972	THR
1	A	987	TYR
1	A	1008	LEU
1	A	1016	PHE
1	A	1031	GLN
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	386	GLU
1	B	397	GLN
1	B	405	VAL

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Mol	Chain	Res	Type
1	B	417	GLU
1	B	482	ASP
1	B	505	THR
1	B	507	LEU
1	B	513	MET
1	B	583	ILE
1	B	590	HIS
1	B	699	CYS
1	B	705	GLU
1	B	710	THR
1	B	727	ILE
1	B	731	VAL
1	B	742	VAL
1	B	745	LEU
1	B	749	ASN
1	B	750	PHE
1	B	764	LEU
1	B	773	THR
1	B	774	LEU
1	B	821	ASP
1	B	829	LEU
1	B	885	GLU
1	B	887	VAL
1	B	895	LEU
1	B	905	THR
1	B	910	THR
1	B	926	SER
1	B	927	LEU
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	972	THR
1	B	987	TYR
1	B	1008	LEU
1	B	1016	PHE
1	B	1031	GLN

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Mol	Chain	Res	Type
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
1	C	379	HIS
1	C	386	GLU
1	C	397	GLN
1	C	402	GLN
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	525	GLN
1	C	583	ILE
1	C	590	HIS
1	C	699	CYS
1	C	705	GLU
1	C	710	THR
1	C	727	ILE
1	C	731	VAL
1	C	742	VAL
1	C	745	LEU
1	C	749	ASN
1	C	750	PHE
1	C	764	LEU
1	C	773	THR
1	C	774	LEU
1	C	793	LEU
1	C	821	ASP
1	C	829	LEU
1	C	885	GLU
1	C	887	VAL
1	C	895	LEU
1	C	905	THR
1	C	910	THR
1	C	926	SER
1	C	927	LEU

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Mol	Chain	Res	Type
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
1	C	972	THR
1	C	987	TYR
1	C	1008	LEU
1	C	1016	PHE
1	C	1031	GLN
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	397	GLN
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	699	CYS
1	D	705	GLU
1	D	710	THR
1	D	727	ILE
1	D	731	VAL
1	D	742	VAL
1	D	745	LEU
1	D	749	ASN
1	D	750	PHE
1	D	764	LEU

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Mol	Chain	Res	Type
1	D	773	THR
1	D	774	LEU
1	D	821	ASP
1	D	829	LEU
1	D	885	GLU
1	D	887	VAL
1	D	895	LEU
1	D	905	THR
1	D	910	THR
1	D	926	SER
1	D	927	LEU
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	972	THR
1	D	987	TYR
1	D	1008	LEU
1	D	1016	PHE
1	D	1031	GLN
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	397	GLN
1	E	402	GLN
1	E	405	VAL
1	E	417	GLU
1	E	482	ASP
1	E	505	THR
1	E	507	LEU

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Mol	Chain	Res	Type
1	E	513	MET
1	E	583	ILE
1	E	590	HIS
1	E	699	CYS
1	E	705	GLU
1	E	710	THR
1	E	727	ILE
1	E	731	VAL
1	E	742	VAL
1	E	745	LEU
1	E	749	ASN
1	E	750	PHE
1	E	764	LEU
1	E	773	THR
1	E	774	LEU
1	E	793	LEU
1	E	821	ASP
1	E	829	LEU
1	E	885	GLU
1	E	887	VAL
1	E	895	LEU
1	E	905	THR
1	E	910	THR
1	E	926	SER
1	E	927	LEU
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	972	THR
1	E	987	TYR
1	E	1003	LEU
1	E	1008	LEU
1	E	1016	PHE
1	E	1031	GLN
1	E	1032	CYS
1	E	1033	THR

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Mol	Chain	Res	Type
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	397	GLN
1	F	405	VAL
1	F	417	GLU
1	F	482	ASP
1	F	505	THR
1	F	507	LEU
1	F	513	MET
1	F	525	GLN
1	F	583	ILE
1	F	590	HIS
1	F	699	CYS
1	F	705	GLU
1	F	710	THR
1	F	727	ILE
1	F	731	VAL
1	F	742	VAL
1	F	745	LEU
1	F	749	ASN
1	F	750	PHE
1	F	764	LEU
1	F	773	THR
1	F	774	LEU
1	F	793	LEU
1	F	821	ASP
1	F	829	LEU
1	F	885	GLU
1	F	887	VAL
1	F	895	LEU
1	F	905	THR
1	F	910	THR
1	F	926	SER
1	F	927	LEU
1	F	932	TYR
1	F	935	ASP

