



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:33 PM UTC

PDB ID : 3EI4 / pdb_00003ei4
Title : Structure of the hsDDB1-hsDDB2 complex
Authors : Scrima, A.; Pavletich, N.P.; Thoma, N.H.
Deposited on : 2008-09-15
Resolution : 3.30 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:

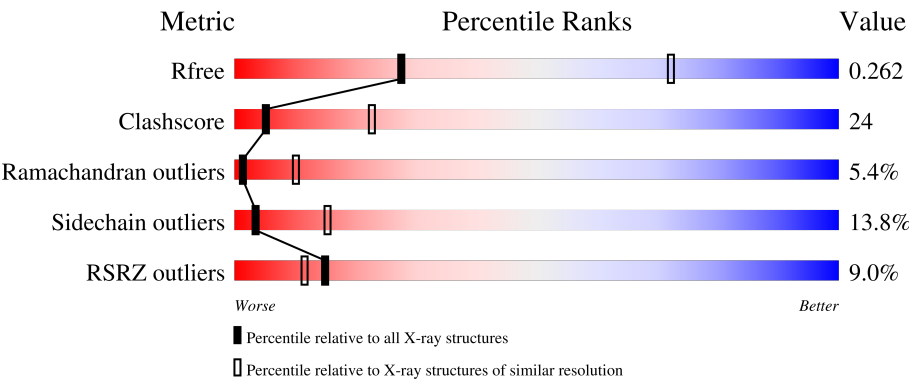
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	1158	9% 53%36%7%..
1	C	1158	10% 54%36%8%..
1	E	1158	9% 53%37%8%..
2	B	436	9% 38%35%10%•16%
2	D	436	5% 39%34%9%•16%

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Mol	Chain	Length	Quality of chain
2	F	436	5% 39% 36% 8% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35241 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0	0
			8861	5610	1493	1709	49			
1	C	1140	Total	C	N	O	S	0	0	0
			8861	5610	1493	1709	49			
1	E	1140	Total	C	N	O	S	0	0	0
			8861	5610	1493	1709	49			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	HIS	-	expression tag	UNP Q16531
A	-11	HIS	-	expression tag	UNP Q16531
A	-10	ARG	-	expression tag	UNP Q16531
A	-9	ARG	-	expression tag	UNP Q16531
A	-8	LEU	-	expression tag	UNP Q16531
A	-7	VAL	-	expression tag	UNP Q16531
A	-6	PRO	-	expression tag	UNP Q16531
A	-5	ARG	-	expression tag	UNP Q16531
A	-4	GLY	-	expression tag	UNP Q16531
A	-3	SER	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	422	TYR	ASP	SEE REMARK 999	UNP Q16531
A	898	ASP	GLU	SEE REMARK 999	UNP Q16531
A	899	VAL	LEU	SEE REMARK 999	UNP Q16531
C	-17	MET	-	expression tag	UNP Q16531
C	-16	HIS	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	HIS	-	expression tag	UNP Q16531
C	-14	HIS	-	expression tag	UNP Q16531
C	-13	HIS	-	expression tag	UNP Q16531
C	-12	HIS	-	expression tag	UNP Q16531
C	-11	HIS	-	expression tag	UNP Q16531
C	-10	ARG	-	expression tag	UNP Q16531
C	-9	ARG	-	expression tag	UNP Q16531
C	-8	LEU	-	expression tag	UNP Q16531
C	-7	VAL	-	expression tag	UNP Q16531
C	-6	PRO	-	expression tag	UNP Q16531
C	-5	ARG	-	expression tag	UNP Q16531
C	-4	GLY	-	expression tag	UNP Q16531
C	-3	SER	-	expression tag	UNP Q16531
C	-2	GLY	-	expression tag	UNP Q16531
C	-1	GLY	-	expression tag	UNP Q16531
C	0	ARG	-	expression tag	UNP Q16531
C	422	TYR	ASP	SEE REMARK 999	UNP Q16531
C	898	ASP	GLU	SEE REMARK 999	UNP Q16531
C	899	VAL	LEU	SEE REMARK 999	UNP Q16531
E	-17	MET	-	expression tag	UNP Q16531
E	-16	HIS	-	expression tag	UNP Q16531
E	-15	HIS	-	expression tag	UNP Q16531
E	-14	HIS	-	expression tag	UNP Q16531
E	-13	HIS	-	expression tag	UNP Q16531
E	-12	HIS	-	expression tag	UNP Q16531
E	-11	HIS	-	expression tag	UNP Q16531
E	-10	ARG	-	expression tag	UNP Q16531
E	-9	ARG	-	expression tag	UNP Q16531
E	-8	LEU	-	expression tag	UNP Q16531
E	-7	VAL	-	expression tag	UNP Q16531
E	-6	PRO	-	expression tag	UNP Q16531
E	-5	ARG	-	expression tag	UNP Q16531
E	-4	GLY	-	expression tag	UNP Q16531
E	-3	SER	-	expression tag	UNP Q16531
E	-2	GLY	-	expression tag	UNP Q16531
E	-1	GLY	-	expression tag	UNP Q16531
E	0	ARG	-	expression tag	UNP Q16531
E	422	TYR	ASP	SEE REMARK 999	UNP Q16531
E	898	ASP	GLU	SEE REMARK 999	UNP Q16531
E	899	VAL	LEU	SEE REMARK 999	UNP Q16531

- Molecule 2 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	368	Total 2886	C 1841	N 513	O 515	S 17	0	0	0
2	D	368	Total 2886	C 1841	N 513	O 515	S 17	0	0	0
2	F	368	Total 2886	C 1841	N 513	O 515	S 17	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP Q92466
B	-7	HIS	-	expression tag	UNP Q92466
B	-6	HIS	-	expression tag	UNP Q92466
B	-5	HIS	-	expression tag	UNP Q92466
B	-4	HIS	-	expression tag	UNP Q92466
B	-3	HIS	-	expression tag	UNP Q92466
B	-2	HIS	-	expression tag	UNP Q92466
B	-1	ARG	-	expression tag	UNP Q92466
B	0	ARG	-	expression tag	UNP Q92466
B	1	LEU	-	expression tag	UNP Q92466
B	2	VAL	-	expression tag	UNP Q92466
B	3	PRO	-	expression tag	UNP Q92466
B	4	ARG	-	expression tag	UNP Q92466
B	5	GLY	-	expression tag	UNP Q92466
B	6	SER	-	expression tag	UNP Q92466
B	7	GLY	-	expression tag	UNP Q92466
B	8	GLY	-	expression tag	UNP Q92466
B	9	ARG	-	expression tag	UNP Q92466
D	-8	MET	-	expression tag	UNP Q92466
D	-7	HIS	-	expression tag	UNP Q92466
D	-6	HIS	-	expression tag	UNP Q92466
D	-5	HIS	-	expression tag	UNP Q92466
D	-4	HIS	-	expression tag	UNP Q92466
D	-3	HIS	-	expression tag	UNP Q92466
D	-2	HIS	-	expression tag	UNP Q92466
D	-1	ARG	-	expression tag	UNP Q92466
D	0	ARG	-	expression tag	UNP Q92466
D	1	LEU	-	expression tag	UNP Q92466
D	2	VAL	-	expression tag	UNP Q92466
D	3	PRO	-	expression tag	UNP Q92466
D	4	ARG	-	expression tag	UNP Q92466
D	5	GLY	-	expression tag	UNP Q92466
D	6	SER	-	expression tag	UNP Q92466

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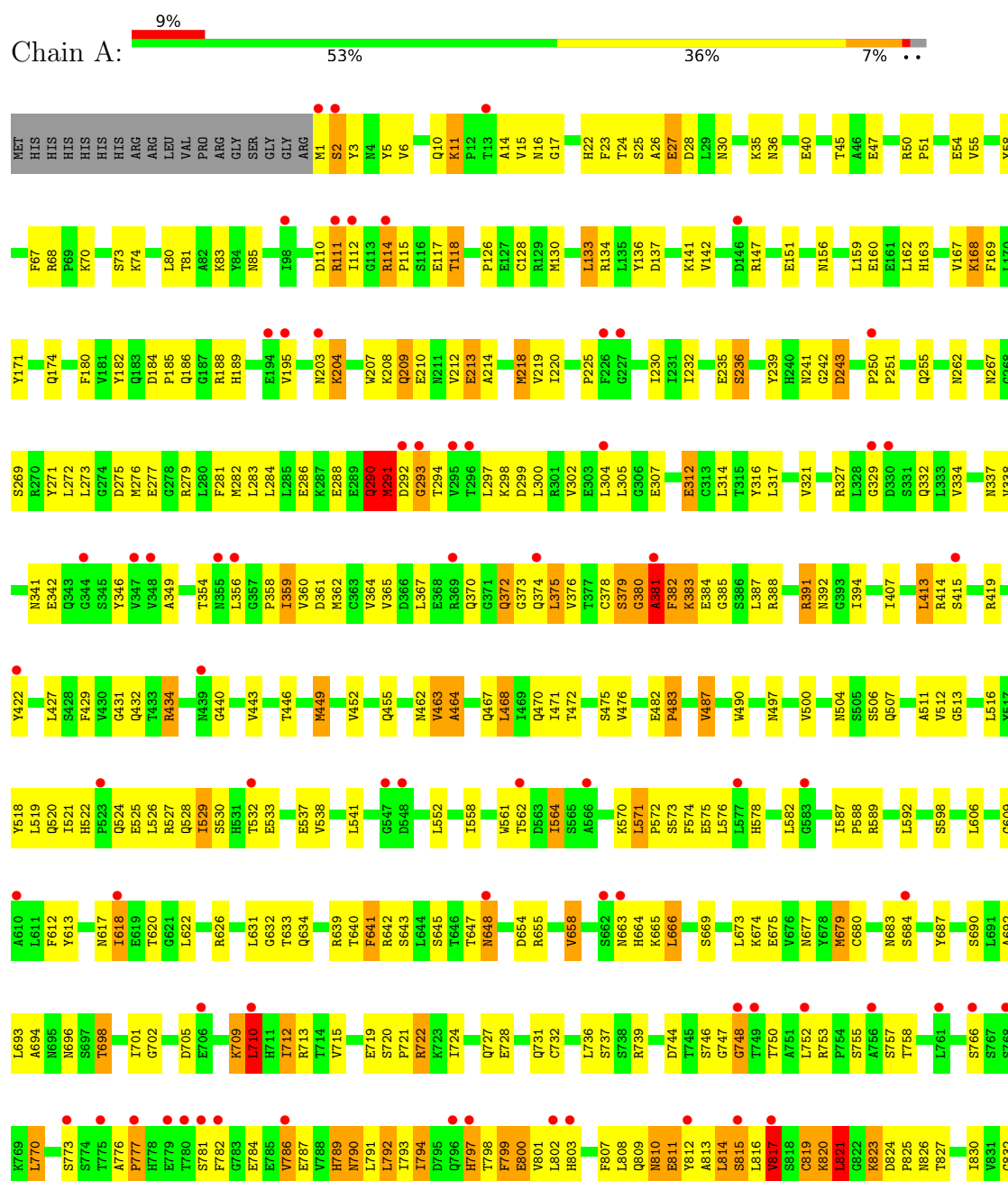
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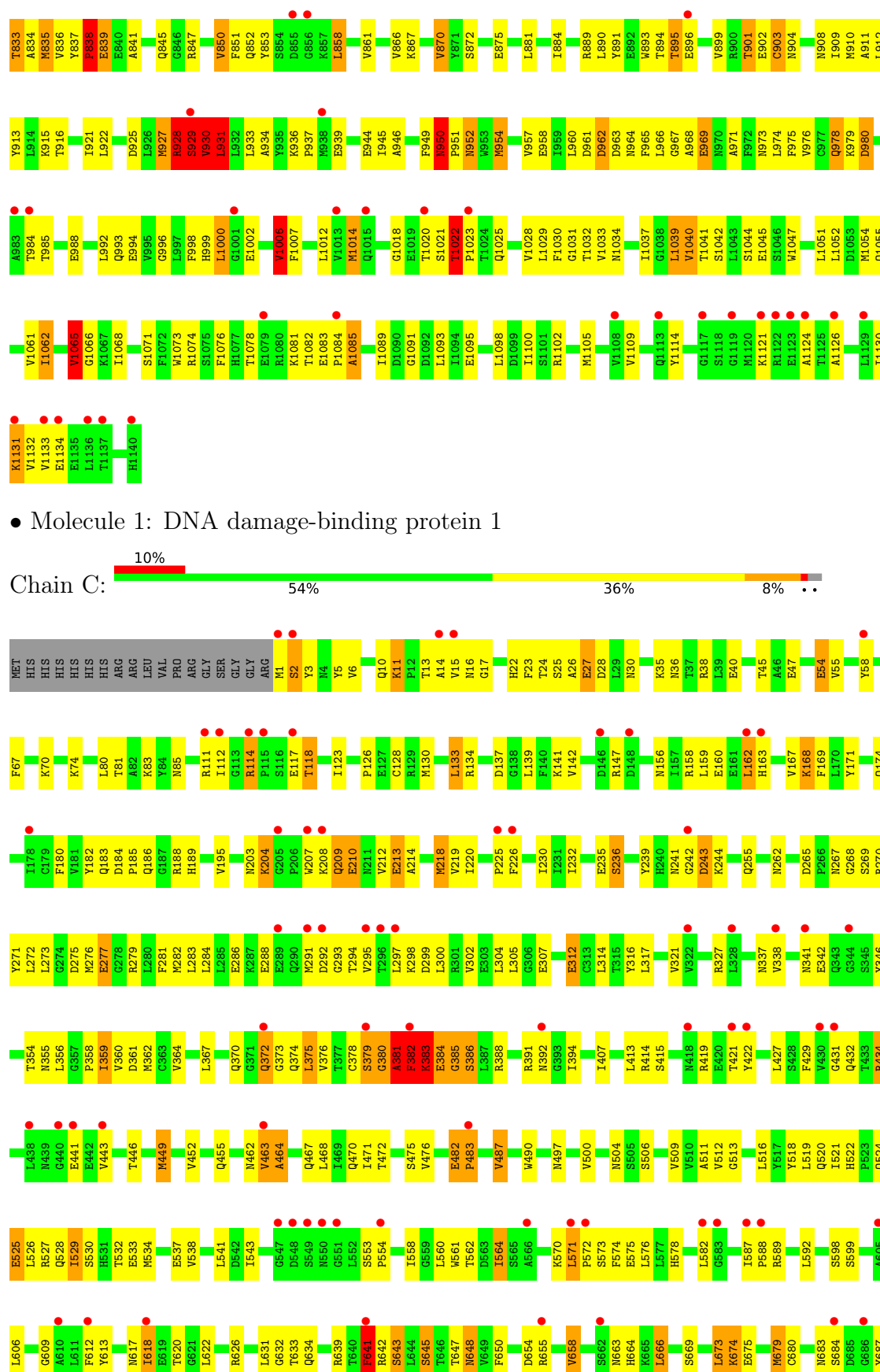
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	GLY	-	expression tag	UNP Q92466
D	8	GLY	-	expression tag	UNP Q92466
D	9	ARG	-	expression tag	UNP Q92466
F	-8	MET	-	expression tag	UNP Q92466
F	-7	HIS	-	expression tag	UNP Q92466
F	-6	HIS	-	expression tag	UNP Q92466
F	-5	HIS	-	expression tag	UNP Q92466
F	-4	HIS	-	expression tag	UNP Q92466
F	-3	HIS	-	expression tag	UNP Q92466
F	-2	HIS	-	expression tag	UNP Q92466
F	-1	ARG	-	expression tag	UNP Q92466
F	0	ARG	-	expression tag	UNP Q92466
F	1	LEU	-	expression tag	UNP Q92466
F	2	VAL	-	expression tag	UNP Q92466
F	3	PRO	-	expression tag	UNP Q92466
F	4	ARG	-	expression tag	UNP Q92466
F	5	GLY	-	expression tag	UNP Q92466
F	6	SER	-	expression tag	UNP Q92466
F	7	GLY	-	expression tag	UNP Q92466
F	8	GLY	-	expression tag	UNP Q92466
F	9	ARG	-	expression tag	UNP Q92466

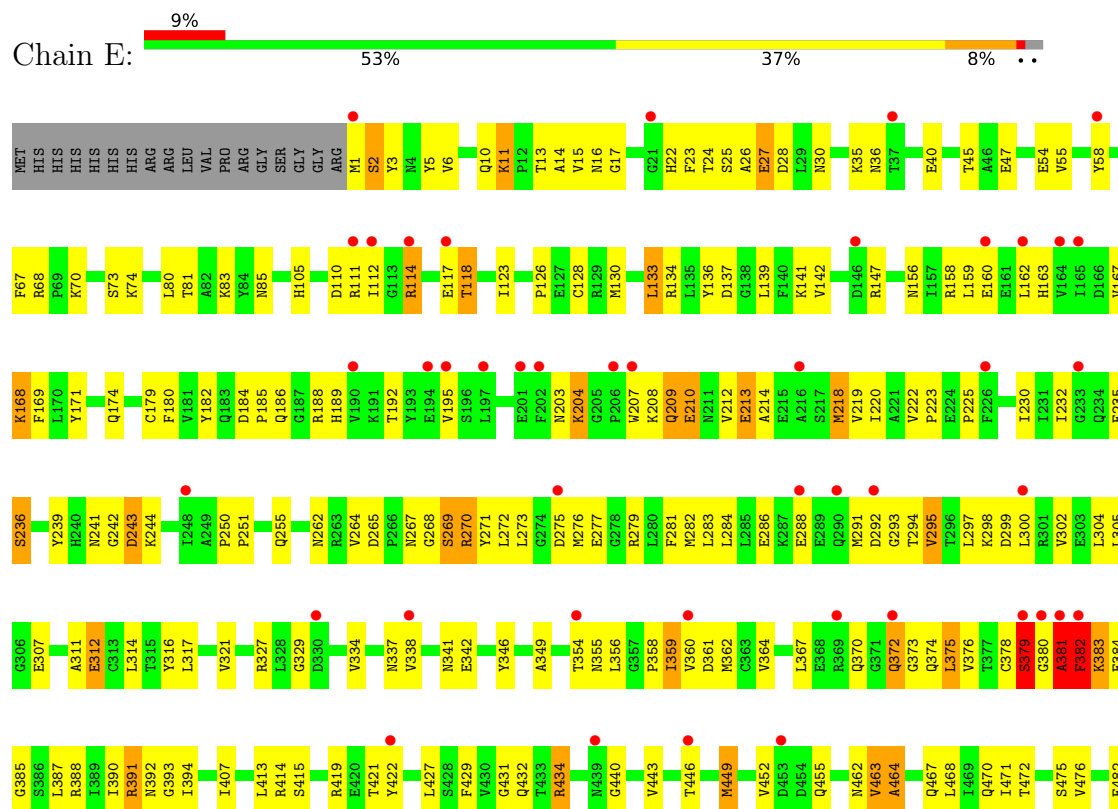
3 Residue-property plots

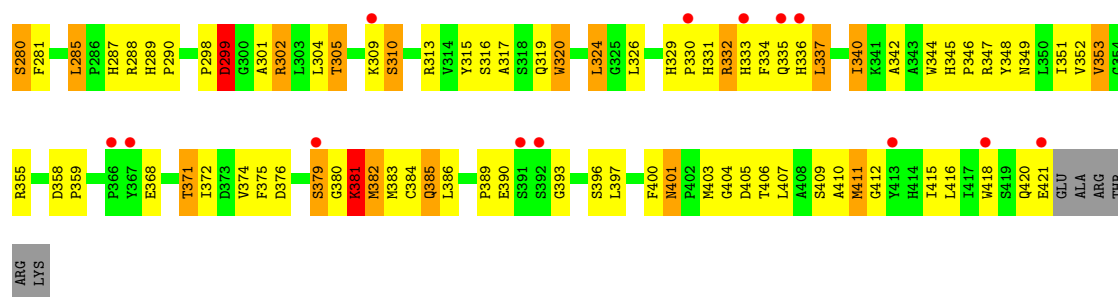
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA damage-binding protein 1

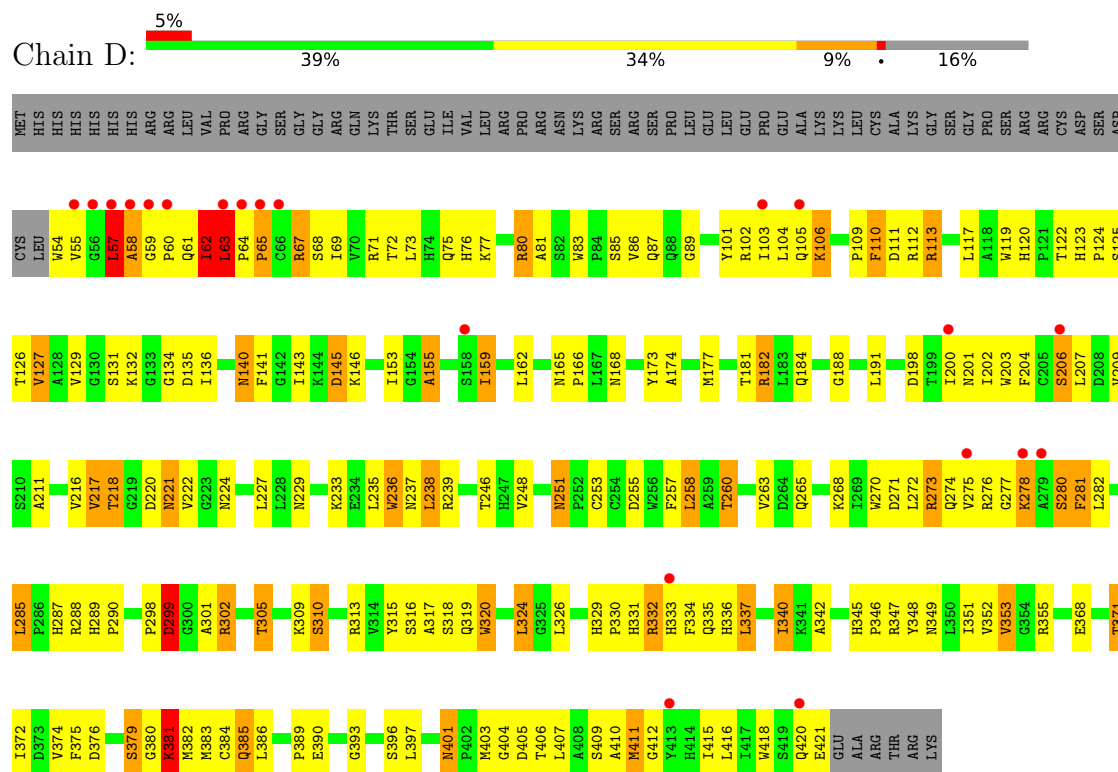




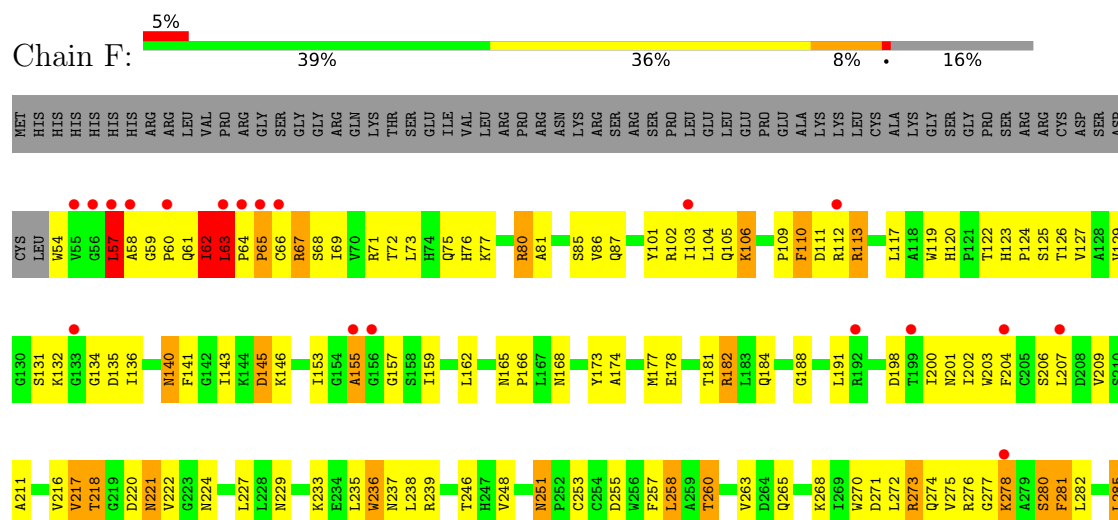


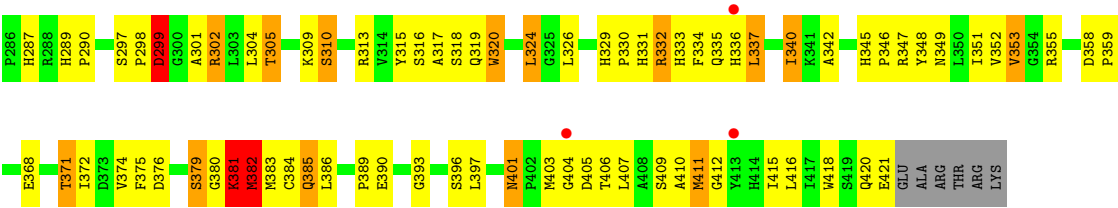


• Molecule 2: DNA damage-binding protein 2



• Molecule 2: DNA damage-binding protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	268.50Å 268.50Å 471.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.30 25.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	80.2 (25.00-3.30) 88.5 (25.00-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.22Å)	Xtrriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.254 , 0.288 0.264 , 0.262	Depositor DCC
R_{free} test set	1368 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtrriage
Anisotropy	0.419	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	35241	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4042e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.76	11/9026 (0.1%)	0.99	30/12239 (0.2%)
1	C	0.65	5/9026 (0.1%)	0.95	21/12239 (0.2%)
1	E	0.66	7/9026 (0.1%)	0.96	30/12239 (0.2%)
2	B	0.82	1/2970 (0.0%)	1.04	9/4042 (0.2%)
2	D	0.72	1/2970 (0.0%)	1.01	6/4042 (0.1%)
2	F	0.73	2/2970 (0.1%)	1.00	4/4042 (0.1%)
All	All	0.71	27/35988 (0.1%)	0.98	100/48843 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	C	0	7
1	E	0	5
2	B	0	2
2	D	0	1
2	F	0	2
All	All	0	23

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	GLU	C-O	-9.14	1.12	1.24
1	E	711	HIS	N-CA	-8.19	1.36	1.46
1	E	381	ALA	CA-CB	-7.84	1.40	1.53
1	A	392	ASN	N-CA	7.58	1.55	1.46
1	E	710	LEU	C-N	-6.66	1.23	1.33
1	A	290	GLN	CA-C	-6.49	1.48	1.52
2	F	381	LYS	CA-C	-6.40	1.44	1.52
1	A	930	VAL	CA-CB	-6.34	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	392	ASN	N-CA	-6.33	1.38	1.46
1	A	899	VAL	CA-CB	6.23	1.60	1.53
1	A	391	ARG	C-N	6.22	1.42	1.33
1	A	391	ARG	CA-C	6.08	1.59	1.52
1	A	381	ALA	C-O	-5.77	1.16	1.24
1	C	899	VAL	CA-CB	5.60	1.60	1.53
1	C	818	SER	C-N	5.56	1.40	1.33
1	C	381	ALA	CA-CB	-5.31	1.44	1.53
1	E	381	ALA	C-O	-5.31	1.17	1.24
2	F	382	MET	C-O	-5.30	1.17	1.23
1	A	928	ARG	C-O	-5.25	1.17	1.24
2	B	206	SER	C-O	-5.24	1.17	1.24
1	C	813	ALA	CA-CB	-5.17	1.45	1.53
1	A	931	LEU	C-O	-5.14	1.17	1.23
1	E	379	SER	C-O	-5.13	1.19	1.24
2	D	381	LYS	C-O	-5.09	1.18	1.24
1	A	930	VAL	C-O	-5.08	1.17	1.23
1	A	713	ARG	C-O	-5.02	1.17	1.24
1	E	813	ALA	CA-CB	-5.00	1.45	1.53

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	SER	N-CA-C	-11.90	101.05	114.62
1	A	821	LEU	N-CA-C	9.08	121.27	108.74
1	C	821	LEU	N-CA-C	8.84	120.94	108.74
1	E	821	LEU	N-CA-C	8.36	120.28	108.74
2	D	206	SER	CA-C-N	7.62	135.48	122.37
2	D	206	SER	C-N-CA	7.62	135.48	122.37
1	A	838	PRO	CA-C-N	7.09	134.46	121.70
1	A	838	PRO	C-N-CA	7.09	134.46	121.70
1	E	838	PRO	CA-C-N	7.08	134.44	121.70
1	E	838	PRO	C-N-CA	7.08	134.44	121.70
1	C	838	PRO	CA-C-N	7.01	134.32	121.70
1	C	838	PRO	C-N-CA	7.01	134.32	121.70
1	E	391	ARG	CA-C-N	-6.97	110.62	122.33
1	E	391	ARG	C-N-CA	-6.97	110.62	122.33
1	A	712	ILE	N-CA-C	6.93	118.78	108.46
2	F	251	ASN	N-CA-C	6.77	117.90	109.57
1	E	381	ALA	N-CA-C	6.70	125.06	110.80
2	B	251	ASN	N-CA-C	6.59	117.67	109.57
2	D	251	ASN	N-CA-C	6.54	117.61	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	ILE	N-CA-C	6.50	117.09	107.15
1	E	432	GLN	N-CA-C	6.41	116.53	108.45
2	D	62	ILE	N-CA-C	6.38	116.92	107.15
1	C	641	PHE	CB-CA-C	-6.34	99.36	111.48
2	F	62	ILE	N-CA-C	6.34	116.85	107.15
2	B	206	SER	CA-C-N	6.32	133.38	122.64
2	B	206	SER	C-N-CA	6.32	133.38	122.64
1	C	432	GLN	N-CA-C	6.32	116.41	108.45
1	C	386	SER	N-CA-C	-6.29	98.95	108.52
2	B	207	LEU	N-CA-C	6.27	120.26	110.17
1	E	641	PHE	CB-CA-C	-6.25	99.54	111.48
1	E	710	LEU	CA-C-N	-6.05	113.63	122.65
1	E	710	LEU	C-N-CA	-6.05	113.63	122.65
1	A	817	VAL	N-CA-C	6.05	117.07	108.42
1	E	988	GLU	N-CA-C	-6.05	105.90	113.28
2	F	63	LEU	N-CA-C	6.04	123.17	109.81
2	F	393	GLY	N-CA-C	-6.04	100.13	111.66
2	B	393	GLY	N-CA-C	-5.97	100.26	111.66
1	C	988	GLU	N-CA-C	-5.95	106.03	113.28
1	A	698	THR	N-CA-C	5.94	119.20	108.69
2	B	63	LEU	N-CA-C	5.90	122.85	109.81
1	A	787	GLU	N-CA-C	5.90	118.32	110.53
2	D	63	LEU	N-CA-C	5.87	122.79	109.81
1	A	432	GLN	N-CA-C	5.87	115.85	108.45
1	A	712	ILE	CB-CA-C	-5.84	101.51	110.50
1	A	988	GLU	N-CA-C	-5.80	106.20	113.28
1	E	787	GLU	N-CA-C	5.78	118.15	110.53
1	A	722	ARG	N-CA-C	5.67	122.89	110.80
1	A	899	VAL	CB-CA-C	5.66	118.44	111.25
1	A	993	GLN	CA-C-N	-5.63	114.95	122.72
1	A	993	GLN	C-N-CA	-5.63	114.95	122.72
1	A	929	SER	N-CA-C	5.62	122.77	110.80
1	E	903	CYS	N-CA-C	5.55	117.70	110.43
1	A	819	CYS	N-CA-C	5.51	118.41	108.48
2	B	207	LEU	CB-CA-C	-5.51	100.19	109.50
1	C	903	CYS	N-CA-C	5.49	117.62	110.43
1	C	787	GLU	N-CA-C	5.47	117.75	110.53
1	A	1006	VAL	N-CA-C	5.47	120.71	109.34
1	C	1083	GLU	CA-C-N	5.41	126.60	119.84
1	C	1083	GLU	C-N-CA	5.41	126.60	119.84
1	E	817	VAL	N-CA-C	5.41	116.16	108.42
1	A	903	CYS	N-CA-C	5.40	117.50	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	393	GLY	N-CA-C	-5.38	101.38	111.66
1	E	311	ALA	N-CA-C	5.36	117.49	108.96
1	C	1006	VAL	N-CA-C	5.36	120.48	109.34
1	E	295	VAL	N-CA-C	5.36	116.16	108.93
1	A	645	SER	N-CA-C	-5.35	105.89	112.90
1	A	391	ARG	CA-C-O	-5.32	114.88	121.11
1	C	698	THR	N-CA-C	5.30	118.08	108.69
1	A	709	LYS	N-CA-C	5.30	119.50	112.72
1	C	899	VAL	CB-CA-C	5.27	117.94	111.25
1	E	1083	GLU	CA-C-N	5.27	126.42	119.84
1	E	1083	GLU	C-N-CA	5.27	126.42	119.84
1	C	722	ARG	N-CA-C	5.25	121.99	110.80
1	E	1006	VAL	N-CA-C	5.24	120.25	109.34
1	A	1083	GLU	CA-C-N	5.24	126.39	119.84
1	A	1083	GLU	C-N-CA	5.24	126.39	119.84
1	E	993	GLN	CA-C-N	-5.24	115.80	122.77
1	E	993	GLN	C-N-CA	-5.24	115.80	122.77
1	C	525	GLU	N-CA-C	5.24	116.93	108.34
1	A	391	ARG	CA-C-N	5.20	129.90	122.72
1	A	391	ARG	C-N-CA	5.20	129.90	122.72
1	E	710	LEU	CA-C-O	5.18	127.92	120.51
1	A	952	ASN	N-CA-C	5.14	121.75	110.80
1	C	655	ARG	CA-C-N	5.13	124.89	119.76
1	C	655	ARG	C-N-CA	5.13	124.89	119.76
1	A	332	GLN	N-CA-C	5.13	115.81	108.74
1	E	722	ARG	N-CA-C	5.11	121.68	110.80
1	E	698	THR	N-CA-C	5.09	117.70	108.69
1	E	525	GLU	N-CA-C	5.07	116.65	108.34
1	E	655	ARG	CA-C-N	5.06	124.82	119.76
1	E	655	ARG	C-N-CA	5.06	124.82	119.76
1	E	899	VAL	CB-CA-C	5.05	117.66	111.25
1	C	645	SER	N-CA-C	-5.04	106.29	112.90
1	E	645	SER	N-CA-C	-5.04	106.30	112.90
1	A	710	LEU	N-CA-C	5.03	121.52	110.80
1	A	837	TYR	CA-C-N	5.02	126.11	119.84
1	A	837	TYR	C-N-CA	5.02	126.11	119.84
1	C	441	GLU	N-CA-C	-5.02	107.00	113.02
2	B	188	GLY	N-CA-C	5.01	125.05	113.18
1	E	1004	VAL	N-CA-C	5.01	114.78	107.37

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide
1	A	293	GLY	Peptide
1	A	379	SER	Peptide
1	A	380	GLY	Peptide
1	A	381	ALA	Peptide
1	A	950	ASN	Peptide
2	B	207	LEU	Peptide
2	B	381	LYS	Peptide
1	C	379	SER	Peptide
1	C	380	GLY	Peptide
1	C	381	ALA	Peptide
1	C	386	SER	Peptide
1	C	482	GLU	Peptide
1	C	641	PHE	Peptide
1	C	950	ASN	Peptide
2	D	380	GLY	Peptide
1	E	379	SER	Peptide
1	E	381	ALA	Peptide
1	E	382	PHE	Peptide
1	E	641	PHE	Peptide
1	E	950	ASN	Peptide
2	F	380	GLY	Peptide
2	F	381	LYS	Peptide