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Mol	Chain	Res	Type
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	972	THR
1	F	987	TYR
1	F	1008	LEU
1	F	1016	PHE
1	F	1031	GLN
1	F	1032	CYS
1	F	1033	THR
1	F	1039	THR
1	G	354	GLU
1	G	364	LEU
1	G	365	HIS
1	G	372	ASN
1	G	386	GLU
1	G	395	PHE
1	G	397	GLN
1	G	405	VAL
1	G	417	GLU
1	G	482	ASP
1	G	505	THR
1	G	507	LEU
1	G	513	MET
1	G	583	ILE
1	G	590	HIS
1	G	699	CYS
1	G	705	GLU
1	G	710	THR
1	G	727	ILE
1	G	731	VAL
1	G	742	VAL
1	G	745	LEU
1	G	749	ASN
1	G	750	PHE
1	G	764	LEU
1	G	773	THR
1	G	774	LEU

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Mol	Chain	Res	Type
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	905	THR
1	G	910	THR
1	G	926	SER
1	G	927	LEU
1	G	932	TYR
1	G	935	ASP
1	G	936	ASN
1	G	940	LEU
1	G	942	ARG
1	G	959	GLU
1	G	960	GLU
1	G	961	ASN
1	G	963	LEU
1	G	972	THR
1	G	987	TYR
1	G	1008	LEU
1	G	1016	PHE
1	G	1031	GLN
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	397	GLN
1	H	405	VAL
1	H	417	GLU
1	H	482	ASP
1	H	505	THR
1	H	507	LEU
1	H	513	MET
1	H	525	GLN

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Mol	Chain	Res	Type
1	H	583	ILE
1	H	590	HIS
1	H	699	CYS
1	H	705	GLU
1	H	710	THR
1	H	727	ILE
1	H	731	VAL
1	H	742	VAL
1	H	745	LEU
1	H	749	ASN
1	H	750	PHE
1	H	764	LEU
1	H	773	THR
1	H	774	LEU
1	H	821	ASP
1	H	829	LEU
1	H	885	GLU
1	H	887	VAL
1	H	895	LEU
1	H	905	THR
1	H	910	THR
1	H	926	SER
1	H	927	LEU
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	972	THR
1	H	987	TYR
1	H	1008	LEU
1	H	1016	PHE
1	H	1031	GLN
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	468	HIS
1	B	697	HIS
1	B	776	ASN
1	B	891	ASN
1	C	350	HIS
1	C	379	HIS
1	C	394	HIS
1	C	427	ASN
1	C	468	HIS
1	C	697	HIS
1	C	776	ASN
1	C	891	ASN
1	D	379	HIS
1	D	394	HIS
1	D	468	HIS
1	D	776	ASN
1	D	891	ASN
1	E	379	HIS
1	E	394	HIS
1	E	449	ASN
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	427	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	449	ASN
1	G	468	HIS