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	8861	0	8781	407	0
1	C	8861	0	8781	395	0
1	E	8861	0	8781	406	0
2	B	2886	0	2836	200	0
2	D	2886	0	2836	185	0
2	F	2886	0	2836	193	0
All	All	35241	0	34851	1716	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1716) 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)
2:B:208:ASP:O	2:B:209:VAL:CG1	1.66	1.43
1:A:791:LEU:HD22	1:A:814:LEU:O	1.25	1.31
1:E:791:LEU:HD22	1:E:814:LEU:O	1.25	1.26
1:C:791:LEU:HD22	1:C:814:LEU:O	1.27	1.23
2:D:287:HIS:CE1	2:D:305:THR:HG21	1.75	1.22
2:F:287:HIS:CE1	2:F:305:THR:HG21	1.78	1.19
1:C:265:ASP:OD2	1:C:270:ARG:HG3	1.41	1.19
1:A:792:LEU:N	1:A:792:LEU:HD12	1.52	1.18
1:C:817:VAL:HG11	1:C:872:SER:HA	1.22	1.18
1:E:817:VAL:HG11	1:E:872:SER:HA	1.22	1.17
2:F:381:LYS:HB2	2:F:381:LYS:NZ	1.58	1.17
2:B:287:HIS:CE1	2:B:305:THR:HG21	1.79	1.16
1:E:792:LEU:HD12	1:E:792:LEU:N	1.51	1.15
2:B:208:ASP:O	2:B:209:VAL:HG12	0.97	1.14
1:C:792:LEU:HD12	1:C:792:LEU:N	1.51	1.12
1:A:817:VAL:HG11	1:A:872:SER:HA	1.24	1.11
1:A:838:PRO:HB2	1:A:839:GLU:HB2	1.32	1.11
1:C:380:GLY:HA3	1:C:721:PRO:HG2	1.31	1.10
2:F:375:PHE:CE2	2:F:382:MET:CE	2.34	1.10
2:B:63:LEU:HB3	2:B:64:PRO:CD	1.78	1.08
2:B:208:ASP:C	2:B:209:VAL:CG1	2.21	1.08
2:D:63:LEU:HB3	2:D:64:PRO:CD	1.80	1.08
2:B:63:LEU:CB	2:B:64:PRO:HD3	1.83	1.07
2:F:375:PHE:CE2	2:F:382:MET:HE2	1.88	1.07
2:F:63:LEU:HB3	2:F:64:PRO:CD	1.80	1.07
2:F:63:LEU:CB	2:F:64:PRO:HD3	1.85	1.06
1:C:383:LYS:O	1:C:383:LYS:HG3	1.55	1.06
2:D:63:LEU:CB	2:D:64:PRO:HD3	1.85	1.06
1:C:838:PRO:HB2	1:C:839:GLU:HB2	1.36	1.05
1:A:927:MET:O	1:A:928:ARG:HB3	1.49	1.05
1:E:838:PRO:HB2	1:E:839:GLU:HB2	1.35	1.05
1:A:380:GLY:HA3	1:A:721:PRO:HG2	1.40	1.02
1:A:927:MET:HE3	2:B:90:LEU:HD22	1.41	1.02
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.41	1.02
1:C:934:ALA:HB2	1:C:945:ILE:HD11	1.41	1.01
2:B:208:ASP:C	2:B:209:VAL:HG13	1.84	0.99
2:F:381:LYS:HB2	2:F:381:LYS:HZ2	1.09	0.99
1:E:934:ALA:HB2	1:E:945:ILE:HD11	1.43	0.96
2:F:63:LEU:HB3	2:F:64:PRO:HD3	0.99	0.96
2:D:63:LEU:HB3	2:D:64:PRO:HD3	0.99	0.96
1:A:449:MET:HA	1:A:449:MET:HE3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:287:HIS:HE1	2:F:305:THR:HG21	1.20	0.95
2:B:63:LEU:HB3	2:B:64:PRO:HD3	0.97	0.95
1:E:449:MET:HA	1:E:449:MET:HE3	1.49	0.95
1:C:792:LEU:HD12	1:C:792:LEU:H	1.14	0.94
2:D:287:HIS:HE1	2:D:305:THR:HG21	1.17	0.94
1:A:838:PRO:CB	1:A:839:GLU:HB2	1.98	0.94
1:E:792:LEU:HD12	1:E:792:LEU:H	1.11	0.93
1:A:792:LEU:HD12	1:A:792:LEU:H	1.18	0.93
2:B:287:HIS:HE1	2:B:305:THR:HG21	1.23	0.93
1:E:294:THR:HG22	1:E:295:VAL:H	1.33	0.92
2:F:110:PHE:HD2	2:F:111:ASP:N	1.67	0.92
1:C:449:MET:HE3	1:C:449:MET:HA	1.52	0.91
1:E:838:PRO:CB	1:E:839:GLU:HB2	1.99	0.91
1:C:838:PRO:CB	1:C:839:GLU:HB2	2.00	0.91
1:C:294:THR:HG22	1:C:295:VAL:H	1.35	0.91
2:F:381:LYS:NZ	2:F:381:LYS:CB	2.30	0.91
1:A:949:PHE:HD2	2:B:122:THR:HG22	1.37	0.90
2:F:80:ARG:HG3	2:F:80:ARG:HH11	1.34	0.90
2:F:375:PHE:CZ	2:F:382:MET:HE1	2.06	0.90
1:C:817:VAL:CG1	1:C:872:SER:HA	2.02	0.89
1:E:817:VAL:CG1	1:E:872:SER:HA	2.02	0.89
2:B:110:PHE:HD2	2:B:111:ASP:N	1.70	0.89
1:C:382:PHE:C	1:C:384:GLU:H	1.81	0.89
2:D:110:PHE:HD2	2:D:111:ASP:N	1.70	0.89
1:A:910:MET:CG	1:A:927:MET:HG3	2.02	0.88
2:D:381:LYS:NZ	2:D:381:LYS:CB	2.29	0.88
2:D:80:ARG:HH11	2:D:80:ARG:HG3	1.38	0.88
2:B:80:ARG:HH11	2:B:80:ARG:HG3	1.36	0.88
1:A:817:VAL:CG1	1:A:872:SER:HA	2.04	0.87
1:A:810:ASN:CG	1:A:813:ALA:HB2	1.99	0.87
1:A:167:VAL:HG12	1:A:180:PHE:HB3	1.57	0.86
1:E:422:TYR:HD1	1:E:683:ASN:H	1.20	0.86
1:A:927:MET:CE	2:B:90:LEU:HD22	2.05	0.86
1:C:383:LYS:HG2	1:C:384:GLU:HG3	1.58	0.86
1:C:810:ASN:CG	1:C:813:ALA:HB2	2.01	0.86
1:A:791:LEU:HD13	1:A:814:LEU:HA	1.58	0.85
1:E:791:LEU:HD13	1:E:814:LEU:HA	1.58	0.85
1:E:810:ASN:CG	1:E:813:ALA:HB2	2.01	0.85
1:C:422:TYR:HD1	1:C:683:ASN:H	1.20	0.84
1:C:791:LEU:HD13	1:C:814:LEU:HA	1.58	0.84
1:A:910:MET:HG3	1:A:927:MET:HG3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ARG:HG3	1:C:647:THR:HG22	1.58	0.84
1:E:167:VAL:HG12	1:E:180:PHE:HB3	1.58	0.84
1:A:293:GLY:C	1:A:294:THR:HG22	2.03	0.84
1:A:422:TYR:HD1	1:A:683:ASN:H	1.25	0.84
1:A:929:SER:OG	1:A:951:PRO:C	2.20	0.84
2:D:381:LYS:CB	2:D:381:LYS:HZ3	1.91	0.84
1:C:81:THR:HG22	1:C:83:LYS:H	1.40	0.84
1:E:642:ARG:HG3	1:E:647:THR:HG22	1.58	0.84
1:A:791:LEU:CD2	1:A:814:LEU:O	2.21	0.83
1:C:242:GLY:O	1:C:243:ASP:HB2	1.78	0.83
1:C:167:VAL:HG12	1:C:180:PHE:HB3	1.58	0.83
1:E:1025:GLN:HB3	1:E:1042:SER:HB2	1.60	0.83
1:A:927:MET:HE3	2:B:90:LEU:CD2	2.08	0.83
1:E:168:LYS:HE2	1:E:219:VAL:O	1.78	0.83
2:F:376:ASP:CG	2:F:379:SER:OG	2.22	0.83
1:C:117:GLU:OE2	2:D:60:PRO:HB3	1.78	0.83
1:E:654:ASP:HA	1:E:675:GLU:HG2	1.61	0.82
1:C:168:LYS:HE2	1:C:219:VAL:O	1.78	0.82
1:C:184:ASP:HB2	1:C:185:PRO:HD2	1.61	0.82
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.59	0.82
1:C:792:LEU:N	1:C:792:LEU:CD1	2.30	0.82
1:E:242:GLY:O	1:E:243:ASP:HB2	1.77	0.82
1:A:810:ASN:ND2	1:A:813:ALA:HB2	1.95	0.81
2:D:381:LYS:HZ3	2:D:381:LYS:HB2	1.45	0.81
1:A:242:GLY:O	1:A:243:ASP:HB2	1.79	0.81
1:C:819:CYS:SG	1:C:873:MET:HE3	2.20	0.81
1:A:168:LYS:HE2	1:A:219:VAL:O	1.80	0.81
1:C:22:HIS:HD2	1:C:28:ASP:O	1.61	0.81
1:E:22:HIS:HD2	1:E:28:ASP:O	1.63	0.81
2:B:198:ASP:HA	2:F:112:ARG:NH2	1.96	0.80
1:A:655:ARG:NH2	1:A:1014:MET:SD	2.55	0.80
1:A:654:ASP:HA	1:A:675:GLU:HG2	1.62	0.80
1:C:487:VAL:HG13	1:C:524:GLN:HA	1.64	0.80
1:E:81:THR:HG22	1:E:83:LYS:H	1.44	0.80
1:A:1025:GLN:HB3	1:A:1042:SER:HB2	1.61	0.80
1:C:383:LYS:O	1:C:383:LYS:CG	2.29	0.80
1:E:14:ALA:HB1	1:E:327:ARG:HG3	1.64	0.79
1:A:22:HIS:HD2	1:A:28:ASP:O	1.65	0.79
1:C:1025:GLN:HB3	1:C:1042:SER:HB2	1.62	0.79
1:E:184:ASP:HB2	1:E:185:PRO:HD2	1.62	0.79
1:E:823:LYS:HG3	1:E:893:TRP:CD1	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:ARG:O	1:A:928:ARG:HG2	1.83	0.79
1:C:380:GLY:HA3	1:C:721:PRO:CG	2.09	0.79
1:E:792:LEU:N	1:E:792:LEU:CD1	2.30	0.79
1:C:810:ASN:ND2	1:C:813:ALA:HB2	1.96	0.79
1:E:487:VAL:CG1	1:E:524:GLN:HA	2.12	0.79
1:A:81:THR:HG22	1:A:83:LYS:H	1.47	0.78
1:A:642:ARG:HG3	1:A:647:THR:HG22	1.64	0.78
1:A:290:GLN:O	1:A:291:MET:CG	2.31	0.78
1:C:654:ASP:HA	1:C:675:GLU:HG2	1.63	0.78
1:C:823:LYS:HG3	1:C:893:TRP:CD1	2.17	0.78
2:D:381:LYS:NZ	2:D:381:LYS:HB2	1.93	0.78
2:B:143:ILE:HG23	2:B:145:ASP:HB2	1.65	0.78
1:E:449:MET:HA	1:E:449:MET:CE	2.13	0.78
1:E:487:VAL:HG13	1:E:524:GLN:HA	1.64	0.78
1:A:449:MET:HA	1:A:449:MET:CE	2.12	0.78
1:A:817:VAL:HG11	1:A:872:SER:CA	2.11	0.78
1:C:487:VAL:CG1	1:C:524:GLN:HA	2.14	0.78
1:C:1032:THR:HG22	1:C:1034:ASN:H	1.49	0.77
1:E:24:THR:H	1:E:30:ASN:ND2	1.82	0.77
1:E:737:SER:HB3	1:E:794:ILE:HD11	1.64	0.77
1:C:380:GLY:CA	1:C:721:PRO:HG2	2.12	0.77
1:A:358:PRO:HD2	1:A:380:GLY:O	1.84	0.77
1:A:634:GLN:HG2	1:A:654:ASP:HB3	1.67	0.77
1:C:634:GLN:HG2	1:C:654:ASP:HB3	1.67	0.77
1:E:163:HIS:HB2	2:F:57:LEU:HB2	1.67	0.77
1:E:792:LEU:HB3	1:E:807:PHE:O	1.85	0.77
1:E:817:VAL:HG11	1:E:872:SER:CA	2.10	0.77
1:A:24:THR:H	1:A:30:ASN:ND2	1.81	0.77
1:A:487:VAL:CG1	1:A:524:GLN:HA	2.14	0.77
1:C:163:HIS:HB2	2:D:57:LEU:HB2	1.66	0.76
1:E:810:ASN:ND2	1:E:813:ALA:HB2	2.00	0.76
1:A:1032:THR:HG22	1:A:1034:ASN:H	1.51	0.76
1:C:449:MET:HA	1:C:449:MET:CE	2.16	0.76
1:C:24:THR:H	1:C:30:ASN:ND2	1.84	0.76
1:C:14:ALA:HB1	1:C:327:ARG:HG3	1.67	0.76
1:A:792:LEU:N	1:A:792:LEU:CD1	2.29	0.76
2:D:143:ILE:HG23	2:D:145:ASP:HB2	1.66	0.76
2:D:309:LYS:HE2	2:D:333:HIS:CD2	2.21	0.76
1:A:487:VAL:HG13	1:A:524:GLN:HA	1.66	0.75
1:A:928:ARG:O	1:A:928:ARG:CG	2.30	0.75
1:C:817:VAL:HG11	1:C:872:SER:CA	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:PHE:HD2	2:D:111:ASP:H	0.85	0.75
1:A:290:GLN:O	1:A:291:MET:HG2	1.85	0.75
1:A:472:THR:HG23	1:A:475:SER:H	1.50	0.75
1:A:927:MET:O	1:A:928:ARG:CB	2.29	0.75
1:C:381:ALA:O	1:C:382:PHE:HB2	1.85	0.75
2:F:143:ILE:HG23	2:F:145:ASP:HB2	1.67	0.74
1:C:385:GLY:HA3	1:C:719:GLU:O	1.86	0.74
1:E:472:THR:HG23	1:E:475:SER:H	1.52	0.74
2:F:140:ASN:O	2:F:143:ILE:HG22	1.87	0.74
2:D:140:ASN:O	2:D:143:ILE:HG22	1.87	0.74
1:E:791:LEU:CD2	1:E:814:LEU:O	2.21	0.74
2:B:376:ASP:CG	2:B:379:SER:OG	2.31	0.74
1:C:791:LEU:CD2	1:C:814:LEU:O	2.23	0.74
1:E:118:THR:HB	1:E:134:ARG:HH22	1.52	0.74
2:F:309:LYS:HE2	2:F:333:HIS:CD2	2.23	0.74
2:D:345:HIS:CD2	2:D:347:ARG:H	2.06	0.74
1:E:23:PHE:H	1:E:30:ASN:HD22	1.34	0.73
1:E:634:GLN:HG2	1:E:654:ASP:HB3	1.70	0.73
2:B:110:PHE:HD2	2:B:111:ASP:H	0.86	0.73
1:C:815:SER:HA	1:C:833:THR:HA	1.68	0.73
1:E:815:SER:HA	1:E:833:THR:HA	1.70	0.73
1:C:118:THR:HB	1:C:134:ARG:HH22	1.54	0.73
1:A:815:SER:HA	1:A:833:THR:HA	1.69	0.73
1:E:375:LEU:HB3	1:E:391:ARG:HB3	1.70	0.73
1:E:1032:THR:HG22	1:E:1034:ASN:H	1.53	0.73
1:A:118:THR:HB	1:A:134:ARG:HH22	1.53	0.73
1:A:823:LYS:HG3	1:A:893:TRP:CD1	2.24	0.73
1:A:23:PHE:H	1:A:30:ASN:HD22	1.35	0.73
1:A:380:GLY:HA3	1:A:721:PRO:CG	2.16	0.73
1:A:641:PHE:N	1:A:641:PHE:CD1	2.53	0.73
1:E:841:ALA:HA	2:F:68:SER:HA	1.69	0.73
1:C:23:PHE:H	1:C:30:ASN:HD22	1.35	0.72
1:C:770:LEU:H	1:C:770:LEU:HD12	1.54	0.72
1:A:792:LEU:HB3	1:A:807:PHE:O	1.90	0.72
2:B:200:ILE:HB	2:F:155:ALA:CB	2.19	0.72
2:B:268:LYS:HB3	2:B:270:TRP:NE1	2.05	0.72
1:C:286:GLU:HG3	1:C:299:ASP:HB3	1.71	0.72
1:A:949:PHE:CD2	2:B:122:THR:HG22	2.23	0.72
1:A:14:ALA:HB1	1:A:327:ARG:HG3	1.70	0.72
1:C:265:ASP:OD2	1:C:270:ARG:CG	2.31	0.72
2:D:268:LYS:HB3	2:D:270:TRP:NE1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:375:PHE:CD2	2:F:382:MET:HE2	2.25	0.72
1:A:979:LYS:O	1:A:980:ASP:HB2	1.90	0.72
1:A:286:GLU:HG3	1:A:299:ASP:HB3	1.72	0.72
1:C:384:GLU:C	1:C:385:GLY:O	2.26	0.72
1:C:472:THR:HG23	1:C:475:SER:H	1.55	0.71
1:A:934:ALA:CB	1:A:945:ILE:HD11	2.19	0.71
2:B:174:ALA:O	2:B:181:THR:HA	1.90	0.71
2:B:140:ASN:O	2:B:143:ILE:HG22	1.91	0.71
2:D:381:LYS:HZ3	2:D:381:LYS:CA	2.04	0.71
1:A:770:LEU:HD12	1:A:770:LEU:H	1.54	0.71
1:C:137:ASP:OD2	2:D:57:LEU:HD23	1.90	0.71
2:B:345:HIS:CD2	2:B:347:ARG:H	2.08	0.71
1:E:934:ALA:CB	1:E:945:ILE:HD11	2.18	0.71
1:E:286:GLU:HG3	1:E:299:ASP:HB3	1.72	0.71
1:A:225:PRO:HG2	1:A:267:ASN:HB2	1.73	0.70
2:D:381:LYS:O	2:D:382:MET:C	2.30	0.70
1:C:792:LEU:H	1:C:792:LEU:CD1	1.98	0.70
2:B:209:VAL:CG2	2:B:209:VAL:O	2.40	0.70
1:C:666:LEU:HD23	1:C:666:LEU:H	1.57	0.70
1:E:770:LEU:H	1:E:770:LEU:HD12	1.54	0.70
1:E:792:LEU:H	1:E:792:LEU:CD1	1.96	0.70
1:A:55:VAL:HG11	1:A:1065:VAL:HG11	1.72	0.70
1:E:55:VAL:HG11	1:E:1065:VAL:HG11	1.71	0.70
2:D:301:ALA:HA	2:D:317:ALA:HB2	1.73	0.70
2:B:301:ALA:HA	2:B:317:ALA:HB2	1.74	0.70
2:B:302:ARG:N	2:B:302:ARG:HD2	2.06	0.70
2:B:309:LYS:HE2	2:B:333:HIS:CD2	2.26	0.70
1:C:810:ASN:HD21	1:C:833:THR:HG21	1.57	0.70
2:D:287:HIS:CE1	2:D:305:THR:CG2	2.68	0.70
1:A:362:MET:HG2	1:A:1006:VAL:HG21	1.74	0.69
2:D:289:HIS:HB3	2:D:290:PRO:CD	2.22	0.69
2:D:302:ARG:HA	2:D:315:TYR:O	1.91	0.69
1:C:823:LYS:HG3	1:C:893:TRP:CG	2.27	0.69
1:A:929:SER:OG	1:A:951:PRO:HA	1.93	0.69
2:F:345:HIS:CD2	2:F:347:ARG:H	2.10	0.69
1:A:1021:SER:C	1:A:1023:PRO:HD2	2.17	0.69
1:C:490:TRP:HE1	1:C:528:GLN:HE21	1.39	0.69
2:F:268:LYS:HB3	2:F:270:TRP:NE1	2.07	0.69
1:E:225:PRO:HG2	1:E:267:ASN:HB2	1.74	0.69
1:C:934:ALA:CB	1:C:945:ILE:HD11	2.19	0.68
1:E:1021:SER:C	1:E:1023:PRO:HD2	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:HIS:CD2	1:C:28:ASP:O	2.45	0.68
1:C:55:VAL:HG11	1:C:1065:VAL:HG11	1.76	0.68
2:B:110:PHE:CZ	2:B:131:SER:HB2	2.28	0.68
2:D:345:HIS:HD2	2:D:347:ARG:H	1.42	0.68
1:E:22:HIS:CD2	1:E:28:ASP:O	2.46	0.68
2:F:289:HIS:HB3	2:F:290:PRO:CD	2.24	0.68
2:F:389:PRO:O	2:F:390:GLU:HG2	1.94	0.68
1:A:23:PHE:N	1:A:30:ASN:HD22	1.92	0.68
1:A:810:ASN:HD21	1:A:833:THR:HG21	1.58	0.68
1:C:225:PRO:HG2	1:C:267:ASN:HB2	1.73	0.68
2:D:401:ASN:ND2	2:D:406:THR:HB	2.09	0.68
1:E:666:LEU:HD23	1:E:666:LEU:H	1.56	0.68
1:A:838:PRO:HB2	1:A:839:GLU:CB	2.18	0.68
2:B:375:PHE:CE2	2:B:382:MET:CE	2.76	0.68
1:C:532:THR:HG22	1:C:533:GLU:H	1.59	0.68
1:C:979:LYS:O	1:C:980:ASP:HB2	1.93	0.68
2:B:289:HIS:HB3	2:B:290:PRO:CD	2.24	0.68
1:C:641:PHE:HZ	1:C:650:PHE:HD1	1.39	0.68
2:D:221:ASN:HD22	2:D:221:ASN:H	1.41	0.68
2:F:302:ARG:HA	2:F:315:TYR:O	1.94	0.68
2:B:401:ASN:ND2	2:B:406:THR:HB	2.09	0.67
2:D:289:HIS:HB3	2:D:290:PRO:HD2	1.75	0.67
2:D:174:ALA:O	2:D:181:THR:HA	1.93	0.67
2:D:389:PRO:O	2:D:390:GLU:HG2	1.94	0.67
1:E:641:PHE:HZ	1:E:650:PHE:HD1	1.40	0.67
1:E:834:ALA:O	1:E:835:MET:HB2	1.93	0.67
1:C:1021:SER:C	1:C:1023:PRO:HD2	2.18	0.67
1:C:1061:VAL:HG12	1:C:1062:ILE:H	1.58	0.67
1:E:823:LYS:HG3	1:E:893:TRP:CG	2.29	0.67
1:A:490:TRP:HE1	1:A:528:GLN:HE21	1.40	0.67
1:A:816:LEU:HD21	1:A:834:ALA:HB2	1.75	0.67
1:C:375:LEU:HB3	1:C:391:ARG:HB3	1.75	0.67
2:F:80:ARG:HH11	2:F:80:ARG:CG	2.07	0.67
1:A:1061:VAL:HG12	1:A:1062:ILE:H	1.60	0.67
2:B:289:HIS:HB3	2:B:290:PRO:HD2	1.76	0.67
1:C:163:HIS:CB	2:D:57:LEU:HB2	2.23	0.67
1:C:757:SER:CB	1:C:792:LEU:HD22	2.24	0.67
1:E:362:MET:HG2	1:E:1006:VAL:HG21	1.75	0.67
1:E:838:PRO:HB2	1:E:839:GLU:CB	2.20	0.67
1:E:1031:GLY:HA2	1:E:1037:ILE:HG22	1.76	0.67
2:F:174:ALA:O	2:F:181:THR:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:221:ASN:H	2:F:221:ASN:HD22	1.42	0.67
1:C:841:ALA:HA	2:D:68:SER:HA	1.76	0.67
1:E:1061:VAL:HG12	1:E:1062:ILE:H	1.59	0.67
2:F:289:HIS:HB3	2:F:290:PRO:HD2	1.75	0.67
1:A:833:THR:CG2	1:A:847:ARG:HB3	2.25	0.67
2:B:62:ILE:HD13	2:B:67:ARG:CB	2.25	0.67
1:A:910:MET:HG2	1:A:927:MET:HG3	1.77	0.67
1:E:23:PHE:N	1:E:30:ASN:HD22	1.92	0.67
1:E:378:CYS:SG	1:E:388:ARG:HB2	2.34	0.67
1:A:532:THR:HG22	1:A:533:GLU:H	1.58	0.66
1:E:810:ASN:HD21	1:E:833:THR:HG21	1.61	0.66
2:F:401:ASN:ND2	2:F:406:THR:HB	2.11	0.66
1:A:22:HIS:CD2	1:A:28:ASP:O	2.48	0.66
1:A:757:SER:CB	1:A:792:LEU:HD22	2.25	0.66
1:A:810:ASN:CG	1:A:813:ALA:CB	2.68	0.66
1:A:934:ALA:HB2	1:A:945:ILE:CD1	2.24	0.66
2:D:173:TYR:CB	2:D:207:LEU:HD21	2.26	0.66
1:E:979:LYS:O	1:E:980:ASP:HB2	1.93	0.66
1:C:834:ALA:O	1:C:835:MET:HB2	1.94	0.66
2:D:217:VAL:HG13	2:D:227:LEU:HD23	1.78	0.66
2:F:173:TYR:CB	2:F:207:LEU:HD21	2.26	0.66
2:F:301:ALA:HA	2:F:317:ALA:HB2	1.76	0.66
1:A:641:PHE:N	1:A:641:PHE:HD1	1.91	0.66
2:B:345:HIS:HD2	2:B:347:ARG:H	1.43	0.66
2:B:221:ASN:H	2:B:221:ASN:HD22	1.43	0.66
1:C:833:THR:CG2	1:C:847:ARG:HB3	2.25	0.66
1:C:1031:GLY:HA2	1:C:1037:ILE:HG22	1.76	0.65
1:C:23:PHE:N	1:C:30:ASN:HD22	1.93	0.65
1:C:838:PRO:HB2	1:C:839:GLU:CB	2.21	0.65
1:A:117:GLU:OE2	2:B:60:PRO:HB3	1.96	0.65
1:C:188:ARG:HD2	1:C:214:ALA:O	1.96	0.65
1:E:946:ALA:CB	1:E:992:LEU:HG	2.25	0.65
1:A:137:ASP:OD2	2:B:57:LEU:HD23	1.97	0.65
1:A:666:LEU:H	1:A:666:LEU:HD23	1.62	0.65
2:B:217:VAL:HG13	2:B:227:LEU:HD23	1.79	0.65
1:C:362:MET:HG2	1:C:1006:VAL:HG21	1.78	0.65
1:E:532:THR:HG22	1:E:533:GLU:H	1.60	0.65
1:A:292:ASP:O	1:A:294:THR:N	2.29	0.65
2:F:227:LEU:H	2:F:236:TRP:HB2	1.62	0.65
1:A:841:ALA:HA	2:B:68:SER:HA	1.79	0.65
1:A:946:ALA:CB	1:A:992:LEU:HG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:PHE:C	1:C:384:GLU:N	2.46	0.65
1:C:946:ALA:CB	1:C:992:LEU:HG	2.27	0.65
1:E:282:MET:HB2	1:E:305:LEU:HD11	1.78	0.65
1:A:823:LYS:HG3	1:A:893:TRP:CG	2.32	0.65
1:C:282:MET:HB2	1:C:305:LEU:HD11	1.79	0.65
1:A:912:LEU:HD21	2:B:73:LEU:HD13	1.79	0.65
2:B:198:ASP:CB	2:F:112:ARG:HH22	2.09	0.65
2:D:63:LEU:CB	2:D:64:PRO:CD	2.57	0.65
2:D:101:TYR:O	2:D:103:ILE:N	2.30	0.65
2:D:62:ILE:HD13	2:D:67:ARG:CB	2.26	0.65
2:D:229:ASN:ND2	2:D:233:LYS:HB2	2.12	0.65
2:D:381:LYS:NZ	2:D:381:LYS:HA	2.12	0.65
1:E:188:ARG:HD2	1:E:214:ALA:O	1.97	0.65
1:E:490:TRP:HE1	1:E:528:GLN:HE21	1.43	0.65
2:F:110:PHE:CZ	2:F:131:SER:HB2	2.31	0.65
1:C:163:HIS:CG	2:D:57:LEU:HB2	2.32	0.64
1:C:381:ALA:HA	1:C:721:PRO:HD3	1.80	0.64
1:C:810:ASN:CG	1:C:813:ALA:CB	2.71	0.64
1:E:288:GLU:HB2	1:E:298:LYS:HB2	1.79	0.64
2:B:63:LEU:CB	2:B:64:PRO:CD	2.55	0.64
1:C:288:GLU:HB2	1:C:298:LYS:HB2	1.78	0.64
1:A:24:THR:H	1:A:30:ASN:HD21	1.43	0.64
1:A:208:LYS:O	1:A:209:GLN:HB3	1.97	0.64
2:B:202:ILE:HA	2:B:221:ASN:HD21	1.63	0.64
1:C:208:LYS:O	1:C:209:GLN:HB3	1.96	0.64
2:F:62:ILE:HD13	2:F:67:ARG:CB	2.28	0.64
1:A:1031:GLY:HA2	1:A:1037:ILE:HG22	1.79	0.64
1:C:792:LEU:HB3	1:C:807:PHE:O	1.98	0.64
1:E:117:GLU:OE2	2:F:60:PRO:HB3	1.97	0.64
1:E:833:THR:CG2	1:E:847:ARG:HB3	2.27	0.64
1:E:641:PHE:CZ	1:E:650:PHE:HD1	2.16	0.64
1:E:1000:LEU:HD13	1:E:1002:GLU:HB2	1.79	0.64
1:A:282:MET:HB2	1:A:305:LEU:HD11	1.80	0.64
2:D:381:LYS:NZ	2:D:381:LYS:CA	2.60	0.64
1:C:382:PHE:O	1:C:384:GLU:N	2.31	0.64
2:F:302:ARG:N	2:F:302:ARG:HD2	2.13	0.64
1:E:422:TYR:HD1	1:E:683:ASN:N	1.96	0.64
1:A:375:LEU:HB3	1:A:391:ARG:HB3	1.79	0.63
1:C:360:VAL:HG13	2:D:77:LYS:HD3	1.80	0.63
1:E:208:LYS:O	1:E:209:GLN:HB3	1.97	0.63
1:A:288:GLU:HB2	1:A:298:LYS:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:912:LEU:HD21	2:F:73:LEU:HD13	1.80	0.63
1:C:24:THR:H	1:C:30:ASN:HD21	1.47	0.63
1:E:391:ARG:O	1:E:710:LEU:HA	1.98	0.63
2:F:202:ILE:HA	2:F:221:ASN:HD21	1.63	0.63
1:E:3:TYR:CE1	1:E:1045:GLU:HG2	2.33	0.63
1:E:24:THR:H	1:E:30:ASN:HD21	1.45	0.63
1:E:642:ARG:NH1	1:E:645:SER:HA	2.13	0.63
1:A:3:TYR:CE1	1:A:1045:GLU:HG2	2.33	0.63
1:A:518:TYR:HB3	1:A:530:SER:HB3	1.81	0.63
1:C:358:PRO:O	1:C:359:ILE:HB	1.99	0.63
1:C:422:TYR:HD1	1:C:683:ASN:N	1.94	0.63
1:C:642:ARG:NH1	1:C:645:SER:HA	2.12	0.63
1:C:912:LEU:HD21	2:D:73:LEU:HD13	1.79	0.63
2:B:101:TYR:O	2:B:103:ILE:N	2.32	0.63
2:B:227:LEU:H	2:B:236:TRP:HB2	1.62	0.63
1:C:813:ALA:HB1	1:C:833:THR:OG1	1.99	0.63
2:F:331:HIS:O	2:F:332:ARG:O	2.16	0.63
1:A:813:ALA:HB1	1:A:833:THR:OG1	1.99	0.63
1:E:518:TYR:HB3	1:E:530:SER:HB3	1.80	0.63
2:F:101:TYR:O	2:F:103:ILE:N	2.32	0.63
1:A:834:ALA:O	1:A:835:MET:HB2	1.99	0.63
1:C:378:CYS:SG	1:C:388:ARG:HB2	2.39	0.63
1:C:641:PHE:CZ	1:C:650:PHE:HD1	2.15	0.63
2:D:268:LYS:HB3	2:D:270:TRP:HE1	1.64	0.63
1:A:791:LEU:C	1:A:792:LEU:HD12	2.23	0.62
2:B:331:HIS:O	2:B:332:ARG:O	2.17	0.62
1:C:1000:LEU:HD13	1:C:1002:GLU:HB2	1.79	0.62
2:F:63:LEU:CB	2:F:64:PRO:CD	2.57	0.62
1:C:518:TYR:HB3	1:C:530:SER:HB3	1.82	0.62
2:D:110:PHE:CZ	2:D:131:SER:HB2	2.33	0.62
1:A:378:CYS:SG	1:A:388:ARG:HB2	2.39	0.62
1:A:927:MET:CE	2:B:90:LEU:CD2	2.75	0.62
2:F:217:VAL:HG13	2:F:227:LEU:HD23	1.80	0.62
2:D:346:PRO:HG3	2:D:401:ASN:O	1.99	0.62
1:E:573:SER:O	1:E:574:PHE:HB2	2.00	0.62
2:B:200:ILE:HB	2:F:155:ALA:HB1	1.79	0.62
2:B:389:PRO:O	2:B:390:GLU:HG2	1.98	0.62
1:E:757:SER:CB	1:E:792:LEU:HD22	2.29	0.62
2:F:229:ASN:ND2	2:F:233:LYS:HB2	2.15	0.62
1:A:188:ARG:HD2	1:A:214:ALA:O	1.98	0.62
2:B:229:ASN:ND2	2:B:233:LYS:HB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:PRO:O	2:D:299:ASP:HB3	1.99	0.62
1:E:929:SER:HB3	1:E:952:ASN:HB2	1.80	0.62
2:B:198:ASP:HB2	2:F:112:ARG:HH22	1.65	0.61
1:C:384:GLU:O	1:C:385:GLY:C	2.40	0.61
1:C:889:ARG:HE	1:C:904:ASN:HD21	1.48	0.61
2:F:375:PHE:CZ	2:F:382:MET:CE	2.72	0.61
1:A:951:PRO:HB2	2:B:347:ARG:CZ	2.31	0.61
1:A:1084:PRO:O	1:A:1085:ALA:HB3	1.99	0.61
2:B:345:HIS:CD2	2:B:348:TYR:H	2.18	0.61
2:B:375:PHE:CE2	2:B:382:MET:HE2	2.35	0.61
1:E:163:HIS:CB	2:F:57:LEU:HB2	2.30	0.61
1:E:381:ALA:H	1:E:385:GLY:HA2	1.65	0.61
1:E:813:ALA:HB1	1:E:833:THR:OG1	2.01	0.61
2:B:268:LYS:HB3	2:B:270:TRP:HE1	1.64	0.61
1:C:537:GLU:HB2	1:C:561:TRP:HB2	1.82	0.61
2:D:302:ARG:N	2:D:302:ARG:HD2	2.15	0.61
1:E:816:LEU:HD21	1:E:834:ALA:HB2	1.83	0.61
1:A:239:TYR:CE2	1:A:241:ASN:HB2	2.35	0.61
2:B:346:PRO:HG3	2:B:401:ASN:O	1.99	0.61
1:C:3:TYR:CE1	1:C:1045:GLU:HG2	2.35	0.61
1:C:186:GLN:HB2	1:C:189:HIS:HE2	1.65	0.61
2:F:346:PRO:HG3	2:F:401:ASN:O	2.00	0.61
2:B:217:VAL:HB	2:B:248:VAL:HG11	1.83	0.61
1:C:1057:ARG:HB2	1:C:1108:VAL:HG13	1.81	0.61
2:D:202:ILE:HA	2:D:221:ASN:HD21	1.64	0.61
2:F:110:PHE:HD2	2:F:111:ASP:H	0.82	0.61
1:A:573:SER:O	1:A:574:PHE:HB2	2.01	0.61
1:E:163:HIS:CG	2:F:57:LEU:HB2	2.36	0.61
1:A:186:GLN:HB2	1:A:189:HIS:HE2	1.65	0.61
1:E:537:GLU:HB2	1:E:561:TRP:HB2	1.82	0.61
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.83	0.61
1:A:537:GLU:HB2	1:A:561:TRP:CB	2.31	0.61
1:E:810:ASN:CG	1:E:813:ALA:CB	2.72	0.61
2:B:302:ARG:HA	2:B:315:TYR:O	2.01	0.60
2:B:345:HIS:HD2	2:B:348:TYR:H	1.49	0.60
1:C:373:GLY:H	1:C:374:GLN:HB3	1.66	0.60
1:C:520:GLN:HE21	1:C:529:ILE:HG21	1.66	0.60
2:D:331:HIS:O	2:D:332:ARG:O	2.18	0.60
1:E:643:SER:HB2	1:E:648:ASN:OD1	2.01	0.60
1:C:934:ALA:HB2	1:C:945:ILE:CD1	2.25	0.60
1:E:866:VAL:HG12	1:E:867:LYS:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1084:PRO:O	1:E:1085:ALA:HB3	1.99	0.60
2:F:173:TYR:HB3	2:F:207:LEU:HD21	1.83	0.60
2:B:110:PHE:CD2	2:B:111:ASP:N	2.56	0.60
2:D:110:PHE:CD2	2:D:111:ASP:N	2.56	0.60
2:F:345:HIS:HD2	2:F:347:ARG:H	1.47	0.60
1:A:293:GLY:C	1:A:294:THR:CG2	2.73	0.60
1:A:810:ASN:OD1	1:A:810:ASN:N	2.35	0.60
1:C:1084:PRO:O	1:C:1085:ALA:HB3	2.00	0.60
1:C:67:PHE:HB2	1:C:128:CYS:SG	2.42	0.60
1:C:203:ASN:O	1:C:204:LYS:CB	2.50	0.60
1:C:573:SER:O	1:C:574:PHE:HB2	2.01	0.60
2:D:129:VAL:HG11	2:D:415:ILE:HD11	1.84	0.60
2:D:227:LEU:H	2:D:236:TRP:HB2	1.67	0.60
1:A:163:HIS:HB2	2:B:57:LEU:HB2	1.82	0.60
1:A:362:MET:HG2	1:A:1006:VAL:CG2	2.32	0.60
1:A:373:GLY:H	1:A:374:GLN:HB3	1.66	0.60
1:A:792:LEU:H	1:A:792:LEU:CD1	1.99	0.60
2:B:129:VAL:HG11	2:B:415:ILE:HD11	1.83	0.60
1:C:928:ARG:NH1	2:D:405:ASP:OD1	2.35	0.60
1:C:929:SER:HB3	1:C:952:ASN:HB2	1.82	0.60
1:A:407:ILE:HD12	1:A:694:ALA:HB1	1.84	0.60
1:A:665:LYS:NZ	1:A:1020:THR:H	1.98	0.60
1:C:382:PHE:HD1	1:C:720:SER:HG	1.50	0.60
1:C:537:GLU:HB2	1:C:561:TRP:CB	2.31	0.60
2:D:173:TYR:HB3	2:D:207:LEU:HD21	1.84	0.60
1:E:390:ILE:HG22	1:E:710:LEU:HG	1.83	0.60
1:E:537:GLU:HB2	1:E:561:TRP:CB	2.32	0.60
1:E:362:MET:HG2	1:E:1006:VAL:CG2	2.32	0.60
1:A:360:VAL:HG13	2:B:77:LYS:HD3	1.82	0.60
1:A:358:PRO:O	1:A:1032:THR:O	2.20	0.59
2:F:129:VAL:HG11	2:F:415:ILE:HD11	1.84	0.59
1:A:930:VAL:HG23	1:A:931:LEU:N	2.12	0.59
1:A:537:GLU:HB2	1:A:561:TRP:HB2	1.83	0.59
1:C:239:TYR:CE2	1:C:241:ASN:HB2	2.38	0.59
1:C:273:LEU:HB2	1:C:281:PHE:HB2	1.84	0.59
1:E:186:GLN:HB2	1:E:189:HIS:HE2	1.67	0.59
1:E:273:LEU:HB2	1:E:281:PHE:HB2	1.84	0.59
1:C:226:PHE:CE1	1:C:268:GLY:O	2.56	0.59
1:A:394:ILE:HG23	1:A:705:ASP:HB2	1.84	0.59
1:E:358:PRO:O	1:E:359:ILE:HB	2.02	0.59
1:C:203:ASN:O	1:C:204:LYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ASP:HB2	1:E:279:ARG:HB2	1.85	0.59
1:E:721:PRO:O	1:E:736:LEU:O	2.21	0.59
1:E:792:LEU:HB3	1:E:807:PHE:C	2.27	0.59
2:F:349:ASN:O	2:F:376:ASP:O	2.20	0.59
1:C:1136:LEU:O	1:C:1139:ILE:HG12	2.03	0.59
1:E:520:GLN:HE21	1:E:529:ILE:HG21	1.66	0.59
2:B:166:PRO:HB2	2:B:211:ALA:HB2	1.85	0.59
1:C:1044:SER:HB3	1:C:1047:TRP:HD1	1.67	0.59
1:E:203:ASN:O	1:E:204:LYS:CB	2.51	0.59
2:B:383:MET:O	2:B:384:CYS:HB3	2.02	0.59
1:C:163:HIS:HB2	2:D:57:LEU:HA	1.84	0.59
1:E:889:ARG:HE	1:E:904:ASN:HD21	1.49	0.59
1:E:902:GLU:HG2	1:E:903:CYS:H	1.68	0.59
2:B:298:PRO:O	2:B:299:ASP:HB3	2.03	0.58
2:B:375:PHE:CZ	2:B:382:MET:HE1	2.37	0.58
1:C:949:PHE:HD2	2:D:122:THR:HG22	1.68	0.58
2:D:319:GLN:O	2:D:320:TRP:HB2	2.03	0.58
1:E:40:GLU:HG2	1:E:54:GLU:HG3	1.85	0.58
1:E:239:TYR:CE2	1:E:241:ASN:HB2	2.38	0.58
1:A:422:TYR:HD1	1:A:683:ASN:N	1.98	0.58
1:C:709:LYS:O	1:C:710:LEU:HB3	2.03	0.58
1:E:373:GLY:H	1:E:374:GLN:HB3	1.68	0.58
1:C:866:VAL:HG12	1:C:867:LYS:H	1.68	0.58
2:F:345:HIS:CD2	2:F:348:TYR:H	2.22	0.58
1:A:910:MET:HG3	1:A:927:MET:CG	2.31	0.58
1:A:275:ASP:HB2	1:A:279:ARG:HB2	1.85	0.58
1:A:520:GLN:HE21	1:A:529:ILE:HG21	1.68	0.58
2:B:112:ARG:O	2:B:113:ARG:HB2	2.04	0.58
2:D:298:PRO:O	2:D:299:ASP:CB	2.51	0.58
1:E:709:LYS:O	1:E:710:LEU:HB3	2.04	0.58
2:B:382:MET:HE2	2:B:382:MET:CA	2.32	0.58
1:C:816:LEU:HD21	1:C:834:ALA:HB2	1.85	0.58
1:E:620:THR:OG1	1:E:622:LEU:HB2	2.04	0.58
1:E:934:ALA:HB2	1:E:945:ILE:CD1	2.25	0.58
1:A:25:SER:O	1:A:74:LYS:HB3	2.03	0.58
1:A:203:ASN:O	1:A:204:LYS:CB	2.51	0.58
2:B:334:PHE:HB3	2:B:337:LEU:HB3	1.84	0.58
1:C:40:GLU:HG2	1:C:54:GLU:HG3	1.86	0.58
1:C:643:SER:HB2	1:C:648:ASN:OD1	2.04	0.58
2:D:345:HIS:CD2	2:D:348:TYR:H	2.21	0.58
1:E:1044:SER:HB3	1:E:1047:TRP:HD1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:HIS:CB	2:F:126:THR:HB	2.34	0.58
2:F:268:LYS:HB3	2:F:270:TRP:HE1	1.67	0.58
2:F:407:LEU:HB3	2:F:418:TRP:HB2	1.84	0.58
2:B:275:VAL:HG11	2:B:280:SER:O	2.04	0.58
2:F:111:ASP:CG	2:F:112:ARG:N	2.62	0.58
1:A:929:SER:OG	1:A:951:PRO:CA	2.52	0.57
1:C:275:ASP:HB2	1:C:279:ARG:HB2	1.86	0.57
1:C:620:THR:OG1	1:C:622:LEU:HB2	2.04	0.57
2:D:217:VAL:HB	2:D:248:VAL:HG11	1.86	0.57
2:D:317:ALA:HA	2:D:320:TRP:CE2	2.39	0.57
1:A:663:ASN:HD22	1:A:1131:LYS:NZ	2.02	0.57
1:A:1044:SER:HB3	1:A:1047:TRP:HD1	1.68	0.57
2:B:80:ARG:HH11	2:B:80:ARG:CG	2.10	0.57
2:B:411:MET:HG3	2:B:416:LEU:HD12	1.86	0.57
1:C:721:PRO:O	1:C:736:LEU:O	2.21	0.57
2:F:376:ASP:CB	2:F:379:SER:OG	2.52	0.57
1:A:744:ASP:H	1:A:748:GLY:HA2	1.68	0.57
1:A:902:GLU:HG2	1:A:903:CYS:H	1.67	0.57
1:E:709:LYS:HB3	1:E:711:HIS:NE2	2.19	0.57
2:F:112:ARG:O	2:F:113:ARG:HB2	2.04	0.57
2:F:317:ALA:HA	2:F:320:TRP:CE2	2.40	0.57
2:B:375:PHE:CE2	2:B:382:MET:HE1	2.39	0.57
1:C:407:ILE:HD12	1:C:694:ALA:HB1	1.85	0.57
1:E:358:PRO:HD2	1:E:380:GLY:O	2.04	0.57
1:E:866:VAL:HG11	1:E:884:ILE:HD13	1.86	0.57
1:A:866:VAL:HG12	1:A:867:LYS:H	1.69	0.57
1:C:158:ARG:NH2	2:D:319:GLN:HE22	2.02	0.57
1:C:362:MET:HG2	1:C:1006:VAL:CG2	2.34	0.57
1:C:902:GLU:HG2	1:C:903:CYS:H	1.68	0.57
1:A:262:ASN:ND2	1:A:316:TYR:H	2.02	0.57
1:A:587:ILE:H	1:A:587:ILE:HD12	1.70	0.57
1:A:866:VAL:HG11	1:A:884:ILE:HD13	1.87	0.57
2:B:140:ASN:ND2	2:B:141:PHE:O	2.37	0.57
1:E:1078:THR:HB	1:E:1081:LYS:H	1.69	0.57
1:A:385:GLY:HA3	1:A:719:GLU:O	2.05	0.57
1:C:463:VAL:HG13	1:C:464:ALA:N	2.20	0.57
1:C:737:SER:HB3	1:C:794:ILE:HD11	1.87	0.57
1:C:744:ASP:H	1:C:748:GLY:HA2	1.70	0.57
2:D:407:LEU:HB3	2:D:418:TRP:HB2	1.87	0.57
1:A:620:THR:OG1	1:A:622:LEU:HB2	2.04	0.57
2:B:317:ALA:HA	2:B:320:TRP:CE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:587:ILE:H	1:E:587:ILE:HD12	1.70	0.57
2:B:298:PRO:O	2:B:299:ASP:CB	2.52	0.57
2:B:319:GLN:O	2:B:320:TRP:HB2	2.05	0.57
1:C:895:THR:O	1:C:896:GLU:HB2	2.05	0.57
1:C:998:PHE:CZ	1:C:1074:ARG:HD2	2.40	0.57
2:D:411:MET:HG3	2:D:416:LEU:HD12	1.86	0.57
1:A:203:ASN:O	1:A:204:LYS:HB2	2.04	0.57
1:A:293:GLY:O	1:A:294:THR:HG22	2.04	0.57
1:A:967:GLY:HA3	1:A:975:PHE:CZ	2.40	0.57
1:C:25:SER:O	1:C:74:LYS:HB3	2.03	0.57
1:C:791:LEU:C	1:C:792:LEU:HD12	2.26	0.57
2:D:166:PRO:HB2	2:D:211:ALA:HB2	1.86	0.57
2:D:275:VAL:HG11	2:D:280:SER:O	2.04	0.57
2:F:57:LEU:O	2:F:59:GLY:N	2.38	0.57
2:F:217:VAL:HB	2:F:248:VAL:HG11	1.87	0.57
2:D:349:ASN:O	2:D:376:ASP:O	2.23	0.56
2:D:383:MET:O	2:D:384:CYS:HB3	2.04	0.56
1:A:709:LYS:O	1:A:710:LEU:CB	2.53	0.56
1:A:732:CYS:HA	1:A:797:HIS:O	2.05	0.56
1:C:126:PRO:HD3	1:C:169:PHE:HB3	1.87	0.56
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.86	0.56
1:A:721:PRO:O	1:A:736:LEU:O	2.23	0.56
1:A:1109:VAL:HG21	1:A:1126:ALA:HA	1.87	0.56
2:B:397:LEU:HB2	2:B:410:ALA:HB3	1.87	0.56
1:C:262:ASN:ND2	1:C:316:TYR:H	2.02	0.56
1:C:358:PRO:O	1:C:1032:THR:O	2.22	0.56
1:C:394:ILE:HG23	1:C:705:ASP:HB2	1.87	0.56
1:C:606:LEU:HD11	1:C:612:PHE:HE1	1.70	0.56
1:C:810:ASN:OD1	1:C:810:ASN:N	2.37	0.56
2:D:104:LEU:HD22	2:D:416:LEU:HB3	1.88	0.56
2:D:181:THR:OG1	2:D:218:THR:HG21	2.05	0.56
2:D:209:VAL:HG12	2:D:216:VAL:HG22	1.88	0.56
2:D:334:PHE:HB3	2:D:337:LEU:HB3	1.86	0.56
1:E:203:ASN:O	1:E:204:LYS:HB2	2.04	0.56
1:E:294:THR:HG22	1:E:295:VAL:N	2.14	0.56
1:E:358:PRO:O	1:E:1032:THR:O	2.23	0.56
1:E:744:ASP:H	1:E:748:GLY:HA2	1.69	0.56
1:E:810:ASN:HD22	1:E:835:MET:HE2	1.71	0.56
1:E:946:ALA:HB1	1:E:992:LEU:HG	1.86	0.56
2:F:173:TYR:HB2	2:F:207:LEU:HD21	1.88	0.56
1:A:40:GLU:HG2	1:A:54:GLU:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:THR:HB	1:A:1081:LYS:H	1.69	0.56
2:B:287:HIS:CE1	2:B:305:THR:CG2	2.73	0.56
2:D:120:HIS:CB	2:D:126:THR:HB	2.36	0.56
2:F:111:ASP:OD2	2:F:112:ARG:N	2.37	0.56
2:F:287:HIS:CE1	2:F:305:THR:CG2	2.71	0.56
2:F:381:LYS:O	2:F:381:LYS:CG	2.49	0.56
1:E:810:ASN:OD1	1:E:810:ASN:N	2.36	0.56
2:F:140:ASN:ND2	2:F:141:PHE:O	2.38	0.56
1:A:242:GLY:O	1:A:243:ASP:CB	2.53	0.56
1:C:5:TYR:O	1:C:1040:VAL:HA	2.06	0.56
1:C:500:VAL:HG12	1:C:541:LEU:HD12	1.87	0.56
1:C:1044:SER:HB3	1:C:1047:TRP:CD1	2.41	0.56
1:C:1109:VAL:HG21	1:C:1126:ALA:HA	1.87	0.56
1:A:737:SER:HB3	1:A:794:ILE:HD11	1.87	0.56
2:B:57:LEU:O	2:B:59:GLY:N	2.38	0.56
1:C:866:VAL:HG11	1:C:884:ILE:HD13	1.87	0.56
1:E:25:SER:O	1:E:74:LYS:HB3	2.05	0.56
1:E:137:ASP:OD2	2:F:57:LEU:HD23	2.06	0.56
1:A:889:ARG:HE	1:A:904:ASN:HD21	1.52	0.56
2:B:407:LEU:HB3	2:B:418:TRP:HB2	1.88	0.56
1:C:757:SER:HB2	1:C:792:LEU:HD22	1.86	0.56
1:C:928:ARG:HB2	2:D:403:MET:SD	2.46	0.56
2:D:173:TYR:HB2	2:D:207:LEU:HD21	1.86	0.56
1:E:407:ILE:HD12	1:E:694:ALA:HB1	1.86	0.56
2:F:275:VAL:HG11	2:F:280:SER:O	2.05	0.56
1:A:5:TYR:O	1:A:1040:VAL:HA	2.06	0.56
1:E:385:GLY:HA3	1:E:719:GLU:O	2.06	0.56
2:F:355:ARG:NH1	2:F:368:GLU:OE2	2.38	0.56
1:A:134:ARG:HD2	1:A:134:ARG:C	2.31	0.56
1:A:663:ASN:CG	1:A:664:HIS:H	2.13	0.56
2:D:401:ASN:HD21	2:D:406:THR:HB	1.70	0.56
1:E:881:LEU:HD12	1:E:889:ARG:O	2.06	0.56
1:E:1032:THR:HG22	1:E:1033:VAL:N	2.20	0.56
1:A:895:THR:O	1:A:896:GLU:HB2	2.06	0.55
2:B:209:VAL:O	2:B:209:VAL:HG23	2.04	0.55
1:E:1130:ILE:O	1:E:1134:GLU:HB2	2.06	0.55
2:F:334:PHE:HB3	2:F:337:LEU:HB3	1.87	0.55
1:A:118:THR:HB	1:A:134:ARG:NH2	2.20	0.55
1:A:317:LEU:HD12	1:A:321:VAL:HG12	1.88	0.55
2:B:355:ARG:NH1	2:B:368:GLU:OE2	2.39	0.55
1:C:927:MET:O	1:C:928:ARG:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:LEU:O	2:D:59:GLY:N	2.39	0.55
1:E:118:THR:HB	1:E:134:ARG:NH2	2.21	0.55
2:F:153:ILE:HG22	2:F:155:ALA:H	1.72	0.55
1:A:3:TYR:HE1	1:A:1045:GLU:HG2	1.71	0.55
2:B:401:ASN:HD21	2:B:406:THR:HB	1.71	0.55
1:C:810:ASN:HD22	1:C:835:MET:HE2	1.71	0.55
1:C:1078:THR:HB	1:C:1081:LYS:H	1.70	0.55
1:E:500:VAL:HG12	1:E:541:LEU:HD12	1.88	0.55
1:E:735:VAL:HB	1:E:794:ILE:HG13	1.88	0.55
2:F:345:HIS:HD2	2:F:348:TYR:H	1.54	0.55
1:A:1130:ILE:O	1:A:1134:GLU:HB2	2.07	0.55
1:C:587:ILE:H	1:C:587:ILE:HD12	1.71	0.55
1:E:606:LEU:HD11	1:E:612:PHE:HE1	1.72	0.55
1:E:715:VAL:HG21	1:E:801:VAL:HG21	1.89	0.55
1:E:1109:VAL:HG21	1:E:1126:ALA:HA	1.87	0.55
2:B:120:HIS:CB	2:B:126:THR:HB	2.36	0.55
1:E:467:GLN:HE22	1:E:524:GLN:H	1.55	0.55
2:F:411:MET:HG3	2:F:416:LEU:HD12	1.86	0.55
1:A:452:VAL:H	1:A:470:GLN:HE22	1.54	0.55
1:E:5:TYR:O	1:E:1040:VAL:HA	2.06	0.55
1:E:1044:SER:HB3	1:E:1047:TRP:CD1	2.41	0.55
2:F:110:PHE:CD2	2:F:111:ASP:N	2.53	0.55
1:A:571:LEU:O	1:A:572:PRO:C	2.49	0.55
1:C:476:VAL:HG12	1:C:526:LEU:HD21	1.88	0.55
2:D:80:ARG:HH11	2:D:80:ARG:CG	2.11	0.55
1:E:3:TYR:HE1	1:E:1045:GLU:HG2	1.72	0.55
1:E:571:LEU:O	1:E:572:PRO:C	2.50	0.55
2:F:166:PRO:HB2	2:F:211:ALA:HB2	1.88	0.55
2:B:153:ILE:HG22	2:B:155:ALA:H	1.72	0.55
1:E:262:ASN:ND2	1:E:316:TYR:H	2.04	0.55
1:E:482:GLU:HB3	1:E:483:PRO:HD2	1.89	0.55
1:E:757:SER:HB2	1:E:792:LEU:HD22	1.88	0.55
1:A:81:THR:HB	1:A:85:ASN:H	1.70	0.55
1:E:394:ILE:HG23	1:E:705:ASP:HB2	1.88	0.55
2:F:298:PRO:O	2:F:299:ASP:HB3	2.06	0.55
1:A:463:VAL:CG1	1:A:521:ILE:HG21	2.37	0.55
1:A:482:GLU:HB3	1:A:483:PRO:HD2	1.89	0.55
2:B:111:ASP:CG	2:B:112:ARG:N	2.64	0.55
1:C:571:LEU:O	1:C:572:PRO:C	2.50	0.55
2:D:112:ARG:O	2:D:113:ARG:HB2	2.06	0.55
2:D:140:ASN:ND2	2:D:141:PHE:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:THR:HB	1:E:85:ASN:H	1.72	0.55
1:E:126:PRO:HD3	1:E:169:PHE:HB3	1.89	0.55
1:E:927:MET:O	1:E:928:ARG:HB3	2.06	0.55
2:F:298:PRO:O	2:F:299:ASP:CB	2.55	0.55
1:A:606:LEU:HD11	1:A:612:PHE:HE1	1.72	0.54
2:B:104:LEU:HD22	2:B:416:LEU:HB3	1.88	0.54
1:C:1057:ARG:NH1	1:C:1112:LEU:HB2	2.21	0.54
2:D:153:ILE:HG22	2:D:155:ALA:H	1.71	0.54
1:E:242:GLY:O	1:E:243:ASP:CB	2.53	0.54
1:E:360:VAL:HG13	2:F:77:LYS:HD3	1.89	0.54
1:E:895:THR:O	1:E:896:GLU:HB2	2.07	0.54
2:F:319:GLN:O	2:F:320:TRP:HB2	2.07	0.54
1:A:830:ILE:HG12	1:A:850:VAL:HG13	1.89	0.54
1:A:1044:SER:HB3	1:A:1047:TRP:CD1	2.42	0.54
1:C:946:ALA:HB1	1:C:992:LEU:HG	1.88	0.54
1:E:67:PHE:HB2	1:E:128:CYS:SG	2.46	0.54
1:E:463:VAL:HG13	1:E:464:ALA:N	2.22	0.54
1:E:667:VAL:HG11	1:E:1138:ARG:HD3	1.89	0.54
1:A:67:PHE:HB2	1:A:128:CYS:SG	2.47	0.54
2:B:111:ASP:OD2	2:B:112:ARG:N	2.39	0.54
2:B:198:ASP:CA	2:F:112:ARG:HH22	2.20	0.54
2:B:222:VAL:HG12	2:B:239:ARG:HH21	1.72	0.54
1:C:739:ARG:NH1	1:C:792:LEU:HD21	2.21	0.54
2:D:381:LYS:HZ3	2:D:381:LYS:HA	1.70	0.54
2:F:104:LEU:HD22	2:F:416:LEU:HB3	1.89	0.54
1:A:126:PRO:HD3	1:A:169:PHE:HB3	1.88	0.54
1:C:866:VAL:HG11	1:C:884:ILE:HG21	1.89	0.54
2:D:222:VAL:HG12	2:D:239:ARG:HH21	1.73	0.54
1:E:25:SER:HB3	1:E:28:ASP:HB2	1.90	0.54
2:F:131:SER:HB3	2:F:135:ASP:HB2	1.89	0.54
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.89	0.54
1:C:139:LEU:HG	2:D:318:SER:HB2	1.89	0.54
2:D:372:ILE:HB	2:D:386:LEU:HB2	1.90	0.54
2:F:222:VAL:HG12	2:F:239:ARG:HH21	1.71	0.54
1:A:220:ILE:HD11	1:A:232:ILE:HD11	1.89	0.54
1:A:463:VAL:HG13	1:A:464:ALA:N	2.22	0.54
1:A:1002:GLU:HB3	1:A:1032:THR:HG23	1.90	0.54
1:A:1032:THR:HG22	1:A:1033:VAL:N	2.22	0.54
2:D:345:HIS:HD2	2:D:348:TYR:H	1.53	0.54
1:A:463:VAL:HG13	1:A:521:ILE:HG21	1.90	0.54
1:C:933:LEU:HD23	1:C:944:GLU:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ILE:HD11	1:E:232:ILE:HD11	1.88	0.54
1:E:317:LEU:HD12	1:E:321:VAL:HG12	1.89	0.54
1:A:715:VAL:HG21	1:A:801:VAL:HG21	1.89	0.54
1:A:946:ALA:HB1	1:A:992:LEU:HG	1.88	0.54
2:B:349:ASN:O	2:B:376:ASP:O	2.26	0.54
1:C:618:ILE:H	1:C:618:ILE:HD13	1.73	0.54
1:A:467:GLN:HE22	1:A:524:GLN:H	1.56	0.54
1:A:790:ASN:C	1:A:790:ASN:HD22	2.16	0.54
1:C:3:TYR:HE1	1:C:1045:GLU:HG2	1.73	0.54
1:C:452:VAL:H	1:C:470:GLN:HE22	1.56	0.54
1:A:522:HIS:CG	1:A:527:ARG:HH21	2.26	0.54
1:C:1057:ARG:HH12	1:C:1112:LEU:HB2	1.73	0.54
1:E:866:VAL:HG11	1:E:884:ILE:HG21	1.90	0.54
1:E:946:ALA:HB3	1:E:992:LEU:HG	1.90	0.54
2:F:181:THR:OG1	2:F:218:THR:HG21	2.07	0.54
1:C:853:TYR:HB2	1:C:858:LEU:HD23	1.89	0.53
1:A:25:SER:HB3	1:A:28:ASP:HB2	1.91	0.53
1:C:81:THR:HB	1:C:85:ASN:H	1.73	0.53
1:C:317:LEU:HD12	1:C:321:VAL:HG12	1.90	0.53
1:C:1002:GLU:HB3	1:C:1032:THR:CG2	2.38	0.53
2:D:379:SER:HB2	2:D:381:LYS:HB2	1.90	0.53
1:E:356:LEU:HD23	1:E:388:ARG:HG3	1.90	0.53
1:E:792:LEU:CB	1:E:807:PHE:O	2.56	0.53
1:E:923:VAL:HB	1:E:931:LEU:HG	1.91	0.53
1:A:358:PRO:O	1:A:359:ILE:HB	2.06	0.53
2:B:198:ASP:HA	2:F:112:ARG:HH22	1.71	0.53
2:B:382:MET:HE2	2:B:382:MET:HA	1.91	0.53
1:C:463:VAL:CG1	1:C:521:ILE:HG21	2.39	0.53
1:C:1130:ILE:O	1:C:1134:GLU:HB2	2.08	0.53
1:C:830:ILE:HG12	1:C:850:VAL:HG13	1.90	0.53
1:E:452:VAL:H	1:E:470:GLN:HE22	1.56	0.53
1:E:463:VAL:HG13	1:E:521:ILE:HG21	1.91	0.53
1:A:792:LEU:CB	1:A:807:PHE:O	2.56	0.53
2:B:131:SER:HB3	2:B:135:ASP:HB2	1.91	0.53
2:D:397:LEU:HB2	2:D:410:ALA:HB3	1.90	0.53
1:E:933:LEU:HD23	1:E:944:GLU:HA	1.91	0.53
2:F:227:LEU:N	2:F:236:TRP:HB2	2.23	0.53
2:F:383:MET:O	2:F:384:CYS:HB3	2.08	0.53
2:D:376:ASP:CG	2:D:379:SER:OG	2.52	0.53
2:B:299:ASP:C	2:B:299:ASP:OD1	2.52	0.53
1:C:118:THR:HB	1:C:134:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLY:O	1:C:243:ASP:CB	2.53	0.53
1:C:833:THR:HG22	1:C:847:ARG:HB3	1.90	0.53
2:D:229:ASN:HD22	2:D:233:LYS:HB2	1.71	0.53
1:E:1051:LEU:HB2	1:E:1089:ILE:HD13	1.91	0.53
1:A:292:ASP:O	1:A:294:THR:HB	2.09	0.53
1:A:1028:VAL:HB	1:A:1040:VAL:HG23	1.90	0.53
2:B:310:SER:HB3	2:B:330:PRO:HA	1.90	0.53
1:E:732:CYS:HA	1:E:797:HIS:O	2.08	0.53
2:F:397:LEU:HB2	2:F:410:ALA:HB3	1.91	0.53
1:A:853:TYR:HB2	1:A:858:LEU:HD23	1.91	0.53
1:A:933:LEU:HD23	1:A:944:GLU:HA	1.90	0.53
2:B:229:ASN:HD22	2:B:233:LYS:HB2	1.73	0.53
1:C:663:ASN:CG	1:C:664:HIS:H	2.17	0.53
2:F:209:VAL:HG12	2:F:216:VAL:HG22	1.90	0.53
1:A:383:LYS:NZ	1:A:384:GLU:OE2	2.32	0.53
1:A:727:GLN:HE21	1:A:820:LYS:HB2	1.74	0.53
1:A:810:ASN:HD22	1:A:835:MET:HE2	1.73	0.53
1:C:463:VAL:HG13	1:C:464:ALA:H	1.74	0.53
1:C:482:GLU:HB3	1:C:483:PRO:HD2	1.90	0.53
1:C:1051:LEU:HB2	1:C:1089:ILE:HD13	1.90	0.53
1:E:134:ARG:HD2	1:E:134:ARG:C	2.33	0.53
1:E:790:ASN:HD22	1:E:790:ASN:C	2.17	0.53
1:E:853:TYR:HB2	1:E:858:LEU:HD23	1.91	0.53
2:F:420:GLN:O	2:F:421:GLU:C	2.52	0.53
1:C:162:LEU:HD13	2:D:55:VAL:O	2.09	0.52
1:C:732:CYS:HA	1:C:797:HIS:O	2.09	0.52
1:C:814:LEU:HB2	1:C:834:ALA:HB3	1.91	0.52
1:E:639:ARG:HB3	1:E:679:MET:HE2	1.91	0.52
1:E:1084:PRO:O	1:E:1085:ALA:CB	2.57	0.52
1:A:378:CYS:SG	1:A:379:SER:N	2.81	0.52
1:C:130:MET:HE3	1:C:195:VAL:HG11	1.90	0.52
1:C:821:LEU:HD13	1:C:830:ILE:HD12	1.91	0.52
1:E:1:MET:O	1:E:2:SER:HB3	2.09	0.52
1:E:618:ILE:HD13	1:E:618:ILE:H	1.74	0.52
2:F:401:ASN:HD21	2:F:406:THR:HB	1.73	0.52
1:A:1002:GLU:HB3	1:A:1032:THR:CG2	2.39	0.52
1:C:634:GLN:HG2	1:C:654:ASP:CB	2.38	0.52
1:C:719:GLU:CG	1:C:755:SER:HB2	2.40	0.52
2:D:134:GLY:HA2	2:D:159:ILE:HD12	1.92	0.52
1:A:500:VAL:HG12	1:A:541:LEU:HD12	1.90	0.52
1:A:618:ILE:HD13	1:A:618:ILE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:VAL:HG11	1:A:884:ILE:HG21	1.90	0.52
1:A:946:ALA:HB3	1:A:992:LEU:HG	1.90	0.52
2:D:119:TRP:CH2	2:D:401:ASN:ND2	2.78	0.52
1:A:522:HIS:CD2	1:A:527:ARG:HH21	2.28	0.52
1:C:715:VAL:HG21	1:C:801:VAL:HG21	1.90	0.52
1:C:969:GLU:OE2	1:C:973:ASN:HB2	2.09	0.52
1:A:538:VAL:HG13	1:A:558:ILE:HD11	1.92	0.52
1:A:807:PHE:CE1	1:A:851:PHE:CZ	2.97	0.52
1:A:969:GLU:OE2	1:A:973:ASN:HB2	2.09	0.52
1:E:361:ASP:HA	1:E:1006:VAL:HG11	1.91	0.52
1:E:429:PHE:HE1	1:E:434:ARG:CG	2.22	0.52
1:E:522:HIS:CG	1:E:527:ARG:HH21	2.28	0.52
1:E:781:SER:O	1:E:786:VAL:HG12	2.10	0.52
2:F:80:ARG:HG3	2:F:80:ARG:NH1	2.15	0.52
1:A:356:LEU:HD23	1:A:388:ARG:HG3	1.92	0.52
2:B:181:THR:OG1	2:B:218:THR:HG21	2.08	0.52
2:B:227:LEU:N	2:B:236:TRP:HB2	2.24	0.52
1:E:381:ALA:HA	1:E:721:PRO:HD3	1.90	0.52
1:A:928:ARG:O	1:A:929:SER:O	2.28	0.52
2:B:420:GLN:O	2:B:421:GLU:C	2.53	0.52
1:C:220:ILE:HD11	1:C:232:ILE:HD11	1.92	0.52
1:C:463:VAL:HG13	1:C:521:ILE:HG21	1.92	0.52
1:C:522:HIS:CG	1:C:527:ARG:HH21	2.28	0.52
1:C:1028:VAL:HB	1:C:1040:VAL:HG23	1.91	0.52
1:A:1:MET:O	1:A:2:SER:HB3	2.10	0.52
2:D:111:ASP:CG	2:D:112:ARG:N	2.67	0.52
1:E:476:VAL:HG12	1:E:526:LEU:HD21	1.90	0.52
1:E:967:GLY:HA3	1:E:975:PHE:CZ	2.45	0.52
1:A:679:MET:HB2	1:A:693:LEU:HD23	1.92	0.52
1:C:807:PHE:CE1	1:C:851:PHE:CZ	2.98	0.52
1:C:1114:TYR:CB	1:C:1124:ALA:HB2	2.40	0.52
1:E:463:VAL:CG1	1:E:521:ILE:HG21	2.40	0.52
1:E:1028:VAL:HB	1:E:1040:VAL:HG23	1.91	0.52
1:A:80:LEU:HD22	1:A:133:LEU:HD22	1.93	0.51
1:A:407:ILE:HD12	1:A:694:ALA:CB	2.40	0.51
1:A:792:LEU:HB3	1:A:807:PHE:C	2.34	0.51
1:C:923:VAL:HB	1:C:931:LEU:HG	1.92	0.51
1:E:925:ASP:O	1:E:928:ARG:O	2.27	0.51
2:F:63:LEU:HG	2:F:85:SER:HB3	1.92	0.51
2:F:381:LYS:HB2	2:F:381:LYS:HZ3	1.63	0.51
1:C:356:LEU:HD23	1:C:388:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:727:GLN:HE21	1:C:820:LYS:HB2	1.74	0.51
1:C:866:VAL:CG1	1:C:884:ILE:HG21	2.40	0.51
1:C:881:LEU:HD12	1:C:889:ARG:O	2.09	0.51
1:E:814:LEU:HB2	1:E:834:ALA:HB3	1.91	0.51
1:A:634:GLN:HG2	1:A:654:ASP:CB	2.39	0.51
1:A:833:THR:HG22	1:A:847:ARG:HB3	1.92	0.51
1:C:504:ASN:ND2	1:C:506:SER:H	2.09	0.51
2:D:345:HIS:CE1	2:D:404:GLY:HA3	2.45	0.51
1:E:823:LYS:CG	1:E:893:TRP:CD1	2.93	0.51
1:A:881:LEU:HD12	1:A:889:ARG:O	2.10	0.51
1:A:909:ILE:HD11	1:A:928:ARG:HH11	1.75	0.51
1:A:1051:LEU:O	1:A:1055:GLN:HG3	2.10	0.51
2:B:342:ALA:HA	2:B:353:VAL:HG13	1.92	0.51
1:C:504:ASN:HD22	1:C:506:SER:H	1.58	0.51
1:C:792:LEU:HB3	1:C:807:PHE:C	2.36	0.51
1:E:663:ASN:CG	1:E:664:HIS:H	2.17	0.51
2:F:119:TRP:CH2	2:F:401:ASN:ND2	2.79	0.51
2:F:229:ASN:HD22	2:F:233:LYS:HB2	1.74	0.51
1:A:532:THR:HG22	1:A:533:GLU:N	2.26	0.51
1:C:80:LEU:HD22	1:C:133:LEU:HD22	1.93	0.51
2:F:76:HIS:HA	2:F:81:ALA:HB3	1.92	0.51
1:A:239:TYR:HE2	1:A:241:ASN:HB2	1.74	0.51
1:A:381:ALA:HB2	1:A:721:PRO:CD	2.40	0.51
1:A:757:SER:HB2	1:A:792:LEU:CD2	2.40	0.51
1:A:781:SER:O	1:A:786:VAL:HG12	2.10	0.51
1:A:821:LEU:HD13	1:A:830:ILE:HD12	1.92	0.51
1:C:1032:THR:HG22	1:C:1033:VAL:N	2.24	0.51
1:E:378:CYS:SG	1:E:379:SER:N	2.82	0.51
2:F:200:ILE:O	2:F:201:ASN:HB2	2.11	0.51
1:E:239:TYR:HE2	1:E:241:ASN:HB2	1.76	0.51
1:E:255:GLN:HB2	1:E:279:ARG:HH12	1.76	0.51
1:E:735:VAL:O	1:E:794:ILE:HG12	2.11	0.51
1:E:799:PHE:O	1:E:800:GLU:HB3	2.10	0.51
1:C:134:ARG:HD2	1:C:134:ARG:C	2.35	0.51
2:D:63:LEU:HG	2:D:85:SER:HB3	1.93	0.51
1:E:969:GLU:OE2	1:E:973:ASN:HB2	2.11	0.51
1:E:998:PHE:CZ	1:E:1074:ARG:HD2	2.46	0.51
1:A:814:LEU:HB2	1:A:834:ALA:HB3	1.92	0.51
1:A:1084:PRO:O	1:A:1085:ALA:CB	2.59	0.51
1:A:1114:TYR:CB	1:A:1124:ALA:HB2	2.41	0.51
2:B:200:ILE:O	2:B:201:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:ASN:ND2	1:C:620:THR:H	2.09	0.51
1:C:790:ASN:C	1:C:790:ASN:HD22	2.19	0.51
2:D:310:SER:HB3	2:D:330:PRO:HA	1.93	0.51
1:E:130:MET:HE3	1:E:195:VAL:HG11	1.93	0.51
2:F:120:HIS:HB2	2:F:126:THR:HB	1.92	0.51
2:B:198:ASP:CA	2:F:112:ARG:NH2	2.71	0.51
1:C:793:ILE:HG22	1:C:807:PHE:HD1	1.75	0.51
2:D:342:ALA:HA	2:D:353:VAL:HG13	1.92	0.51
1:E:807:PHE:CE1	1:E:851:PHE:CZ	2.99	0.51
1:A:476:VAL:HG12	1:A:526:LEU:HD21	1.92	0.50
1:A:835:MET:HB2	1:A:845:GLN:O	2.12	0.50
1:E:830:ILE:HG12	1:E:850:VAL:HG13	1.94	0.50
2:F:342:ALA:HA	2:F:353:VAL:HG13	1.92	0.50
1:A:130:MET:HE3	1:A:195:VAL:HG11	1.92	0.50
2:B:63:LEU:CD1	2:B:72:THR:HG23	2.42	0.50
1:C:799:PHE:O	1:C:800:GLU:HB3	2.11	0.50
2:D:200:ILE:O	2:D:201:ASN:HB2	2.11	0.50
1:E:821:LEU:HD13	1:E:830:ILE:HD12	1.91	0.50
1:E:1114:TYR:CB	1:E:1124:ALA:HB2	2.41	0.50
1:A:394:ILE:HD12	1:A:658:VAL:HG11	1.93	0.50
1:A:617:ASN:ND2	1:A:620:THR:H	2.10	0.50
1:A:1102:ARG:NH2	1:A:1126:ALA:HB3	2.26	0.50
1:E:532:THR:HG22	1:E:533:GLU:N	2.26	0.50
1:A:361:ASP:HA	1:A:1006:VAL:HG11	1.93	0.50
1:A:998:PHE:CZ	1:A:1074:ARG:HD2	2.47	0.50
2:B:345:HIS:CG	2:B:346:PRO:HD2	2.47	0.50
1:C:1:MET:O	1:C:2:SER:HB3	2.12	0.50
1:C:25:SER:HB3	1:C:28:ASP:HB2	1.92	0.50
2:D:111:ASP:OD2	2:D:112:ARG:N	2.43	0.50
1:E:522:HIS:CD2	1:E:527:ARG:HH21	2.30	0.50
1:C:378:CYS:SG	1:C:379:SER:N	2.85	0.50
1:C:781:SER:O	1:C:786:VAL:HG12	2.12	0.50
1:C:946:ALA:HB3	1:C:992:LEU:HG	1.91	0.50
1:E:381:ALA:N	1:E:385:GLY:HA2	2.25	0.50
1:E:727:GLN:HE21	1:E:820:LYS:HB2	1.76	0.50
2:F:310:SER:HB3	2:F:330:PRO:HA	1.93	0.50
1:A:292:ASP:C	1:A:294:THR:N	2.69	0.50
1:A:504:ASN:ND2	1:A:506:SER:H	2.10	0.50
2:B:376:ASP:CB	2:B:379:SER:OG	2.59	0.50
1:C:294:THR:HG22	1:C:295:VAL:N	2.15	0.50
1:C:1084:PRO:O	1:C:1085:ALA:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:LEU:N	2:D:236:TRP:HB2	2.26	0.50
2:D:289:HIS:CB	2:D:290:PRO:CD	2.89	0.50
1:E:821:LEU:O	1:E:827:THR:HA	2.12	0.50
1:E:1102:ARG:NH2	1:E:1126:ALA:HB3	2.26	0.50
1:C:639:ARG:HB3	1:C:679:MET:HE2	1.94	0.50
1:C:1102:ARG:NH2	1:C:1126:ALA:HB3	2.26	0.50
1:E:634:GLN:HG2	1:E:654:ASP:CB	2.40	0.50
1:A:255:GLN:HB2	1:A:279:ARG:HH12	1.75	0.50
1:C:114:ARG:H	1:C:114:ARG:NE	2.10	0.50
1:C:1002:GLU:HB3	1:C:1032:THR:HG23	1.92	0.50
2:D:355:ARG:NH1	2:D:368:GLU:OE2	2.44	0.50
1:E:294:THR:CG2	1:E:295:VAL:H	2.15	0.50
1:A:799:PHE:O	1:A:800:GLU:HB3	2.11	0.49
1:A:866:VAL:CG1	1:A:884:ILE:HG21	2.41	0.49
1:A:927:MET:HE2	2:B:90:LEU:HB3	1.94	0.49
1:C:407:ILE:HD12	1:C:694:ALA:CB	2.42	0.49
1:C:467:GLN:HE22	1:C:524:GLN:H	1.60	0.49
1:C:522:HIS:CD2	1:C:527:ARG:HH21	2.30	0.49
1:E:815:SER:H	1:E:834:ALA:H	1.60	0.49
1:E:866:VAL:HG12	1:E:867:LYS:N	2.26	0.49
1:E:963:ASP:C	1:E:964:ASN:HD22	2.20	0.49
1:E:1057:ARG:HB2	1:E:1108:VAL:HG13	1.93	0.49
1:A:817:VAL:HG23	1:A:832:GLY:HA3	1.93	0.49
1:A:866:VAL:HG12	1:A:867:LYS:N	2.27	0.49
1:A:1029:LEU:HD23	1:A:1039:LEU:HB2	1.94	0.49
2:D:420:GLN:O	2:D:421:GLU:C	2.55	0.49
1:E:373:GLY:H	1:E:374:GLN:HE21	1.60	0.49
2:B:221:ASN:HD22	2:B:221:ASN:N	2.10	0.49
2:B:345:HIS:CE1	2:B:404:GLY:HA3	2.47	0.49
2:D:166:PRO:CB	2:D:211:ALA:HB2	2.43	0.49
1:E:504:ASN:ND2	1:E:506:SER:H	2.10	0.49
2:F:401:ASN:CB	2:F:404:GLY:H	2.25	0.49
1:A:414:ARG:H	1:A:462:ASN:HD21	1.59	0.49
1:A:429:PHE:HE1	1:A:434:ARG:CG	2.24	0.49
1:A:663:ASN:CB	1:A:1131:LYS:HE2	2.41	0.49
1:C:255:GLN:HB2	1:C:279:ARG:HH12	1.77	0.49
1:E:382:PHE:H	1:E:385:GLY:N	2.10	0.49
1:E:617:ASN:ND2	1:E:620:THR:H	2.09	0.49
2:F:112:ARG:HD2	2:F:132:LYS:HB3	1.94	0.49
1:A:504:ASN:HD22	1:A:506:SER:H	1.59	0.49
1:A:709:LYS:O	1:A:710:LEU:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LEU:HD11	2:B:81:ALA:HB1	1.94	0.49
2:B:140:ASN:C	2:B:140:ASN:HD22	2.20	0.49
1:C:239:TYR:HE2	1:C:241:ASN:HB2	1.76	0.49
1:C:1061:VAL:O	1:C:1062:ILE:HB	2.13	0.49
1:C:1114:TYR:HB2	1:C:1124:ALA:HB2	1.94	0.49
1:A:290:GLN:O	1:A:291:MET:CB	2.56	0.49
1:A:810:ASN:ND2	1:A:813:ALA:CB	2.73	0.49
1:A:1114:TYR:HB2	1:A:1124:ALA:HB2	1.95	0.49
1:A:821:LEU:O	1:A:827:THR:HA	2.11	0.49
2:B:200:ILE:HB	2:F:155:ALA:HB3	1.93	0.49
1:C:429:PHE:HE1	1:C:434:ARG:CG	2.25	0.49
1:C:679:MET:HA	1:C:692:ALA:O	2.13	0.49
2:D:401:ASN:CB	2:D:404:GLY:H	2.24	0.49
1:E:10:GLN:HG3	1:E:11:LYS:H	1.77	0.49
1:A:130:MET:HE2	1:A:142:VAL:HG13	1.95	0.49
1:A:757:SER:CB	1:A:792:LEU:CD2	2.91	0.49
1:A:790:ASN:C	1:A:790:ASN:ND2	2.71	0.49
1:A:793:ILE:HG22	1:A:807:PHE:HD1	1.77	0.49
1:A:969:GLU:HG2	1:A:971:ALA:H	1.77	0.49
2:B:401:ASN:CB	2:B:404:GLY:H	2.25	0.49
1:C:866:VAL:HG12	1:C:867:LYS:N	2.27	0.49
1:C:889:ARG:HD3	1:C:901:THR:CG2	2.43	0.49
2:D:299:ASP:C	2:D:299:ASP:OD1	2.55	0.49
1:E:80:LEU:HD22	1:E:133:LEU:HD22	1.93	0.49
1:A:114:ARG:H	1:A:114:ARG:NE	2.11	0.49
1:A:373:GLY:H	1:A:374:GLN:HE21	1.61	0.49
1:A:722:ARG:HB3	1:A:736:LEU:O	2.12	0.49
1:C:679:MET:HB2	1:C:693:LEU:HD23	1.94	0.49
2:D:131:SER:HB3	2:D:135:ASP:HB2	1.94	0.49
2:D:251:ASN:HB2	2:D:257:PHE:HB3	1.94	0.49
1:E:719:GLU:CG	1:E:755:SER:HB2	2.42	0.49
1:E:866:VAL:CG1	1:E:884:ILE:HG21	2.42	0.49
2:F:345:HIS:CE1	2:F:404:GLY:HA3	2.48	0.49
2:F:351:ILE:O	2:F:374:VAL:HA	2.13	0.49
2:F:401:ASN:HB2	2:F:404:GLY:H	1.78	0.49
2:F:401:ASN:HB3	2:F:403:MET:N	2.28	0.49
1:C:163:HIS:HB2	2:D:57:LEU:CB	2.39	0.49
1:C:532:THR:HG22	1:C:533:GLU:N	2.25	0.49
1:C:810:ASN:O	1:C:811:GLU:HB3	2.13	0.49
1:E:793:ILE:HG22	1:E:807:PHE:HD1	1.78	0.49
1:E:838:PRO:CA	1:E:839:GLU:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:928:ARG:NH1	2:F:405:ASP:OD1	2.46	0.49
1:E:1002:GLU:HB3	1:E:1032:THR:CG2	2.43	0.49
2:B:98:LEU:O	2:B:101:TYR:HB2	2.13	0.48
1:C:384:GLU:O	1:C:385:GLY:O	2.29	0.48
1:C:500:VAL:HB	1:C:511:ALA:HB3	1.95	0.48
1:C:797:HIS:HB3	1:C:800:GLU:OE1	2.13	0.48
1:C:821:LEU:O	1:C:827:THR:HA	2.13	0.48
1:C:823:LYS:CG	1:C:893:TRP:CD1	2.92	0.48
1:C:15:VAL:HG12	1:C:17:GLY:H	1.78	0.48
1:C:163:HIS:CD2	2:D:57:LEU:HD22	2.48	0.48
1:A:665:LYS:NZ	1:A:1020:THR:N	2.62	0.48
2:B:248:VAL:HG22	2:B:260:THR:HG23	1.95	0.48
2:B:329:HIS:CE1	2:B:353:VAL:HB	2.48	0.48
1:C:838:PRO:CA	1:C:839:GLU:HB2	2.42	0.48
2:D:63:LEU:CD1	2:D:72:THR:HG23	2.43	0.48
1:A:163:HIS:CG	2:B:57:LEU:HB2	2.47	0.48
2:B:134:GLY:HA2	2:B:159:ILE:HD12	1.95	0.48
2:B:206:SER:HB3	2:B:246:THR:O	2.14	0.48
2:B:401:ASN:HB3	2:B:403:MET:N	2.29	0.48
1:C:958:GLU:HG2	1:C:1028:VAL:HG11	1.95	0.48
2:D:76:HIS:HA	2:D:81:ALA:HB3	1.95	0.48
2:D:248:VAL:HG13	2:D:258:LEU:HD21	1.96	0.48
2:D:401:ASN:HB3	2:D:403:MET:N	2.28	0.48
1:E:390:ILE:CG2	1:E:710:LEU:HG	2.44	0.48
1:E:114:ARG:NE	1:E:114:ARG:H	2.12	0.48
2:F:340:ILE:HG13	2:F:396:SER:HA	1.95	0.48
1:A:218:MET:HG3	1:A:232:ILE:HB	1.95	0.48
1:A:471:ILE:HG23	1:A:476:VAL:HG22	1.95	0.48
1:A:500:VAL:HB	1:A:511:ALA:HB3	1.96	0.48
2:B:76:HIS:HA	2:B:81:ALA:HB3	1.94	0.48
2:B:372:ILE:HB	2:B:386:LEU:HB2	1.94	0.48
1:C:312:GLU:HG3	1:C:327:ARG:HB2	1.95	0.48
2:D:140:ASN:HD22	2:D:140:ASN:C	2.20	0.48
1:E:833:THR:HG22	1:E:847:ARG:HB3	1.94	0.48
1:E:1114:TYR:HB2	1:E:1124:ALA:HB2	1.94	0.48
2:B:173:TYR:HB3	2:B:207:LEU:HD11	1.96	0.48
2:B:263:VAL:C	2:B:265:GLN:H	2.21	0.48
1:C:967:GLY:HA3	1:C:975:PHE:CZ	2.49	0.48
2:D:112:ARG:HD2	2:D:132:LYS:HB3	1.95	0.48
1:E:158:ARG:NH2	2:F:319:GLN:HE22	2.10	0.48
1:E:835:MET:HB2	1:E:845:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:101:TYR:OH	2:F:405:ASP:HA	2.13	0.48
2:F:204:PHE:HA	2:F:220:ASP:HA	1.95	0.48
2:F:381:LYS:CB	2:F:381:LYS:HZ3	2.19	0.48
2:F:409:SER:HB2	2:F:416:LEU:HB2	1.95	0.48
1:A:719:GLU:CG	1:A:755:SER:HB2	2.43	0.48
2:B:204:PHE:HA	2:B:220:ASP:HA	1.94	0.48
2:D:345:HIS:CG	2:D:346:PRO:HD2	2.47	0.48
2:D:401:ASN:HB2	2:D:404:GLY:H	1.78	0.48
1:E:163:HIS:CD2	2:F:57:LEU:HD22	2.49	0.48
2:F:248:VAL:HG13	2:F:258:LEU:HD21	1.95	0.48
1:A:312:GLU:HG3	1:A:327:ARG:HB2	1.95	0.48
1:E:1051:LEU:O	1:E:1055:GLN:HG3	2.14	0.48
2:F:345:HIS:CG	2:F:346:PRO:HD2	2.49	0.48
1:A:789:HIS:HB2	2:B:71:ARG:HH22	1.78	0.48
2:B:120:HIS:HB2	2:B:126:THR:HB	1.96	0.48
2:B:401:ASN:HB2	2:B:404:GLY:H	1.79	0.48
1:C:167:VAL:CG1	1:C:180:PHE:HB3	2.37	0.48
1:C:1076:PHE:O	1:C:1082:THR:HA	2.14	0.48
1:E:272:LEU:O	1:E:273:LEU:HD23	2.13	0.48
1:A:213:GLU:HG3	1:A:236:SER:HB3	1.96	0.47
1:A:757:SER:HB2	1:A:792:LEU:HD22	1.96	0.47
1:C:218:MET:HG3	1:C:232:ILE:HB	1.96	0.47
1:C:835:MET:HB2	1:C:845:GLN:O	2.14	0.47
2:D:101:TYR:OH	2:D:405:ASP:HA	2.14	0.47
1:E:500:VAL:HB	1:E:511:ALA:HB3	1.96	0.47
2:F:134:GLY:HA2	2:F:159:ILE:HD12	1.96	0.47
2:F:376:ASP:CG	2:F:379:SER:HG	2.22	0.47
1:A:838:PRO:CA	1:A:839:GLU:HB2	2.44	0.47
1:A:1074:ARG:HD3	1:A:1074:ARG:HA	1.58	0.47
2:B:101:TYR:OH	2:B:405:ASP:HA	2.14	0.47
1:E:504:ASN:HD22	1:E:506:SER:H	1.61	0.47
1:E:958:GLU:HG2	1:E:1028:VAL:HG11	1.95	0.47
2:F:221:ASN:HD22	2:F:221:ASN:N	2.10	0.47
1:A:163:HIS:CB	2:B:57:LEU:HB2	2.44	0.47
1:C:358:PRO:HD2	1:C:380:GLY:O	2.14	0.47
1:C:361:ASP:HA	1:C:1006:VAL:HG11	1.96	0.47
2:D:63:LEU:HD13	2:D:72:THR:HG23	1.96	0.47
2:D:76:HIS:CG	2:D:86:VAL:HG21	2.49	0.47
2:D:204:PHE:HA	2:D:220:ASP:HA	1.96	0.47
1:E:797:HIS:HB3	1:E:800:GLU:OE1	2.14	0.47
1:E:928:ARG:HB2	2:F:403:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1061:VAL:O	1:E:1062:ILE:HB	2.14	0.47
2:F:253:CYS:SG	2:F:299:ASP:HA	2.54	0.47
1:A:212:VAL:O	1:A:213:GLU:C	2.57	0.47
1:A:951:PRO:HB2	2:B:347:ARG:NH1	2.30	0.47
2:B:376:ASP:HB3	2:B:380:GLY:H	1.79	0.47
1:E:538:VAL:HG13	1:E:558:ILE:HD11	1.96	0.47
2:F:63:LEU:CD1	2:F:72:THR:HG23	2.45	0.47
1:A:815:SER:H	1:A:834:ALA:H	1.62	0.47
1:A:889:ARG:HD3	1:A:901:THR:CG2	2.45	0.47
1:E:407:ILE:HD12	1:E:694:ALA:CB	2.44	0.47
2:F:273:ARG:HE	2:F:274:GLN:HB2	1.80	0.47
2:B:409:SER:HB2	2:B:416:LEU:HB2	1.96	0.47
1:C:394:ILE:HD12	1:C:658:VAL:HG11	1.97	0.47
1:C:969:GLU:HG2	1:C:971:ALA:H	1.80	0.47
1:C:1029:LEU:HD23	1:C:1039:LEU:HB2	1.97	0.47
2:D:80:ARG:CG	2:D:80:ARG:NH1	2.76	0.47
2:D:101:TYR:C	2:D:103:ILE:N	2.72	0.47
2:D:221:ASN:HD22	2:D:221:ASN:N	2.09	0.47
1:E:312:GLU:HG3	1:E:327:ARG:HB2	1.97	0.47
1:E:414:ARG:H	1:E:462:ASN:HD21	1.62	0.47
2:B:351:ILE:O	2:B:374:VAL:HA	2.15	0.47
1:C:373:GLY:H	1:C:374:GLN:HE21	1.62	0.47
2:D:411:MET:HG3	2:D:416:LEU:CD1	2.45	0.47
1:E:265:ASP:OD2	1:E:270:ARG:HG3	2.14	0.47
1:E:429:PHE:CE1	1:E:434:ARG:CG	2.97	0.47
1:E:790:ASN:C	1:E:790:ASN:ND2	2.73	0.47
2:F:289:HIS:CB	2:F:290:PRO:CD	2.91	0.47
2:B:63:LEU:HG	2:B:85:SER:HB3	1.97	0.47
2:B:208:ASP:CG	2:B:209:VAL:H	2.23	0.47
1:C:429:PHE:HE1	1:C:434:ARG:HG2	1.80	0.47
1:C:810:ASN:ND2	1:C:813:ALA:CB	2.76	0.47
1:C:975:PHE:HA	1:C:996:GLY:O	2.15	0.47
1:E:662:SER:CB	1:E:1138:ARG:NH2	2.78	0.47
1:E:1022:THR:N	1:E:1023:PRO:HD2	2.30	0.47
2:F:101:TYR:C	2:F:103:ILE:N	2.73	0.47
2:F:329:HIS:CE1	2:F:353:VAL:HB	2.50	0.47
1:C:337:ASN:HB2	1:C:346:TYR:HA	1.97	0.47
1:C:392:ASN:ND2	1:C:1140:HIS:O	2.48	0.47
2:F:372:ILE:HB	2:F:386:LEU:HB2	1.96	0.47
1:A:1061:VAL:O	1:A:1062:ILE:HB	2.13	0.46