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Mol	Chain	Res	Type
1	G	697	HIS
1	G	776	ASN
1	G	891	ASN
1	H	379	HIS
1	H	394	HIS
1	H	449	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	11 (1%)	66	41	58, 105, 158, 185	0
1	B	585/696 (84%)	0.34	16 (2%)	56	34	67, 105, 151, 179	0
1	C	585/696 (84%)	0.05	8 (1%)	73	47	55, 95, 141, 181	0
1	D	585/696 (84%)	0.28	21 (3%)	46	27	57, 102, 155, 217	0
1	E	585/696 (84%)	0.18	12 (2%)	63	39	50, 86, 134, 180	0
1	F	585/696 (84%)	0.33	29 (4%)	34	21	59, 96, 149, 200	0
1	G	585/696 (84%)	0.32	14 (2%)	59	36	68, 108, 160, 198	0
1	H	585/696 (84%)	0.31	14 (2%)	59	36	75, 112, 161, 203	0
All	All	4680/5568 (84%)	0.25	125 (2%)	56	34	50, 101, 154, 217	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	513	MET	4.7
1	F	963	LEU	4.3
1	B	513	MET	4.2
1	D	513	MET	4.2
1	C	949	ALA	4.2
1	H	949	ALA	3.9
1	B	511	PHE	3.9
1	B	949	ALA	3.9
1	F	961	ASN	3.9
1	G	513	MET	3.6
1	F	954	GLU	3.6
1	B	837	ASP	3.6
1	A	1024	ALA	3.6
1	F	949	ALA	3.4
1	A	949	ALA	3.4
1	D	1024	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	1024	ALA	3.4
1	H	367	ASP	3.4
1	G	367	ASP	3.4
1	D	949	ALA	3.4
1	E	1024	ALA	3.3
1	D	837	ASP	3.3
1	F	953	LEU	3.2
1	E	1029	PRO	3.2
1	G	970	PRO	3.2
1	F	513	MET	3.1
1	F	967	TYR	3.1
1	B	817	ALA	3.1
1	D	717	THR	3.1
1	B	566	ILE	3.0
1	F	962	ALA	3.0
1	C	513	MET	3.0
1	F	367	ASP	3.0
1	G	1029	PRO	3.0
1	B	536	MET	3.0
1	H	566	ILE	3.0
1	A	953	LEU	2.9
1	B	953	LEU	2.9
1	G	984	LEU	2.9
1	C	953	LEU	2.9
1	F	726	CYS	2.9
1	D	836	PHE	2.9
1	H	956	LEU	2.8
1	F	1024	ALA	2.8
1	G	949	ALA	2.8
1	H	837	ASP	2.8
1	C	535	GLU	2.8
1	D	367	ASP	2.8
1	D	422	CYS	2.7
1	G	817	ALA	2.7
1	E	961	ASN	2.7
1	B	955	ALA	2.7
1	E	817	ALA	2.6
1	E	799	ASN	2.6
1	D	955	ALA	2.6
1	F	810	ASN	2.6
1	H	799	ASN	2.6
1	E	988	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	960	GLU	2.6
1	F	817	ALA	2.6
1	G	810	ASN	2.6
1	G	837	ASP	2.6
1	H	889	ASP	2.6
1	F	595	GLU	2.5
1	B	367	ASP	2.5
1	G	953	LEU	2.5
1	D	1029	PRO	2.5
1	E	949	ALA	2.5
1	H	836	PHE	2.5
1	C	1024	ALA	2.5
1	D	719	LEU	2.5
1	F	570	TYR	2.5
1	A	367	ASP	2.5
1	E	953	LEU	2.5
1	D	947	GLY	2.5
1	F	365	HIS	2.4
1	E	821	ASP	2.4
1	H	414	VAL	2.4
1	G	1015	CYS	2.4
1	G	968	SER	2.4
1	B	836	PHE	2.4
1	F	736	VAL	2.4
1	E	837	ASP	2.4
1	E	836	PHE	2.4
1	D	953	LEU	2.4
1	A	513	MET	2.3
1	A	817	ALA	2.3
1	F	837	ASP	2.3
1	A	799	ASN	2.3
1	C	810	ASN	2.3
1	F	556	LEU	2.3
1	H	416	ILE	2.3
1	B	570	TYR	2.3
1	D	714	ALA	2.3
1	D	535	GLU	2.3
1	A	837	ASP	2.2
1	F	516	TYR	2.2
1	B	875	THR	2.2
1	G	544	ALA	2.2
1	B	1024	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	836	PHE	2.2
1	G	1024	ALA	2.1
1	D	718	VAL	2.1
1	A	903	PRO	2.1
1	A	353	LEU	2.1
1	E	986	LEU	2.1
1	F	388	GLU	2.1
1	H	953	LEU	2.1
1	D	810	ASN	2.1
1	F	819	LEU	2.1
1	F	957	LEU	2.1
1	B	595	GLU	2.1
1	D	961	ASN	2.1
1	F	548	LEU	2.1
1	A	966	GLY	2.1
1	D	436	GLU	2.1
1	F	422	CYS	2.1
1	F	799	ASN	2.1
1	F	944	LEU	2.1
1	D	875	THR	2.0
1	H	366	LYS	2.0
1	C	817	ALA	2.0
1	F	544	ALA	2.0
1	B	799	ASN	2.0
1	C	989	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
2	CA	A	2001	1/1	0.99	0.02	68,68,68,68	0
2	CA	B	2001	1/1	0.99	0.03	73,73,73,73	0
2	CA	C	2001	1/1	0.99	0.03	61,61,61,61	0
2	CA	D	2001	1/1	0.99	0.04	50,50,50,50	0
2	CA	E	2001	1/1	0.99	0.03	57,57,57,57	0
2	CA	F	2001	1/1	0.99	0.04	72,72,72,72	0
2	CA	G	2001	1/1	0.99	0.02	57,57,57,57	0
2	CA	H	2001	1/1	1.00	0.04	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.