1:C:10:GLN:HG3	1:C:11:LYS:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ARG:H	1:C:462:ASN:HD21	1.63	0.46
2:F:140:ASN:C	2:F:140:ASN:HD22	2.22	0.46
1:A:381:ALA:HB2	1:A:721:PRO:HD3	1.96	0.46
1:A:467:GLN:NE2	1:A:524:GLN:H	2.13	0.46
1:E:387:LEU:HB2	1:E:715:VAL:HB	1.97	0.46
1:E:390:ILE:HG22	1:E:710:LEU:CG	2.44	0.46
2:F:285:LEU:HD13	2:F:315:TYR:CE2	2.50	0.46
1:A:24:THR:N	1:A:30:ASN:HD21	2.13	0.46
1:A:665:LYS:HZ1	1:A:1020:THR:N	2.13	0.46
1:A:810:ASN:O	1:A:811:GLU:HB3	2.15	0.46
1:A:1022:THR:N	1:A:1023:PRO:HD2	2.30	0.46
1:A:1091:GLY:O	1:A:1095:GLU:N	2.35	0.46
2:B:177:MET:HA	2:B:203:TRP:CD1	2.51	0.46
1:A:823:LYS:CG	1:A:893:TRP:CD1	2.97	0.46
1:A:936:LYS:HB2	1:A:936:LYS:HE3	1.66	0.46
2:B:198:ASP:HA	2:F:112:ARG:HH21	1.74	0.46
1:C:373:GLY:N	1:C:374:GLN:HB3	2.30	0.46
1:C:963:ASP:C	1:C:964:ASN:HD22	2.23	0.46
2:D:177:MET:HA	2:D:203:TRP:CD1	2.50	0.46
2:D:220:ASP:C	2:D:220:ASP:OD2	2.59	0.46
2:D:316:SER:HB2	2:D:324:LEU:HD12	1.97	0.46
1:E:15:VAL:HG12	1:E:17:GLY:H	1.80	0.46
2:B:63:LEU:HD13	2:B:72:THR:HG23	1.96	0.46
2:B:166:PRO:CB	2:B:211:ALA:HB2	2.45	0.46
1:C:1022:THR:N	1:C:1023:PRO:HD2	2.31	0.46
2:D:235:LEU:C	2:D:236:TRP:HE3	2.24	0.46
2:D:263:VAL:C	2:D:265:GLN:H	2.23	0.46
1:E:487:VAL:HG11	1:E:524:GLN:HA	1.95	0.46
1:E:967:GLY:O	1:E:974:LEU:HA	2.15	0.46
1:E:1076:PHE:O	1:E:1082:THR:HA	2.16	0.46
2:F:301:ALA:C	2:F:302:ARG:HD2	2.41	0.46
1:A:15:VAL:HG12	1:A:17:GLY:H	1.81	0.46
1:C:815:SER:H	1:C:834:ALA:H	1.64	0.46
2:D:301:ALA:C	2:D:302:ARG:HD2	2.40	0.46
1:E:126:PRO:HB3	1:E:171:TYR:CE2	2.50	0.46
1:E:684:SER:HB3	1:E:687:TYR:HB2	1.98	0.46
2:F:177:MET:HA	2:F:203:TRP:CD1	2.50	0.46
1:C:582:LEU:HD13	1:C:606:LEU:HD21	1.98	0.46
1:C:1133:VAL:O	1:C:1137:THR:HG23	2.16	0.46
1:E:218:MET:HG3	1:E:232:ILE:HB	1.96	0.46
1:A:337:ASN:HB2	1:A:346:TYR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:PHE:HE1	1:A:434:ARG:HG2	1.81	0.46
2:B:76:HIS:CG	2:B:86:VAL:HG21	2.51	0.46
2:B:386:LEU:HD23	2:B:386:LEU:HA	1.76	0.46
1:C:936:LYS:O	1:C:939:GLU:HB3	2.15	0.46
1:C:1105:MET:O	1:C:1109:VAL:HG23	2.16	0.46
2:D:63:LEU:HD11	2:D:81:ALA:HB1	1.98	0.46
2:D:285:LEU:HD13	2:D:315:TYR:CE2	2.51	0.46
1:E:817:VAL:HG23	1:E:832:GLY:HA3	1.97	0.46
2:F:281:PHE:HB2	2:F:282:LEU:H	1.59	0.46
1:A:126:PRO:HB3	1:A:171:TYR:CE2	2.51	0.46
1:A:965:PHE:O	1:A:976:VAL:HA	2.15	0.46
1:C:212:VAL:O	1:C:213:GLU:C	2.58	0.46
1:C:790:ASN:C	1:C:790:ASN:ND2	2.74	0.46
1:C:1044:SER:HB3	1:C:1047:TRP:HB2	1.98	0.46
1:C:1051:LEU:O	1:C:1055:GLN:HG3	2.15	0.46
2:D:120:HIS:HB2	2:D:126:THR:HB	1.98	0.46
2:D:351:ILE:O	2:D:374:VAL:HA	2.16	0.46
1:E:975:PHE:HA	1:E:996:GLY:O	2.16	0.46
1:A:961:ASP:C	1:A:963:ASP:H	2.23	0.46
1:A:967:GLY:O	1:A:974:LEU:HA	2.15	0.46
2:B:301:ALA:C	2:B:302:ARG:HD2	2.41	0.46
1:C:538:VAL:HG13	1:C:558:ILE:HD11	1.97	0.46
1:E:937:PRO:C	1:E:939:GLU:N	2.73	0.46
1:E:1002:GLU:HB3	1:E:1032:THR:HG23	1.98	0.46
1:E:1105:MET:O	1:E:1109:VAL:HG23	2.15	0.46
1:A:387:LEU:HB2	1:A:715:VAL:HB	1.96	0.45
2:B:165:ASN:HB3	2:B:168:ASN:O	2.17	0.45
2:D:54:TRP:HA	2:D:324:LEU:O	2.15	0.45
1:E:213:GLU:HG3	1:E:236:SER:HB3	1.98	0.45
1:E:810:ASN:O	1:E:811:GLU:HB3	2.17	0.45
1:E:1021:SER:OG	1:E:1135:GLU:HG3	2.15	0.45
1:A:958:GLU:HG2	1:A:1028:VAL:HG11	1.98	0.45
2:B:248:VAL:HG13	2:B:258:LEU:HD21	1.98	0.45
2:D:101:TYR:C	2:D:103:ILE:H	2.24	0.45
2:D:342:ALA:CB	2:D:353:VAL:HG13	2.46	0.45
2:F:63:LEU:HD11	2:F:81:ALA:HB1	1.98	0.45
2:F:248:VAL:HG22	2:F:260:THR:HG23	1.98	0.45
2:F:304:LEU:HD21	2:F:351:ILE:HG23	1.98	0.45
2:B:119:TRP:CH2	2:B:401:ASN:ND2	2.85	0.45
2:B:333:HIS:CD2	2:B:333:HIS:H	2.35	0.45
1:E:367:LEU:HB2	1:E:375:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:ILE:HG23	1:E:712:ILE:HD13	1.98	0.45
2:F:235:LEU:C	2:F:236:TRP:HE3	2.24	0.45
2:F:263:VAL:C	2:F:265:GLN:H	2.24	0.45
2:F:299:ASP:OD1	2:F:299:ASP:C	2.59	0.45
1:A:413:LEU:HD21	1:A:468:LEU:HG	1.99	0.45
1:A:429:PHE:CE1	1:A:434:ARG:CG	2.98	0.45
1:A:582:LEU:HD13	1:A:606:LEU:HD21	1.99	0.45
1:A:679:MET:HE3	1:A:680:CYS:HA	1.98	0.45
1:A:684:SER:HB3	1:A:687:TYR:HB2	1.98	0.45
1:C:965:PHE:O	1:C:976:VAL:HA	2.17	0.45
1:C:1074:ARG:HD3	1:C:1074:ARG:HA	1.63	0.45
2:D:371:THR:OG1	2:D:385:GLN:HB3	2.15	0.45
2:D:409:SER:HB2	2:D:416:LEU:HB2	1.96	0.45
1:E:612:PHE:HE2	1:E:626:ARG:NH1	2.14	0.45
2:F:165:ASN:HB3	2:F:168:ASN:O	2.17	0.45
1:A:23:PHE:N	1:A:30:ASN:ND2	2.63	0.45
1:A:792:LEU:HB3	1:A:808:LEU:HA	1.99	0.45
1:A:1105:MET:O	1:A:1109:VAL:HG23	2.16	0.45
2:B:251:ASN:HB2	2:B:257:PHE:HB3	1.98	0.45
1:E:264:VAL:HG23	1:E:270:ARG:O	2.16	0.45
1:E:364:VAL:HG22	1:E:376:VAL:HG22	1.99	0.45
1:E:394:ILE:HD12	1:E:658:VAL:HG11	1.97	0.45
1:A:329:GLY:HA3	1:A:384:GLU:HB3	1.99	0.45
1:A:367:LEU:HB2	1:A:375:LEU:HD11	1.98	0.45
1:A:833:THR:HG21	1:A:847:ARG:HB3	1.96	0.45
1:A:975:PHE:HA	1:A:996:GLY:O	2.16	0.45
2:B:119:TRP:CE3	2:B:127:VAL:HG23	2.51	0.45
2:B:208:ASP:HB3	2:B:250:LEU:CD2	2.47	0.45
1:C:928:ARG:O	1:C:929:SER:O	2.34	0.45
1:E:673:LEU:C	1:E:674:LYS:O	2.57	0.45
1:E:679:MET:HB2	1:E:693:LEU:HD23	1.99	0.45
1:E:722:ARG:NH2	1:E:789:HIS:HE1	2.14	0.45
2:F:166:PRO:CB	2:F:211:ALA:HB2	2.47	0.45
1:A:722:ARG:NH2	1:A:789:HIS:HE1	2.14	0.45
1:A:797:HIS:HB3	1:A:800:GLU:OE1	2.17	0.45
2:B:253:CYS:SG	2:B:299:ASP:HA	2.56	0.45
1:E:139:LEU:HG	2:F:318:SER:HB2	1.97	0.45
1:E:757:SER:HB2	1:E:792:LEU:CD2	2.46	0.45
1:E:791:LEU:C	1:E:792:LEU:HD12	2.30	0.45
1:C:383:LYS:CG	1:C:384:GLU:HG3	2.39	0.45
1:E:167:VAL:CG1	1:E:180:PHE:HB3	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:VAL:O	1:E:213:GLU:C	2.59	0.45
1:E:961:ASP:C	1:E:963:ASP:H	2.25	0.45
1:A:380:GLY:CA	1:A:721:PRO:HG2	2.28	0.45
1:A:720:SER:HA	1:A:721:PRO:HD3	1.75	0.45
1:A:1076:PHE:O	1:A:1082:THR:HA	2.16	0.45
1:C:1091:GLY:O	1:C:1095:GLU:N	2.36	0.45
1:E:467:GLN:NE2	1:E:524:GLN:H	2.13	0.45
1:E:969:GLU:HG2	1:E:971:ALA:H	1.82	0.45
1:E:1029:LEU:HD23	1:E:1039:LEU:HB2	1.97	0.45
2:B:101:TYR:C	2:B:103:ILE:H	2.25	0.45
2:B:273:ARG:HE	2:B:274:GLN:HB2	1.82	0.45
1:C:673:LEU:C	1:C:674:LYS:O	2.59	0.45
1:C:766:SER:N	1:C:807:PHE:HE2	2.14	0.45
1:C:951:PRO:HB2	2:D:347:ARG:NH1	2.32	0.45
1:E:679:MET:HE3	1:E:680:CYS:HA	1.98	0.45
1:A:643:SER:HB2	1:A:648:ASN:OD1	2.17	0.44
1:A:679:MET:HA	1:A:692:ALA:O	2.16	0.44
2:B:235:LEU:C	2:B:236:TRP:HE3	2.25	0.44
2:B:340:ILE:HG13	2:B:396:SER:HA	1.99	0.44
1:C:126:PRO:HB3	1:C:171:TYR:CE2	2.51	0.44
1:C:463:VAL:CG1	1:C:464:ALA:N	2.80	0.44
1:C:722:ARG:HB3	1:C:736:LEU:O	2.17	0.44
1:C:833:THR:HG21	1:C:847:ARG:HB3	1.98	0.44
2:D:253:CYS:SG	2:D:299:ASP:HA	2.57	0.44
2:D:273:ARG:HE	2:D:274:GLN:HB2	1.82	0.44
1:E:337:ASN:HB2	1:E:346:TYR:HA	1.99	0.44
1:E:582:LEU:HD13	1:E:606:LEU:HD21	1.99	0.44
1:E:766:SER:N	1:E:807:PHE:HE2	2.15	0.44
1:A:272:LEU:O	1:A:273:LEU:HD23	2.17	0.44
1:A:999:HIS:HB3	1:A:1074:ARG:O	2.17	0.44
2:B:209:VAL:O	2:B:209:VAL:HG22	2.14	0.44
1:C:471:ILE:HG23	1:C:476:VAL:HG22	1.99	0.44
1:C:825:PRO:HB2	1:C:826:ASN:H	1.57	0.44
1:C:1054:MET:HE2	1:C:1054:MET:HA	1.99	0.44
1:E:463:VAL:HG13	1:E:464:ALA:H	1.81	0.44
1:E:1023:PRO:HB2	1:E:1136:LEU:HD21	1.98	0.44
1:E:1044:SER:HB3	1:E:1047:TRP:HB2	1.99	0.44
1:A:359:ILE:HG21	1:A:362:MET:HE3	1.98	0.44
1:A:960:LEU:HD12	1:A:964:ASN:HB3	1.99	0.44
2:B:101:TYR:C	2:B:103:ILE:N	2.73	0.44
2:B:112:ARG:HD2	2:B:132:LYS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:LEU:HD13	2:B:235:LEU:HD13	1.99	0.44
1:C:130:MET:CE	1:C:195:VAL:HG11	2.48	0.44
1:C:709:LYS:O	1:C:710:LEU:CB	2.64	0.44
1:C:967:GLY:O	1:C:974:LEU:HA	2.16	0.44
2:D:342:ALA:HB2	2:D:353:VAL:HG13	1.98	0.44
1:C:414:ARG:HG2	1:C:421:THR:O	2.18	0.44
1:C:925:ASP:O	1:C:928:ARG:O	2.35	0.44
1:E:265:ASP:O	1:E:268:GLY:N	2.49	0.44
1:A:463:VAL:HG13	1:A:464:ALA:H	1.81	0.44
1:A:963:ASP:C	1:A:964:ASN:HD22	2.26	0.44
2:B:381:LYS:O	2:B:381:LYS:CG	2.61	0.44
1:C:382:PHE:HB3	1:C:383:LYS:H	1.58	0.44
2:D:182:ARG:NH2	2:D:184:GLN:HE22	2.15	0.44
1:E:373:GLY:N	1:E:374:GLN:HB3	2.32	0.44
1:E:429:PHE:HE1	1:E:434:ARG:HG2	1.81	0.44
1:A:1051:LEU:CB	1:A:1089:ILE:HD13	2.48	0.44
2:B:110:PHE:CE2	2:B:131:SER:HB2	2.53	0.44
1:C:367:LEU:HB2	1:C:375:LEU:HD11	1.99	0.44
1:C:766:SER:H	1:C:807:PHE:HE2	1.66	0.44
1:C:937:PRO:C	1:C:939:GLU:N	2.74	0.44
2:D:123:HIS:HA	2:D:124:PRO:HD3	1.81	0.44
2:D:248:VAL:HG22	2:D:260:THR:HG23	2.00	0.44
1:E:23:PHE:N	1:E:30:ASN:ND2	2.62	0.44
1:E:58:TYR:O	1:E:1068:ILE:HG21	2.18	0.44
2:F:411:MET:HG3	2:F:416:LEU:CD1	2.48	0.44
1:A:293:GLY:O	1:A:294:THR:O	2.35	0.44
1:C:213:GLU:HG3	1:C:236:SER:HB3	1.99	0.44
1:C:292:ASP:O	1:C:294:THR:N	2.51	0.44
1:C:964:ASN:ND2	1:C:978:GLN:NE2	2.66	0.44
1:E:13:THR:HB	1:E:355:ASN:HA	2.00	0.44
2:F:220:ASP:C	2:F:220:ASP:OD2	2.60	0.44
2:F:386:LEU:HD23	2:F:386:LEU:HA	1.79	0.44
1:A:612:PHE:HE2	1:A:626:ARG:NH1	2.16	0.44
1:A:910:MET:HB3	1:A:912:LEU:HD13	2.00	0.44
1:C:429:PHE:CE1	1:C:434:ARG:HG2	2.53	0.44
1:C:998:PHE:CE1	1:C:1074:ARG:HD2	2.52	0.44
2:D:401:ASN:HB2	2:D:404:GLY:N	2.33	0.44
1:E:720:SER:HA	1:E:721:PRO:HD3	1.78	0.44
1:E:936:LYS:O	1:E:939:GLU:HB3	2.18	0.44
1:A:639:ARG:HB3	1:A:679:MET:HE2	1.99	0.44
2:B:227:LEU:HB3	2:B:236:TRP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:LYS:O	2:B:381:LYS:HG3	2.10	0.44
1:C:564:ILE:HG23	1:C:588:PRO:HD3	1.98	0.44
2:D:342:ALA:CA	2:D:353:VAL:HG13	2.48	0.44
1:A:757:SER:HB3	1:A:792:LEU:HD22	1.98	0.43
2:B:411:MET:HG3	2:B:416:LEU:CD1	2.48	0.43
1:C:372:GLN:HA	1:C:373:GLY:HA2	1.50	0.43
1:C:431:GLY:O	1:C:455:GLN:HA	2.18	0.43
1:C:1007:PHE:CD2	1:C:1030:PHE:HB3	2.53	0.43
1:E:329:GLY:HA3	1:E:384:GLU:HB3	2.00	0.43
1:E:612:PHE:HE2	1:E:626:ARG:HH11	1.65	0.43
1:E:1054:MET:HE2	1:E:1054:MET:HA	1.99	0.43
1:A:1054:MET:HA	1:A:1054:MET:HE2	2.01	0.43
2:B:80:ARG:HG3	2:B:80:ARG:NH1	2.16	0.43
2:B:285:LEU:HD13	2:B:315:TYR:CE2	2.53	0.43
1:C:684:SER:HB3	1:C:687:TYR:HB2	2.00	0.43
1:C:722:ARG:NH2	1:C:789:HIS:HE1	2.15	0.43
2:D:119:TRP:CZ2	2:D:401:ASN:ND2	2.86	0.43
1:E:222:VAL:HA	1:E:223:PRO:HD3	1.90	0.43
2:F:104:LEU:HD21	2:F:418:TRP:CE2	2.53	0.43
2:F:203:TRP:H	2:F:221:ASN:ND2	2.16	0.43
1:A:207:TRP:CE3	1:A:242:GLY:HA3	2.53	0.43
1:A:373:GLY:N	1:A:374:GLN:HB3	2.31	0.43
1:A:866:VAL:HG11	1:A:884:ILE:CD1	2.48	0.43
1:A:937:PRO:C	1:A:939:GLU:N	2.75	0.43
2:B:223:GLY:HA3	2:B:241:HIS:O	2.19	0.43
1:C:429:PHE:CE1	1:C:434:ARG:CG	3.00	0.43
1:C:1051:LEU:CB	1:C:1089:ILE:HD13	2.49	0.43
1:E:511:ALA:HB2	1:E:516:LEU:HD23	1.99	0.43
1:E:744:ASP:HB3	1:E:747:GLY:O	2.19	0.43
2:F:64:PRO:O	2:F:65:PRO:C	2.62	0.43
2:F:227:LEU:HB3	2:F:236:TRP:HB2	2.00	0.43
1:A:522:HIS:HB2	1:A:525:GLU:HB3	2.00	0.43
1:A:866:VAL:CG1	1:A:884:ILE:HD13	2.47	0.43
2:B:190:ILE:HG22	2:B:191:LEU:N	2.33	0.43
2:B:207:LEU:HA	2:B:207:LEU:HD23	1.56	0.43
1:C:817:VAL:HG23	1:C:832:GLY:HA3	1.99	0.43
1:E:429:PHE:CE1	1:E:434:ARG:HG2	2.53	0.43
1:E:564:ILE:HG23	1:E:588:PRO:HD3	2.00	0.43
1:E:999:HIS:HB3	1:E:1074:ARG:O	2.19	0.43
2:F:401:ASN:HB2	2:F:404:GLY:N	2.33	0.43
1:C:141:LYS:HD2	1:C:156:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:ILE:HG23	1:E:476:VAL:HG22	2.00	0.43
1:E:527:ARG:HG2	1:E:529:ILE:HG22	2.00	0.43
1:E:722:ARG:HB3	1:E:736:LEU:O	2.17	0.43
1:E:866:VAL:HG11	1:E:884:ILE:CD1	2.49	0.43
1:E:1057:ARG:HH12	1:E:1112:LEU:HB2	1.82	0.43
2:F:63:LEU:HD13	2:F:72:THR:HG23	1.99	0.43
1:A:16:ASN:ND2	1:A:35:LYS:O	2.51	0.43
1:A:382:PHE:HB3	1:A:383:LYS:H	1.63	0.43
2:B:64:PRO:O	2:B:65:PRO:C	2.61	0.43
1:C:719:GLU:HG3	1:C:755:SER:HB2	1.99	0.43
1:C:951:PRO:HB2	2:D:347:ARG:CZ	2.49	0.43
2:D:281:PHE:HB2	2:D:282:LEU:H	1.60	0.43
2:D:329:HIS:CE1	2:D:353:VAL:HB	2.53	0.43
2:D:401:ASN:HB3	2:D:403:MET:H	1.83	0.43
2:F:76:HIS:CG	2:F:86:VAL:HG21	2.54	0.43
1:A:766:SER:H	1:A:807:PHE:HE2	1.67	0.43
1:A:964:ASN:ND2	1:A:978:GLN:NE2	2.66	0.43
1:C:130:MET:HE2	1:C:142:VAL:HG13	1.99	0.43
1:C:917:LYS:HZ2	1:C:962:ASP:H	1.66	0.43
2:D:271:ASP:HB2	2:D:282:LEU:HD11	2.00	0.43
1:E:833:THR:HG21	1:E:847:ARG:HB3	1.99	0.43
2:F:110:PHE:CE2	2:F:131:SER:HB2	2.54	0.43
1:A:663:ASN:HB3	1:A:1131:LYS:HE2	2.01	0.43
1:A:1098:LEU:HD21	1:A:1133:VAL:HB	2.00	0.43
1:C:207:TRP:CE3	1:C:242:GLY:HA3	2.53	0.43
2:D:227:LEU:HB3	2:D:236:TRP:HB2	2.01	0.43
2:D:375:PHE:CE2	2:D:382:MET:HE2	2.54	0.43
1:E:141:LYS:HD2	1:E:156:ASN:ND2	2.34	0.43
2:F:64:PRO:HG3	2:F:75:GLN:HG3	2.01	0.43
1:A:739:ARG:NH1	1:A:792:LEU:HD21	2.34	0.43
1:A:973:ASN:OD1	1:A:999:HIS:HD2	2.02	0.43
1:C:58:TYR:O	1:C:1068:ILE:HG21	2.18	0.43
2:D:64:PRO:O	2:D:65:PRO:C	2.62	0.43
1:E:130:MET:HE2	1:E:142:VAL:HG13	2.00	0.43
2:F:101:TYR:C	2:F:103:ILE:H	2.26	0.43
1:A:429:PHE:CE1	1:A:434:ARG:HG2	2.53	0.43
1:A:719:GLU:HG3	1:A:755:SER:HB2	2.01	0.43
1:A:916:THR:HG22	1:A:921:ILE:HG12	2.00	0.43
2:B:104:LEU:HD21	2:B:418:TRP:CE2	2.54	0.43
1:C:23:PHE:N	1:C:30:ASN:ND2	2.63	0.43
1:C:220:ILE:HB	1:C:230:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ASN:O	1:C:512:VAL:HG13	2.19	0.43
1:C:916:THR:HG22	1:C:921:ILE:HG12	2.00	0.43
2:D:386:LEU:HD23	2:D:386:LEU:HA	1.85	0.43
1:E:889:ARG:HD3	1:E:901:THR:CG2	2.48	0.43
2:F:227:LEU:HD13	2:F:235:LEU:HD13	1.99	0.43
2:F:333:HIS:CD2	2:F:333:HIS:H	2.36	0.43
1:A:511:ALA:HB2	1:A:516:LEU:HD23	2.01	0.42
1:A:564:ILE:HG23	1:A:588:PRO:HD3	2.01	0.42
1:C:16:ASN:ND2	1:C:35:LYS:O	2.51	0.42
1:C:511:ALA:HB2	1:C:516:LEU:HD23	1.99	0.42
1:C:612:PHE:HE2	1:C:626:ARG:HH11	1.67	0.42
2:D:54:TRP:C	2:D:54:TRP:CD1	2.97	0.42
2:D:340:ILE:HG13	2:D:396:SER:HA	2.00	0.42
1:E:126:PRO:HB3	1:E:171:TYR:CD2	2.54	0.42
1:E:163:HIS:HB2	2:F:57:LEU:CB	2.42	0.42
1:E:207:TRP:CE3	1:E:242:GLY:HA3	2.53	0.42
1:E:852:GLN:HB2	1:E:861:VAL:CG2	2.49	0.42
1:E:886:SER:O	1:E:908:ASN:HB2	2.19	0.42
1:A:663:ASN:CG	1:A:664:HIS:N	2.77	0.42
1:A:744:ASP:HB3	1:A:747:GLY:O	2.19	0.42
1:A:908:ASN:OD1	1:A:931:LEU:HD21	2.19	0.42
2:B:304:LEU:HB2	2:B:344:TRP:CE2	2.55	0.42
1:C:522:HIS:HB2	1:C:525:GLU:HB3	2.01	0.42
1:C:612:PHE:HE2	1:C:626:ARG:NH1	2.16	0.42
1:E:130:MET:CE	1:E:195:VAL:HG11	2.49	0.42
1:E:250:PRO:HA	1:E:251:PRO:HD3	1.89	0.42
1:E:356:LEU:HD21	1:E:712:ILE:HD12	2.01	0.42
2:F:54:TRP:CD1	2:F:54:TRP:C	2.97	0.42
2:F:411:MET:HE3	2:F:411:MET:HB3	1.59	0.42
1:A:50:ARG:HA	1:A:51:PRO:HD3	1.81	0.42
1:A:1044:SER:HB3	1:A:1047:TRP:HB2	2.01	0.42
2:B:54:TRP:C	2:B:54:TRP:CD1	2.97	0.42
2:B:289:HIS:CB	2:B:290:PRO:CD	2.92	0.42
1:C:163:HIS:HB2	2:D:57:LEU:CA	2.47	0.42
1:C:910:MET:HB3	1:C:912:LEU:HD13	2.01	0.42
1:E:294:THR:HG22	1:E:295:VAL:HG22	2.01	0.42
1:A:334:VAL:HG12	1:A:349:ALA:HA	2.02	0.42
1:A:936:LYS:O	1:A:939:GLU:HB3	2.19	0.42
2:B:316:SER:HB2	2:B:324:LEU:HD12	2.00	0.42
1:C:25:SER:OG	1:C:27:GLU:HG2	2.20	0.42
1:C:500:VAL:CG1	1:C:541:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ARG:HG2	1:C:529:ILE:HG22	2.00	0.42
1:C:613:TYR:CE1	1:C:666:LEU:HD21	2.54	0.42
1:C:757:SER:HB2	1:C:792:LEU:CD2	2.49	0.42
1:C:866:VAL:HG11	1:C:884:ILE:CD1	2.49	0.42
1:C:911:ALA:H	1:C:925:ASP:HA	1.84	0.42
1:C:961:ASP:C	1:C:963:ASP:H	2.27	0.42
1:E:965:PHE:O	1:E:976:VAL:HA	2.19	0.42
2:F:123:HIS:HA	2:F:124:PRO:HD3	1.81	0.42
1:A:182:TYR:CE2	1:A:189:HIS:HB2	2.55	0.42
1:A:297:LEU:HD21	1:A:300:LEU:CD1	2.50	0.42
1:A:497:ASN:O	1:A:512:VAL:HG13	2.19	0.42
1:A:613:TYR:CE1	1:A:666:LEU:HD21	2.54	0.42
1:A:950:ASN:HD21	1:A:994:GLU:CD	2.27	0.42
2:D:333:HIS:CD2	2:D:333:HIS:H	2.37	0.42
1:E:158:ARG:CZ	2:F:319:GLN:HE22	2.32	0.42
1:E:613:TYR:CE1	1:E:666:LEU:HD21	2.54	0.42
1:E:911:ALA:H	1:E:925:ASP:HA	1.83	0.42
2:F:316:SER:HB2	2:F:324:LEU:HD12	2.00	0.42
1:C:294:THR:CG2	1:C:295:VAL:H	2.17	0.42
1:C:679:MET:HE3	1:C:680:CYS:HA	2.02	0.42
1:C:792:LEU:CB	1:C:807:PHE:O	2.65	0.42
2:D:165:ASN:HB3	2:D:168:ASN:O	2.19	0.42
2:D:227:LEU:HD13	2:D:235:LEU:HD13	2.01	0.42
2:D:382:MET:HE2	2:D:382:MET:HB2	1.36	0.42
1:E:393:GLY:O	1:E:711:HIS:NE2	2.53	0.42
1:E:429:PHE:HE1	1:E:434:ARG:HG3	1.84	0.42
1:E:490:TRP:HB2	1:E:526:LEU:HD23	2.02	0.42
1:E:500:VAL:CG1	1:E:541:LEU:HD12	2.49	0.42
1:E:928:ARG:O	1:E:929:SER:O	2.38	0.42
1:E:964:ASN:ND2	1:E:978:GLN:NE2	2.67	0.42
1:A:141:LYS:HD2	1:A:156:ASN:ND2	2.35	0.42
1:A:909:ILE:HB	1:A:927:MET:HB2	2.00	0.42
2:B:358:ASP:HA	2:B:359:PRO:HD2	1.90	0.42
1:E:163:HIS:HB2	2:F:57:LEU:HA	2.01	0.42
1:E:666:LEU:HD23	1:E:666:LEU:N	2.31	0.42
1:E:964:ASN:HD22	1:E:964:ASN:N	2.17	0.42
2:F:271:ASP:HB2	2:F:282:LEU:HD11	2.02	0.42
2:F:342:ALA:HB2	2:F:353:VAL:HG13	2.02	0.42
2:F:371:THR:OG1	2:F:385:GLN:HB3	2.18	0.42
1:A:507:GLN:NE2	1:A:552:LEU:HG	2.35	0.42
1:A:609:GLY:HA3	1:A:632:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:PRO:HG3	2:B:75:GLN:HG3	2.01	0.42
2:B:342:ALA:CA	2:B:353:VAL:HG13	2.50	0.42
1:C:286:GLU:HB2	1:C:299:ASP:H	1.84	0.42
1:C:487:VAL:HG11	1:C:524:GLN:HA	1.98	0.42
1:C:490:TRP:HB2	1:C:526:LEU:HD23	2.01	0.42
1:C:719:GLU:HG2	1:C:755:SER:HB2	2.01	0.42
1:C:866:VAL:CG1	1:C:884:ILE:HD13	2.49	0.42
1:E:25:SER:OG	1:E:27:GLU:HG2	2.20	0.42
1:E:269:SER:HB3	1:E:270:ARG:HG2	2.01	0.42
1:E:286:GLU:HB2	1:E:299:ASP:H	1.85	0.42
1:E:679:MET:HA	1:E:692:ALA:O	2.19	0.42
1:E:825:PRO:HB2	1:E:826:ASN:H	1.58	0.42
1:A:766:SER:N	1:A:807:PHE:HE2	2.17	0.42
2:B:123:HIS:HA	2:B:124:PRO:HD3	1.83	0.42
2:B:342:ALA:HB2	2:B:353:VAL:HG13	2.02	0.42
1:C:886:SER:O	1:C:908:ASN:HB2	2.20	0.42
1:C:999:HIS:HB3	1:C:1074:ARG:O	2.19	0.42
2:D:411:MET:HE3	2:D:411:MET:HB3	1.56	0.42
1:E:998:PHE:CE1	1:E:1074:ARG:HD2	2.55	0.42
1:A:487:VAL:HG11	1:A:524:GLN:HA	1.96	0.42
1:A:949:PHE:CD1	1:A:949:PHE:N	2.87	0.42
2:B:199:THR:HB	2:B:202:ILE:HD12	2.01	0.42
1:C:147:ARG:HA	1:C:147:ARG:CZ	2.50	0.42
1:C:182:TYR:CE2	1:C:189:HIS:HB2	2.54	0.42
1:C:634:GLN:HB2	1:C:654:ASP:H	1.85	0.42
1:E:179:CYS:HA	1:E:192:THR:HG22	2.02	0.42
1:E:275:ASP:HB3	1:E:279:ARG:H	1.85	0.42
1:E:292:ASP:O	1:E:294:THR:N	2.53	0.42
1:E:367:LEU:HD11	1:E:798:THR:CG2	2.50	0.42
2:F:251:ASN:HB2	2:F:257:PHE:HB3	2.01	0.42
2:F:342:ALA:CB	2:F:353:VAL:HG13	2.49	0.42
1:A:852:GLN:HB2	1:A:861:VAL:CG2	2.49	0.41
2:B:304:LEU:HD21	2:B:351:ILE:HG23	2.02	0.41
1:C:209:GLN:C	1:C:210:GLU:HG2	2.45	0.41
1:C:297:LEU:HD21	1:C:300:LEU:CD1	2.50	0.41
1:C:570:LYS:HB3	1:C:575:GLU:HB3	2.02	0.41
2:D:206:SER:HB3	2:D:246:THR:O	2.19	0.41
1:E:522:HIS:HB2	1:E:525:GLU:HB3	2.02	0.41
1:E:839:GLU:N	2:F:66:CYS:HB2	2.35	0.41
1:A:25:SER:OG	1:A:27:GLU:HG2	2.20	0.41
1:A:111:ARG:HD2	1:A:111:ARG:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LYS:HB3	1:A:575:GLU:HB3	2.01	0.41
1:A:612:PHE:HE2	1:A:626:ARG:HH11	1.67	0.41
2:B:140:ASN:ND2	2:B:140:ASN:C	2.78	0.41
1:C:277:GLU:O	1:C:383:LYS:HE2	2.21	0.41
1:C:720:SER:HA	1:C:721:PRO:HD3	1.76	0.41
1:C:723:LYS:HB2	1:C:736:LEU:HD12	2.02	0.41
1:E:656:PRO:HB2	1:E:671:VAL:HB	2.02	0.41
1:E:814:LEU:HD23	1:E:836:VAL:HB	2.02	0.41
1:E:1051:LEU:CB	1:E:1089:ILE:HD13	2.49	0.41
2:F:342:ALA:CA	2:F:353:VAL:HG13	2.50	0.41
1:A:10:GLN:HG3	1:A:11:LYS:H	1.85	0.41
1:A:126:PRO:HB3	1:A:171:TYR:CD2	2.55	0.41
1:A:690:SER:HB3	1:A:702:GLY:O	2.20	0.41
1:A:913:TYR:CE1	1:A:954:MET:CE	3.04	0.41
2:D:203:TRP:H	2:D:221:ASN:ND2	2.18	0.41
1:E:182:TYR:CE2	1:E:189:HIS:HB2	2.55	0.41
1:E:910:MET:HB3	1:E:912:LEU:HD13	2.02	0.41
1:A:275:ASP:HB3	1:A:279:ARG:H	1.85	0.41
1:C:183:GLN:HG2	2:D:58:ALA:HB3	2.02	0.41
2:D:104:LEU:HD21	2:D:418:TRP:CE2	2.56	0.41
1:E:147:ARG:CZ	1:E:147:ARG:HA	2.51	0.41
1:E:709:LYS:O	1:E:710:LEU:CB	2.64	0.41
1:E:1057:ARG:NH1	1:E:1112:LEU:HB2	2.35	0.41
1:A:68:ARG:NH2	1:A:73:SER:O	2.54	0.41
1:A:147:ARG:CZ	1:A:147:ARG:HA	2.50	0.41
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.90	0.41
1:A:791:LEU:O	1:A:809:GLN:HG2	2.20	0.41
2:B:160:THR:OG1	2:B:205:CYS:HA	2.20	0.41
2:B:401:ASN:HB2	2:B:404:GLY:N	2.35	0.41
1:C:553:SER:HA	1:C:554:PRO:HD3	1.87	0.41
1:C:852:GLN:HB2	1:C:861:VAL:CG2	2.50	0.41
1:C:875:GLU:CD	1:C:875:GLU:C	2.89	0.41
1:E:553:SER:HA	1:E:554:PRO:HD3	1.87	0.41
1:E:770:LEU:HD12	1:E:770:LEU:N	2.29	0.41
1:E:916:THR:HG22	1:E:921:ILE:HG12	2.03	0.41
1:E:927:MET:O	1:E:928:ARG:CB	2.67	0.41
1:E:949:PHE:HD2	2:F:122:THR:HG22	1.85	0.41
1:A:490:TRP:HB2	1:A:526:LEU:HD23	2.03	0.41
2:B:342:ALA:CB	2:B:353:VAL:HG13	2.50	0.41
1:C:126:PRO:HB3	1:C:171:TYR:CD2	2.56	0.41
1:C:792:LEU:HB3	1:C:808:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ILE:HB	1:E:230:ILE:HB	2.01	0.41
1:E:813:ALA:HB1	1:E:833:THR:HG1	1.85	0.41
1:E:852:GLN:HB2	1:E:861:VAL:HG21	2.03	0.41
2:F:401:ASN:HB3	2:F:403:MET:H	1.84	0.41
1:A:889:ARG:HD3	1:A:901:THR:HG23	2.03	0.41
2:B:68:SER:O	2:B:69:ILE:C	2.64	0.41
1:C:38:ARG:HD2	1:C:54:GLU:CD	2.46	0.41
1:C:927:MET:O	1:C:928:ARG:CB	2.68	0.41
2:D:64:PRO:HG3	2:D:75:GLN:HG3	2.02	0.41
2:D:119:TRP:CE3	2:D:127:VAL:HG23	2.56	0.41
2:D:224:ASN:HA	2:D:239:ARG:HA	2.03	0.41
1:E:209:GLN:C	1:E:210:GLU:HG2	2.46	0.41
1:A:271:TYR:HB2	1:A:283:LEU:HB3	2.02	0.41
1:A:527:ARG:HG2	1:A:529:ILE:HG22	2.02	0.41
1:A:776:ALA:HA	1:A:777:PRO:HD2	1.86	0.41
1:A:969:GLU:CD	1:A:973:ASN:HB2	2.46	0.41
2:B:346:PRO:HD3	2:B:400:PHE:HB2	2.03	0.41
1:C:271:TYR:HB2	1:C:283:LEU:HB3	2.03	0.41
1:E:16:ASN:ND2	1:E:35:LYS:O	2.54	0.41
1:E:570:LYS:HB3	1:E:575:GLU:HB3	2.02	0.41
1:E:723:LYS:HB2	1:E:736:LEU:HD12	2.03	0.41
1:E:794:ILE:HG23	1:E:794:ILE:HD13	1.69	0.41
1:E:866:VAL:CG1	1:E:884:ILE:HD13	2.49	0.41
1:E:936:LYS:HB2	1:E:936:LYS:HE3	1.67	0.41
1:E:1007:PHE:CD2	1:E:1030:PHE:HB3	2.56	0.41
1:A:58:TYR:O	1:A:1068:ILE:HG21	2.21	0.41
1:A:114:ARG:HA	1:A:115:PRO:HD3	1.91	0.41
1:A:431:GLY:O	1:A:455:GLN:HA	2.21	0.41
1:A:800:GLU:O	1:A:800:GLU:HG2	2.21	0.41
1:A:814:LEU:HD23	1:A:836:VAL:HB	2.02	0.41
1:A:839:GLU:N	2:B:66:CYS:HB2	2.36	0.41
1:A:911:ALA:H	1:A:925:ASP:HA	1.85	0.41
1:A:1007:PHE:CD2	1:A:1030:PHE:HB3	2.55	0.41
2:B:401:ASN:HB3	2:B:403:MET:H	1.86	0.41
1:C:13:THR:HB	1:C:355:ASN:HA	2.02	0.41
1:C:382:PHE:HD1	1:C:720:SER:OG	2.01	0.41
1:C:852:GLN:HB2	1:C:861:VAL:HG21	2.03	0.41
1:C:1023:PRO:HB2	1:C:1136:LEU:HD21	2.03	0.41
2:D:62:ILE:HG13	2:D:89:GLY:CA	2.51	0.41
2:D:110:PHE:CE2	2:D:131:SER:HB2	2.56	0.41
1:E:24:THR:N	1:E:30:ASN:HD21	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:GLU:CG	1:E:54:GLU:HG3	2.51	0.41
1:E:105:HIS:CD2	1:E:1067:LYS:HB2	2.56	0.41
1:E:110:ASP:HB2	1:E:136:TYR:CE1	2.56	0.41
1:E:241:ASN:HB3	1:E:244:LYS:HB2	2.03	0.41
1:E:264:VAL:C	1:E:265:ASP:OD1	2.64	0.41
1:E:390:ILE:HG22	1:E:710:LEU:CD1	2.51	0.41
1:E:431:GLY:O	1:E:455:GLN:HA	2.21	0.41
2:F:206:SER:HB3	2:F:246:THR:O	2.21	0.41
1:A:130:MET:CE	1:A:195:VAL:HG11	2.50	0.41
1:A:220:ILE:HB	1:A:230:ILE:HB	2.02	0.41
1:A:677:ASN:HD21	1:A:696:ASN:CG	2.29	0.41
1:C:744:ASP:HB3	1:C:747:GLY:O	2.20	0.41
1:E:271:TYR:HB2	1:E:283:LEU:HB3	2.02	0.41
1:E:719:GLU:HG2	1:E:755:SER:HB2	2.02	0.41
1:E:726:TYR:O	1:E:820:LYS:HG2	2.20	0.41
2:F:105:GLN:O	2:F:106:LYS:CB	2.69	0.41
1:A:463:VAL:CG1	1:A:464:ALA:N	2.83	0.40
1:A:998:PHE:CE1	1:A:1074:ARG:HD2	2.56	0.40
2:B:54:TRP:HA	2:B:324:LEU:O	2.22	0.40
1:C:123:ILE:HG21	1:C:168:LYS:HA	2.03	0.40
1:E:68:ARG:NH2	1:E:73:SER:O	2.55	0.40
1:E:123:ILE:HG21	1:E:168:LYS:HA	2.02	0.40
1:E:297:LEU:HD21	1:E:300:LEU:CD1	2.51	0.40
1:E:334:VAL:HG12	1:E:349:ALA:HA	2.02	0.40
1:E:875:GLU:CD	1:E:875:GLU:C	2.89	0.40
1:E:1095:GLU:C	1:E:1097:PHE:H	2.29	0.40
1:A:372:GLN:HA	1:A:373:GLY:HA2	1.46	0.40
2:B:208:ASP:O	2:B:209:VAL:HG13	1.76	0.40
1:C:241:ASN:HB3	1:C:244:LYS:HB2	2.04	0.40
1:C:509:VAL:HG23	1:C:543:ILE:HD13	2.02	0.40
1:C:609:GLY:HA3	1:C:632:GLY:O	2.20	0.40
1:C:810:ASN:HB2	1:C:835:MET:HE2	2.03	0.40
1:C:855:ASP:C	1:C:857:LYS:H	2.29	0.40
1:C:970:ASN:ND2	2:D:83:TRP:CE2	2.89	0.40
1:E:414:ARG:HG2	1:E:421:THR:O	2.21	0.40
1:E:609:GLY:HA3	1:E:632:GLY:O	2.21	0.40
2:F:224:ASN:HA	2:F:239:ARG:HA	2.03	0.40
1:A:364:VAL:HG22	1:A:376:VAL:HG22	2.03	0.40
2:B:160:THR:HB	2:B:205:CYS:O	2.21	0.40
1:C:275:ASP:HB3	1:C:279:ARG:H	1.86	0.40
1:E:359:ILE:HG21	1:E:362:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:PHE:HD2	1:E:382:PHE:HA	1.69	0.40
1:E:383:LYS:HG3	1:E:384:GLU:N	2.35	0.40
1:E:810:ASN:HB2	1:E:835:MET:HE2	2.03	0.40
1:E:950:ASN:HD21	1:E:994:GLU:CD	2.29	0.40
1:E:951:PRO:O	1:E:952:ASN:O	2.39	0.40
1:E:1032:THR:CG2	1:E:1033:VAL:N	2.84	0.40
2:F:297:SER:OG	2:F:301:ALA:O	2.21	0.40
2:F:376:ASP:OD1	2:F:379:SER:OG	2.34	0.40
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	2.03	0.40
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.56	0.40
1:A:1100:ILE:O	1:A:1105:MET:HE3	2.22	0.40
2:B:319:GLN:O	2:B:320:TRP:CB	2.70	0.40
1:C:364:VAL:HG22	1:C:376:VAL:HG22	2.02	0.40
1:C:1057:ARG:HD2	1:C:1108:VAL:O	2.21	0.40
2:D:238:LEU:N	2:D:238:LEU:HD22	2.36	0.40
1:E:372:GLN:HA	1:E:373:GLY:HA2	1.51	0.40
1:E:719:GLU:HG3	1:E:755:SER:HB2	2.03	0.40
1:E:794:ILE:HD12	1:E:794:ILE:HG21	1.76	0.40
2:F:119:TRP:CZ2	2:F:401:ASN:ND2	2.90	0.40
2:F:157:GLY:HA2	2:F:178:GLU:HG3	2.03	0.40
2:F:177:MET:HG3	2:F:203:TRP:CE2	2.56	0.40
2:F:358:ASP:HA	2:F:359:PRO:HD2	1.86	0.40
1:A:114:ARG:O	1:A:114:ARG:HG2	2.21	0.40
1:A:665:LYS:HZ1	1:A:1020:THR:H	1.64	0.40
1:A:770:LEU:H	1:A:770:LEU:CD1	2.30	0.40
1:A:789:HIS:CD2	2:B:71:ARG:NH2	2.90	0.40
1:A:875:GLU:C	1:A:875:GLU:CD	2.89	0.40
1:A:968:ALA:HA	1:A:973:ASN:O	2.21	0.40
2:B:371:THR:OG1	2:B:385:GLN:HB3	2.22	0.40
1:C:272:LEU:O	1:C:273:LEU:HD23	2.22	0.40
1:C:534:MET:HE3	1:C:560:LEU:HD11	2.03	0.40
2:D:105:GLN:O	2:D:106:LYS:CB	2.69	0.40
2:D:140:ASN:ND2	2:D:140:ASN:C	2.80	0.40
1:E:800:GLU:OE1	1:E:801:VAL:N	2.55	0.40
2:F:182:ARG:NH2	2:F:184:GLN:HE22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1138/1158 (98%)	953 (84%)	130 (11%)	55 (5%)	2	12
1	C	1138/1158 (98%)	944 (83%)	135 (12%)	59 (5%)	1	11
1	E	1138/1158 (98%)	949 (83%)	131 (12%)	58 (5%)	1	11
2	B	366/436 (84%)	303 (83%)	39 (11%)	24 (7%)	1	7
2	D	366/436 (84%)	303 (83%)	40 (11%)	23 (6%)	1	8
2	F	366/436 (84%)	308 (84%)	35 (10%)	23 (6%)	1	8
All	All	4512/4782 (94%)	3760 (83%)	510 (11%)	242 (5%)	1	10

All (242) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	26	ALA
1	A	204	LYS
1	A	243	ASP
1	A	381	ALA
1	A	464	ALA
1	A	483	PRO
1	A	674	LYS
1	A	797	HIS
1	A	838	PRO
1	A	891	TYR
1	A	928	ARG
1	A	929	SER
1	A	952	ASN
2	B	58	ALA
2	B	63	LEU
2	B	102	ARG
2	B	106	LYS
2	B	209	VAL
2	B	278	LYS

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Mol	Chain	Res	Type
2	B	281	PHE
2	B	332	ARG
1	C	2	SER
1	C	26	ALA
1	C	204	LYS
1	C	243	ASP
1	C	382	PHE
1	C	383	LYS
1	C	464	ALA
1	C	483	PRO
1	C	674	LYS
1	C	797	HIS
1	C	838	PRO
1	C	891	TYR
1	C	928	ARG
1	C	929	SER
1	C	952	ASN
2	D	58	ALA
2	D	63	LEU
2	D	102	ARG
2	D	106	LYS
2	D	278	LYS
2	D	281	PHE
2	D	332	ARG
1	E	2	SER
1	E	26	ALA
1	E	204	LYS
1	E	243	ASP
1	E	381	ALA
1	E	382	PHE
1	E	464	ALA
1	E	483	PRO
1	E	674	LYS
1	E	797	HIS
1	E	838	PRO
1	E	891	TYR
1	E	928	ARG
1	E	929	SER
1	E	952	ASN
2	F	58	ALA
2	F	63	LEU
2	F	102	ARG

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Mol	Chain	Res	Type
2	F	106	LYS
2	F	278	LYS
2	F	281	PHE
2	F	332	ARG
1	A	36	ASN
1	A	291	MET
1	A	513	GLY
1	A	784	GLU
1	A	811	GLU
1	A	824	ASP
1	A	825	PRO
1	A	835	MET
1	A	839	GLU
1	A	980	ASP
1	A	1006	VAL
2	B	57	LEU
2	B	109	PRO
2	B	113	ARG
2	B	155	ALA
2	B	188	GLY
2	B	237	ASN
2	B	277	GLY
2	B	320	TRP
1	C	36	ASN
1	C	291	MET
1	C	293	GLY
1	C	381	ALA
1	C	385	GLY
1	C	513	GLY
1	C	748	GLY
1	C	784	GLU
1	C	811	GLU
1	C	824	ASP
1	C	825	PRO
1	C	835	MET
1	C	839	GLU
1	C	950	ASN
1	C	980	ASP
1	C	1006	VAL
2	D	57	LEU
2	D	109	PRO
2	D	113	ARG

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Mol	Chain	Res	Type
2	D	155	ALA
2	D	188	GLY
2	D	237	ASN
2	D	277	GLY
1	E	36	ASN
1	E	291	MET
1	E	293	GLY
1	E	513	GLY
1	E	784	GLU
1	E	811	GLU
1	E	824	ASP
1	E	825	PRO
1	E	835	MET
1	E	839	GLU
1	E	870	VAL
1	E	980	ASP
1	E	1006	VAL
2	F	57	LEU
2	F	109	PRO
2	F	113	ARG
2	F	155	ALA
2	F	188	GLY
2	F	237	ASN
2	F	277	GLY
1	A	578	HIS
1	A	710	LEU
1	A	746	SER
1	A	748	GLY
1	A	753	ARG
1	A	782	PHE
1	A	798	THR
1	A	815	SER
1	A	870	VAL
1	A	950	ASN
2	B	299	ASP
2	B	302	ARG
1	C	276	MET
1	C	578	HIS
1	C	746	SER
1	C	753	ARG
1	C	782	PHE
1	C	815	SER

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Mol	Chain	Res	Type
1	C	870	VAL
2	D	299	ASP
2	D	302	ARG
2	D	320	TRP
1	E	578	HIS
1	E	748	GLY
1	E	753	ARG
1	E	782	PHE
1	E	815	SER
1	E	950	ASN
1	E	1085	ALA
2	F	299	ASP
2	F	320	TRP
1	A	11	LYS
1	A	235	GLU
1	A	276	MET
1	A	341	ASN
1	A	576	LEU
1	A	750	THR
1	A	962	ASP
1	A	985	THR
1	A	1085	ALA
2	B	255	ASP
1	C	209	GLN
1	C	235	GLU
1	C	341	ASN
1	C	576	LEU
1	C	750	THR
1	C	798	THR
1	C	962	ASP
1	C	985	THR
1	C	1085	ALA
2	D	255	ASP
2	D	335	GLN
1	E	235	GLU
1	E	276	MET
1	E	341	ASN
1	E	576	LEU
1	E	746	SER
1	E	750	THR
1	E	798	THR
1	E	985	THR

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Mol	Chain	Res	Type
2	F	255	ASP
2	F	302	ARG
1	A	209	GLN
1	A	370	GLN
1	A	1022	THR
1	A	1062	ILE
1	A	1066	GLY
2	B	65	PRO
2	B	67	ARG
2	B	335	GLN
2	B	412	GLY
1	C	11	LYS
1	C	359	ILE
1	C	370	GLN
1	C	643	SER
1	C	1022	THR
1	C	1062	ILE
1	C	1066	GLY
2	D	65	PRO
1	E	11	LYS
1	E	209	GLN
1	E	359	ILE
1	E	643	SER
1	E	1022	THR
1	E	1062	ILE
2	F	65	PRO
2	F	67	ARG
2	F	335	GLN
1	A	359	ILE
2	D	67	ARG
2	D	412	GLY
1	E	370	GLN
1	E	962	ASP
1	E	1066	GLY
2	F	412	GLY
1	A	777	PRO
1	C	777	PRO
1	E	1018	GLY
2	B	146	LYS
1	C	1018	GLY
1	E	440	GLY
1	E	777	PRO

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Mol	Chain	Res	Type
1	A	440	GLY
1	A	1018	GLY
1	A	1065	VAL
1	C	1065	VAL
2	D	146	LYS
1	E	721	PRO
1	E	1065	VAL
2	F	146	LYS
1	E	564	ILE
1	A	564	ILE
1	C	564	ILE
1	C	801	VAL

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	984/1014 (97%)	852 (87%)	132 (13%)	4	16
1	C	984/1014 (97%)	860 (87%)	124 (13%)	4	18
1	E	984/1014 (97%)	857 (87%)	127 (13%)	4	17
2	B	315/378 (83%)	261 (83%)	54 (17%)	2	10
2	D	315/378 (83%)	265 (84%)	50 (16%)	2	12
2	F	315/378 (83%)	266 (84%)	49 (16%)	2	12
All	All	3897/4176 (93%)	3361 (86%)	536 (14%)	3	15

All (536) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	27	GLU
1	A	45	THR
1	A	47	GLU
1	A	70	LYS
1	A	111	ARG

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Mol	Chain	Res	Type
1	A	112	ILE
1	A	114	ARG
1	A	118	THR
1	A	133	LEU
1	A	151	GLU
1	A	159	LEU
1	A	160	GLU
1	A	162	LEU
1	A	168	LYS
1	A	174	GLN
1	A	210	GLU
1	A	213	GLU
1	A	218	MET
1	A	236	SER
1	A	269	SER
1	A	277	GLU
1	A	284	LEU
1	A	290	GLN
1	A	291	MET
1	A	302	VAL
1	A	304	LEU
1	A	307	GLU
1	A	312	GLU
1	A	314	LEU
1	A	338	VAL
1	A	342	GLU
1	A	354	THR
1	A	365	VAL
1	A	372	GLN
1	A	375	LEU
1	A	382	PHE
1	A	383	LYS
1	A	413	LEU
1	A	415	SER
1	A	419	ARG
1	A	427	LEU
1	A	434	ARG
1	A	443	VAL
1	A	446	THR
1	A	449	MET
1	A	463	VAL
1	A	468	LEU

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Mol	Chain	Res	Type
1	A	487	VAL
1	A	519	LEU
1	A	529	ILE
1	A	562	THR
1	A	571	LEU
1	A	589	ARG
1	A	592	LEU
1	A	598	SER
1	A	618	ILE
1	A	631	LEU
1	A	633	THR
1	A	640	THR
1	A	641	PHE
1	A	648	ASN
1	A	658	VAL
1	A	666	LEU
1	A	669	SER
1	A	673	LEU
1	A	679	MET
1	A	698	THR
1	A	701	ILE
1	A	710	LEU
1	A	712	ILE
1	A	724	ILE
1	A	728	GLU
1	A	731	GLN
1	A	752	LEU
1	A	758	THR
1	A	770	LEU
1	A	773	SER
1	A	786	VAL
1	A	789	HIS
1	A	790	ASN
1	A	792	LEU
1	A	794	ILE
1	A	799	PHE
1	A	800	GLU
1	A	802	LEU
1	A	803	HIS
1	A	810	ASN
1	A	812	TYR
1	A	814	LEU

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Mol	Chain	Res	Type
1	A	817	VAL
1	A	819	CYS
1	A	820	LYS
1	A	821	LEU
1	A	823	LYS
1	A	826	ASN
1	A	833	THR
1	A	850	VAL
1	A	858	LEU
1	A	870	VAL
1	A	890	LEU
1	A	894	THR
1	A	895	THR
1	A	901	THR
1	A	915	LYS
1	A	922	LEU
1	A	927	MET
1	A	928	ARG
1	A	930	VAL
1	A	931	LEU
1	A	950	ASN
1	A	954	MET
1	A	957	VAL
1	A	962	ASP
1	A	966	LEU
1	A	969	GLU
1	A	978	GLN
1	A	984	THR
1	A	1000	LEU
1	A	1012	LEU
1	A	1014	MET
1	A	1022	THR
1	A	1039	LEU
1	A	1040	VAL
1	A	1041	THR
1	A	1052	LEU
1	A	1065	VAL
1	A	1071	SER
1	A	1093	LEU
1	A	1121	LYS
1	A	1131	LYS
1	A	1132	VAL

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Mol	Chain	Res	Type
2	B	57	LEU
2	B	61	GLN
2	B	62	ILE
2	B	69	ILE
2	B	71	ARG
2	B	80	ARG
2	B	82	SER
2	B	87	GLN
2	B	110	PHE
2	B	117	LEU
2	B	125	SER
2	B	127	VAL
2	B	136	ILE
2	B	140	ASN
2	B	145	ASP
2	B	159	ILE
2	B	162	LEU
2	B	182	ARG
2	B	191	LEU
2	B	198	ASP
2	B	207	LEU
2	B	209	VAL
2	B	217	VAL
2	B	218	THR
2	B	221	ASN
2	B	236	TRP
2	B	238	LEU
2	B	258	LEU
2	B	260	THR
2	B	272	LEU
2	B	273	ARG
2	B	276	ARG
2	B	278	LYS
2	B	280	SER
2	B	285	LEU
2	B	288	ARG
2	B	299	ASP
2	B	305	THR
2	B	310	SER
2	B	313	ARG
2	B	324	LEU
2	B	326	LEU

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Mol	Chain	Res	Type
2	B	336	HIS
2	B	337	LEU
2	B	340	ILE
2	B	352	VAL
2	B	353	VAL
2	B	371	THR
2	B	379	SER
2	B	381	LYS
2	B	382	MET
2	B	385	GLN
2	B	401	ASN
2	B	411	MET
1	C	6	VAL
1	C	27	GLU
1	C	45	THR
1	C	47	GLU
1	C	54	GLU
1	C	70	LYS
1	C	111	ARG
1	C	112	ILE
1	C	114	ARG
1	C	118	THR
1	C	133	LEU
1	C	159	LEU
1	C	160	GLU
1	C	162	LEU
1	C	168	LYS
1	C	174	GLN
1	C	210	GLU
1	C	213	GLU
1	C	218	MET
1	C	236	SER
1	C	277	GLU
1	C	284	LEU
1	C	302	VAL
1	C	304	LEU
1	C	307	GLU
1	C	312	GLU
1	C	314	LEU
1	C	338	VAL
1	C	342	GLU
1	C	354	THR

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Mol	Chain	Res	Type
1	C	372	GLN
1	C	375	LEU
1	C	382	PHE
1	C	383	LYS
1	C	413	LEU
1	C	415	SER
1	C	419	ARG
1	C	427	LEU
1	C	434	ARG
1	C	443	VAL
1	C	446	THR
1	C	449	MET
1	C	463	VAL
1	C	468	LEU
1	C	487	VAL
1	C	519	LEU
1	C	529	ILE
1	C	562	THR
1	C	571	LEU
1	C	589	ARG
1	C	592	LEU
1	C	598	SER
1	C	599	SER
1	C	618	ILE
1	C	631	LEU
1	C	633	THR
1	C	648	ASN
1	C	658	VAL
1	C	666	LEU
1	C	669	SER
1	C	673	LEU
1	C	679	MET
1	C	698	THR
1	C	701	ILE
1	C	712	ILE
1	C	724	ILE
1	C	728	GLU
1	C	731	GLN
1	C	752	LEU
1	C	758	THR
1	C	770	LEU
1	C	773	SER

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Mol	Chain	Res	Type
1	C	786	VAL
1	C	789	HIS
1	C	790	ASN
1	C	791	LEU
1	C	792	LEU
1	C	794	ILE
1	C	799	PHE
1	C	800	GLU
1	C	802	LEU
1	C	803	HIS
1	C	810	ASN
1	C	812	TYR
1	C	814	LEU
1	C	817	VAL
1	C	820	LYS
1	C	821	LEU
1	C	823	LYS
1	C	826	ASN
1	C	833	THR
1	C	845	GLN
1	C	850	VAL
1	C	858	LEU
1	C	870	VAL
1	C	890	LEU
1	C	894	THR
1	C	895	THR
1	C	901	THR
1	C	915	LYS
1	C	922	LEU
1	C	950	ASN
1	C	954	MET
1	C	957	VAL
1	C	962	ASP
1	C	966	LEU
1	C	969	GLU
1	C	978	GLN
1	C	984	THR
1	C	1000	LEU
1	C	1013	VAL
1	C	1014	MET
1	C	1022	THR
1	C	1039	LEU

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Mol	Chain	Res	Type
1	C	1040	VAL
1	C	1041	THR
1	C	1052	LEU
1	C	1065	VAL
1	C	1071	SER
1	C	1093	LEU
1	C	1121	LYS
1	C	1131	LYS
1	C	1132	VAL
1	C	1137	THR
2	D	57	LEU
2	D	61	GLN
2	D	62	ILE
2	D	69	ILE
2	D	71	ARG
2	D	80	ARG
2	D	87	GLN
2	D	110	PHE
2	D	117	LEU
2	D	125	SER
2	D	127	VAL
2	D	136	ILE
2	D	140	ASN
2	D	145	ASP
2	D	159	ILE
2	D	162	LEU
2	D	182	ARG
2	D	191	LEU
2	D	198	ASP
2	D	217	VAL
2	D	218	THR
2	D	221	ASN
2	D	236	TRP
2	D	238	LEU
2	D	258	LEU
2	D	260	THR
2	D	272	LEU
2	D	273	ARG
2	D	276	ARG
2	D	278	LYS
2	D	280	SER
2	D	285	LEU

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Mol	Chain	Res	Type
2	D	288	ARG
2	D	299	ASP
2	D	305	THR
2	D	310	SER
2	D	313	ARG
2	D	324	LEU
2	D	326	LEU
2	D	336	HIS
2	D	337	LEU
2	D	340	ILE
2	D	352	VAL
2	D	353	VAL
2	D	371	THR
2	D	379	SER
2	D	381	LYS
2	D	385	GLN
2	D	401	ASN
2	D	411	MET
1	E	6	VAL
1	E	27	GLU
1	E	45	THR
1	E	47	GLU
1	E	70	LYS
1	E	111	ARG
1	E	112	ILE
1	E	114	ARG
1	E	118	THR
1	E	133	LEU
1	E	159	LEU
1	E	160	GLU
1	E	162	LEU
1	E	168	LYS
1	E	174	GLN
1	E	210	GLU
1	E	213	GLU
1	E	218	MET
1	E	236	SER
1	E	269	SER
1	E	270	ARG
1	E	277	GLU
1	E	284	LEU
1	E	302	VAL

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Mol	Chain	Res	Type
1	E	304	LEU
1	E	307	GLU
1	E	312	GLU
1	E	314	LEU
1	E	338	VAL
1	E	342	GLU
1	E	354	THR
1	E	372	GLN
1	E	375	LEU
1	E	382	PHE
1	E	383	LYS
1	E	413	LEU
1	E	415	SER
1	E	419	ARG
1	E	427	LEU
1	E	434	ARG
1	E	443	VAL
1	E	446	THR
1	E	449	MET
1	E	463	VAL
1	E	468	LEU
1	E	487	VAL
1	E	519	LEU
1	E	529	ILE
1	E	562	THR
1	E	571	LEU
1	E	589	ARG
1	E	592	LEU
1	E	598	SER
1	E	599	SER
1	E	618	ILE
1	E	631	LEU
1	E	633	THR
1	E	648	ASN
1	E	658	VAL
1	E	666	LEU
1	E	669	SER
1	E	673	LEU
1	E	679	MET
1	E	698	THR
1	E	701	ILE
1	E	712	ILE

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Mol	Chain	Res	Type
1	E	724	ILE
1	E	728	GLU
1	E	731	GLN
1	E	752	LEU
1	E	758	THR
1	E	770	LEU
1	E	773	SER
1	E	775	THR
1	E	786	VAL
1	E	789	HIS
1	E	790	ASN
1	E	791	LEU
1	E	792	LEU
1	E	794	ILE
1	E	799	PHE
1	E	800	GLU
1	E	803	HIS
1	E	810	ASN
1	E	812	TYR
1	E	814	LEU
1	E	817	VAL
1	E	819	CYS
1	E	820	LYS
1	E	821	LEU
1	E	823	LYS
1	E	826	ASN
1	E	833	THR
1	E	842	GLU
1	E	845	GLN
1	E	850	VAL
1	E	858	LEU
1	E	870	VAL
1	E	886	SER
1	E	890	LEU
1	E	894	THR
1	E	895	THR
1	E	901	THR
1	E	915	LYS
1	E	922	LEU
1	E	950	ASN
1	E	954	MET
1	E	957	VAL

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Mol	Chain	Res	Type
1	E	962	ASP
1	E	966	LEU
1	E	969	GLU
1	E	978	GLN
1	E	984	THR
1	E	1000	LEU
1	E	1012	LEU
1	E	1013	VAL
1	E	1014	MET
1	E	1022	THR
1	E	1039	LEU
1	E	1040	VAL
1	E	1041	THR
1	E	1052	LEU
1	E	1065	VAL
1	E	1071	SER
1	E	1093	LEU
1	E	1121	LYS
1	E	1131	LYS
2	F	57	LEU
2	F	61	GLN
2	F	62	ILE
2	F	69	ILE
2	F	71	ARG
2	F	80	ARG
2	F	87	GLN
2	F	110	PHE
2	F	117	LEU
2	F	125	SER
2	F	127	VAL
2	F	136	ILE
2	F	140	ASN
2	F	145	ASP
2	F	162	LEU
2	F	182	ARG
2	F	191	LEU
2	F	198	ASP
2	F	217	VAL
2	F	218	THR
2	F	221	ASN
2	F	236	TRP
2	F	238	LEU

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Mol	Chain	Res	Type
2	F	258	LEU
2	F	260	THR
2	F	272	LEU
2	F	273	ARG
2	F	276	ARG
2	F	278	LYS
2	F	280	SER
2	F	285	LEU
2	F	299	ASP
2	F	305	THR
2	F	310	SER
2	F	313	ARG
2	F	324	LEU
2	F	326	LEU
2	F	336	HIS
2	F	337	LEU
2	F	340	ILE
2	F	352	VAL
2	F	353	VAL
2	F	371	THR
2	F	379	SER
2	F	381	LYS
2	F	382	MET
2	F	385	GLN
2	F	401	ASN
2	F	411	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	22	HIS
1	A	30	ASN
1	A	105	HIS
1	A	109	GLN
1	A	156	ASN
1	A	255	GLN
1	A	262	ASN
1	A	290	GLN
1	A	341	ASN
1	A	355	ASN
1	A	370	GLN

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Mol	Chain	Res	Type
1	A	374	GLN
1	A	397	HIS
1	A	439	ASN
1	A	462	ASN
1	A	465	HIS
1	A	467	GLN
1	A	470	GLN
1	A	497	ASN
1	A	504	ASN
1	A	520	GLN
1	A	522	HIS
1	A	528	GLN
1	A	617	ASN
1	A	677	ASN
1	A	727	GLN
1	A	731	GLN
1	A	789	HIS
1	A	790	ASN
1	A	796	GLN
1	A	845	GLN
1	A	877	ASN
1	A	885	ASN
1	A	904	ASN
1	A	950	ASN
1	A	964	ASN
1	A	999	HIS
1	A	1025	GLN
1	A	1034	ASN
1	A	1049	ASN
1	A	1070	HIS
1	A	1113	GLN
1	A	1140	HIS
2	B	74	HIS
2	B	92	GLN
2	B	140	ASN
2	B	184	GLN
2	B	221	ASN
2	B	237	ASN
2	B	247	HIS
2	B	251	ASN
2	B	287	HIS
2	B	289	HIS

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Mol	Chain	Res	Type
2	B	333	HIS
2	B	335	GLN
2	B	345	HIS
2	B	349	ASN
2	B	385	GLN
2	B	401	ASN
2	B	414	HIS
2	B	420	GLN
1	C	16	ASN
1	C	22	HIS
1	C	30	ASN
1	C	105	HIS
1	C	109	GLN
1	C	156	ASN
1	C	262	ASN
1	C	290	GLN
1	C	341	ASN
1	C	355	ASN
1	C	370	GLN
1	C	372	GLN
1	C	374	GLN
1	C	397	HIS
1	C	439	ASN
1	C	462	ASN
1	C	465	HIS
1	C	470	GLN
1	C	504	ASN
1	C	520	GLN
1	C	522	HIS
1	C	528	GLN
1	C	617	ASN
1	C	677	ASN
1	C	727	GLN
1	C	731	GLN
1	C	789	HIS
1	C	796	GLN
1	C	845	GLN
1	C	877	ASN
1	C	885	ASN
1	C	904	ASN
1	C	950	ASN
1	C	964	ASN

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Mol	Chain	Res	Type
1	C	978	GLN
1	C	999	HIS
1	C	1009	HIS
1	C	1034	ASN
1	C	1049	ASN
1	C	1070	HIS
1	C	1113	GLN
2	D	87	GLN
2	D	92	GLN
2	D	140	ASN
2	D	184	GLN
2	D	221	ASN
2	D	224	ASN
2	D	237	ASN
2	D	247	HIS
2	D	251	ASN
2	D	287	HIS
2	D	289	HIS
2	D	333	HIS
2	D	335	GLN
2	D	345	HIS
2	D	349	ASN
2	D	385	GLN
2	D	401	ASN
2	D	414	HIS
2	D	420	GLN
1	E	16	ASN
1	E	22	HIS
1	E	30	ASN
1	E	105	HIS
1	E	109	GLN
1	E	156	ASN
1	E	262	ASN
1	E	267	ASN
1	E	290	GLN
1	E	341	ASN
1	E	355	ASN
1	E	370	GLN
1	E	372	GLN
1	E	374	GLN
1	E	397	HIS
1	E	439	ASN

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Mol	Chain	Res	Type
1	E	462	ASN
1	E	465	HIS
1	E	467	GLN
1	E	470	GLN
1	E	504	ASN
1	E	520	GLN
1	E	522	HIS
1	E	528	GLN
1	E	617	ASN
1	E	727	GLN
1	E	731	GLN
1	E	789	HIS
1	E	790	ASN
1	E	796	GLN
1	E	845	GLN
1	E	877	ASN
1	E	885	ASN
1	E	904	ASN
1	E	950	ASN
1	E	964	ASN
1	E	999	HIS
1	E	1009	HIS
1	E	1034	ASN
1	E	1049	ASN
1	E	1070	HIS
1	E	1113	GLN
1	E	1140	HIS
2	F	87	GLN
2	F	92	GLN
2	F	123	HIS
2	F	140	ASN
2	F	184	GLN
2	F	221	ASN
2	F	237	ASN
2	F	247	HIS
2	F	251	ASN
2	F	287	HIS
2	F	289	HIS
2	F	319	GLN
2	F	333	HIS
2	F	335	GLN
2	F	345	HIS

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Mol	Chain	Res	Type
2	F	349	ASN
2	F	401	ASN
2	F	414	HIS
2	F	420	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1140/1158 (98%)	0.93	100 (8%)	15 12	23, 63, 97, 120	0
1	C	1140/1158 (98%)	0.97	117 (10%)	12 10	23, 63, 95, 120	0
1	E	1140/1158 (98%)	0.95	108 (9%)	14 11	22, 64, 96, 120	0
2	B	368/436 (84%)	0.91	40 (10%)	10 9	24, 55, 86, 141	0
2	D	368/436 (84%)	0.66	21 (5%)	29 20	24, 55, 88, 136	0
2	F	368/436 (84%)	0.75	22 (5%)	27 19	25, 56, 85, 139	0
All	All	4524/4782 (94%)	0.91	408 (9%)	15 11	22, 62, 94, 141	0

All (408) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	58	ALA	6.7
1	C	566	ALA	5.5
1	C	548	ASP	5.0
1	A	547	GLY	4.6
1	C	1121	LYS	4.5
1	C	1108	VAL	4.5
1	A	439	ASN	4.4
1	C	796	GLN	4.4
2	F	64	PRO	4.2
1	C	819	CYS	4.2
1	A	293	GLY	4.1
1	E	780	THR	4.0
2	D	58	ALA	4.0
1	C	550	ASN	4.0
1	A	984	THR	4.0
2	F	199	THR	3.9
2	B	206	SER	3.8
2	F	63	LEU	3.8
2	F	55	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	618	ILE	3.7
2	B	103	ILE	3.7
1	A	856	GLY	3.7
1	C	781	SER	3.7
1	E	1019	GLU	3.6
2	F	58	ALA	3.6
2	B	391	SER	3.6
1	E	1020	THR	3.6
1	E	111	ARG	3.6
1	E	984	THR	3.6
1	C	1117	GLY	3.5
1	C	988	GLU	3.5
1	A	195	VAL	3.5
1	C	803	HIS	3.5
1	E	112	ILE	3.4
1	A	780	THR	3.4
1	C	58	TYR	3.4
1	E	1120	MET	3.4
1	E	146	ASP	3.4
1	C	207	TRP	3.4
1	E	781	SER	3.4
1	C	571	LEU	3.4
1	E	114	ARG	3.3
1	E	372	GLN	3.3
1	C	774	SER	3.3
1	C	547	GLY	3.3
1	E	548	ASP	3.3
1	E	292	ASP	3.3
1	A	146	ASP	3.3
1	C	1138	ARG	3.3
2	D	64	PRO	3.3
1	C	790	ASN	3.3
1	A	775	THR	3.2
1	A	381	ALA	3.2
1	A	983	ALA	3.2
2	D	59	GLY	3.2
1	E	1103	PRO	3.2
1	E	534	MET	3.2
2	F	192	ARG	3.2
1	C	935	TYR	3.2
1	C	146	ASP	3.2
1	C	422	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	780	THR	3.2
1	E	1121	LYS	3.1
2	B	379	SER	3.1
1	A	566	ALA	3.1
1	A	1126	ALA	3.1
1	E	381	ALA	3.1
1	A	1136	LEU	3.1
1	A	748	GLY	3.1
1	E	662	SER	3.1
1	E	710	LEU	3.1
1	C	760	ALA	3.1
1	A	766	SER	3.1
1	E	803	HIS	3.0
1	E	535	GLU	3.0
1	E	766	SER	3.0
2	B	54	TRP	3.0
1	C	112	ILE	3.0
1	C	775	THR	3.0
1	C	773	SER	3.0
1	A	855	ASP	3.0
1	C	1136	LEU	3.0
1	E	571	LEU	3.0
1	C	341	ASN	3.0
1	C	551	GLY	3.0
2	F	156	GLY	3.0
1	E	985	THR	3.0
1	E	796	GLN	3.0
2	D	103	ILE	3.0
2	D	333	HIS	3.0
1	A	112	ILE	3.0
1	A	803	HIS	2.9
1	E	290	GLN	2.9
1	A	1137	THR	2.9
1	C	582	LEU	2.9
2	D	55	VAL	2.9
2	B	62	ILE	2.9
1	E	162	LEU	2.9
2	B	279	ALA	2.9
2	D	279	ALA	2.9
1	E	561	TRP	2.9
1	C	1054	MET	2.9
1	E	202	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	291	MET	2.9
1	C	769	LYS	2.9
1	C	1021	SER	2.8
1	E	1115	ASP	2.8
1	A	1134	GLU	2.8
1	A	773	SER	2.8
1	E	983	ALA	2.8
1	A	782	PHE	2.8
1	E	783	GLY	2.8
1	E	772	SER	2.8
1	E	703	THR	2.8
2	F	66	CYS	2.8
1	A	1013	VAL	2.8
1	E	582	LEU	2.8
1	E	207	TRP	2.8
1	A	1133	VAL	2.8
1	C	662	SER	2.8
1	A	562	THR	2.8
1	C	985	THR	2.8
1	E	566	ALA	2.7
1	E	1126	ALA	2.7
2	B	278	LYS	2.7
2	B	335	GLN	2.7
2	B	366	PRO	2.7
1	C	1	MET	2.7
1	E	563	ASP	2.7
2	B	367	TYR	2.7
1	A	802	LEU	2.7
2	B	65	PRO	2.7
2	B	102	ARG	2.7
1	A	374	GLN	2.7
1	A	796	GLN	2.7
1	A	779	GLU	2.7
1	C	702	GLY	2.7
1	E	1119	GLY	2.7
1	C	549	SER	2.7
1	E	422	TYR	2.7
1	E	1111	ASN	2.7
1	A	532	THR	2.7
1	C	296	THR	2.7
1	E	117	GLU	2.6
1	A	929	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	2	SER	2.6
1	E	164	VAL	2.6
1	E	226	PHE	2.6
1	A	583	GLY	2.6
1	E	233	GLY	2.6
1	E	577	LEU	2.6
2	B	57	LEU	2.6
2	B	63	LEU	2.6
2	F	278	LYS	2.6
1	E	782	PHE	2.6
2	D	60	PRO	2.6
2	D	65	PRO	2.6
1	E	439	ASN	2.6
2	B	216	VAL	2.6
1	A	2	SER	2.6
1	A	292	ASP	2.6
1	E	1113	GLN	2.6
1	A	203	ASN	2.6
1	A	896	GLU	2.6
1	E	644	LEU	2.6
2	B	104	LEU	2.6
1	C	1110	ALA	2.6
2	F	112	ARG	2.6
1	A	812	TYR	2.6
1	C	766	SER	2.6
2	F	65	PRO	2.6
2	B	157	GLY	2.6
1	A	1131	LYS	2.6
1	A	13	THR	2.6
1	C	984	THR	2.6
1	C	884	ILE	2.5
1	E	641	PHE	2.5
1	C	583	GLY	2.5
2	B	105	GLN	2.5
1	E	369	ARG	2.5
2	B	200	ILE	2.5
1	A	422	TYR	2.5
2	B	205	CYS	2.5
1	E	549	SER	2.5
1	E	330	ASP	2.5
2	B	198	ASP	2.5
2	B	201	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	421	THR	2.5
1	A	797	HIS	2.5
2	F	60	PRO	2.5
1	E	623	LEU	2.5
1	C	1133	VAL	2.5
1	E	786	VAL	2.5
1	A	663	ASN	2.5
2	F	103	ILE	2.5
1	C	115	PRO	2.5
1	C	588	PRO	2.5
1	E	206	PRO	2.5
2	B	413	TYR	2.5
2	F	404	GLY	2.5
1	C	430	VAL	2.5
1	A	662	SER	2.5
1	C	684	SER	2.5
1	C	328	LEU	2.5
1	A	786	VAL	2.5
1	C	15	VAL	2.5
1	C	338	VAL	2.5
2	D	275	VAL	2.5
2	D	105	GLN	2.5
1	E	502	SER	2.4
2	D	200	ILE	2.4
1	A	330	ASP	2.4
1	A	1129	LEU	2.4
2	D	57	LEU	2.4
1	A	777	PRO	2.4
1	A	98	ILE	2.4
1	C	587	ILE	2.4
1	A	684	SER	2.4
1	C	441	GLU	2.4
1	E	379	SER	2.4
1	E	1104	LYS	2.4
1	A	356	LEU	2.4
1	A	761	LEU	2.4
1	C	438	LEU	2.4
1	E	37	THR	2.4
1	C	431	GLY	2.4
1	E	935	TYR	2.4
1	A	756	ALA	2.4
1	C	618	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1121	LYS	2.4
1	C	114	ARG	2.4
1	C	117	GLU	2.4
1	C	289	GLU	2.4
1	C	655	ARG	2.4
1	E	1067	LYS	2.4
1	E	288	GLU	2.4
1	C	818	SER	2.4
1	E	624	SER	2.4
1	E	338	VAL	2.4
1	C	1035	GLY	2.4
2	F	56	GLY	2.4
2	F	413	TYR	2.4
1	C	226	PHE	2.4
1	C	710	LEU	2.4
1	A	1020	THR	2.4
1	A	1108	VAL	2.4
1	E	778	HIS	2.4
1	A	114	ARG	2.4
1	C	372	GLN	2.4
1	E	767	SER	2.4
2	B	236	TRP	2.4
1	A	1117	GLY	2.3
2	B	56	GLY	2.3
2	F	336	HIS	2.3
1	A	369	ARG	2.3
1	E	453	ASP	2.3
2	B	101	TYR	2.3
1	E	1108	VAL	2.3
2	B	55	VAL	2.3
2	F	155	ALA	2.3
1	A	355	ASN	2.3
1	A	752	LEU	2.3
1	C	1045	GLU	2.3
1	A	749	THR	2.3
1	A	781	SER	2.3
1	C	178	ILE	2.3
1	E	794	ILE	2.3
1	E	446	THR	2.3
1	C	163	HIS	2.3
2	B	333	HIS	2.3
2	B	336	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	418	ASN	2.3
1	A	706	GLU	2.3
1	C	295	VAL	2.3
1	C	777	PRO	2.3
1	C	1084	PRO	2.3
1	C	205	GLY	2.3
1	C	786	VAL	2.3
1	E	195	VAL	2.3
1	A	250	PRO	2.3
1	C	721	PRO	2.3
1	C	686	GLY	2.3
1	C	1126	ALA	2.3
1	C	758	THR	2.3
2	B	392	SER	2.3
2	D	158	SER	2.3
2	D	413	TYR	2.3
1	E	663	ASN	2.3
1	E	877	ASN	2.3
1	C	292	ASP	2.3
1	E	618	ILE	2.2
1	A	1124	ALA	2.2
1	E	354	THR	2.2
1	E	382	PHE	2.2
2	D	206	SER	2.2
1	A	348	VAL	2.2
1	A	648	ASN	2.2
1	E	190	VAL	2.2
1	A	610	ALA	2.2
1	C	14	ALA	2.2
1	C	610	ALA	2.2
2	D	63	LEU	2.2
1	A	296	THR	2.2
1	C	208	LYS	2.2
1	E	1044	SER	2.2
1	E	1015	GLN	2.2
1	E	1107	GLU	2.2
2	B	421	GLU	2.2
1	A	710	LEU	2.2
1	E	275	ASP	2.2
1	C	225	PRO	2.2
1	C	483	PRO	2.2
1	E	1112	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	57	LEU	2.2
1	A	226	PHE	2.2
1	E	165	ILE	2.2
1	C	826	ASN	2.2
2	B	330	PRO	2.2
1	A	548	ASP	2.2
2	B	309	LYS	2.2
1	C	641	PHE	2.2
1	C	1020	THR	2.2
1	C	812	TYR	2.2
1	E	812	TYR	2.2
1	C	162	LEU	2.2
1	C	761	LEU	2.2
1	E	1	MET	2.2
1	E	216	ALA	2.2
1	E	550	ASN	2.2
1	C	572	PRO	2.2
2	D	56	GLY	2.2
2	B	418	TRP	2.2
1	A	1140	HIS	2.2
1	A	817	VAL	2.1
1	C	463	VAL	2.1
1	A	415	SER	2.1
1	C	605	ALA	2.1
1	A	111	ARG	2.1
1	A	1119	GLY	2.1
2	F	133	GLY	2.1
1	A	1122	ARG	2.1
1	A	1023	PRO	2.1
1	E	1023	PRO	2.1
2	B	133	GLY	2.1
1	C	382	PHE	2.1
1	E	1065	VAL	2.1
1	A	304	LEU	2.1
1	A	194	GLU	2.1
1	A	523	PRO	2.1
1	C	344	GLY	2.1
1	C	746	SER	2.1
1	C	322	VAL	2.1
1	C	823	LYS	2.1
1	A	577	LEU	2.1
1	E	197	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	938	MET	2.1
2	D	420	GLN	2.1
1	A	344	GLY	2.1
1	A	1001	GLY	2.1
1	C	440	GLY	2.1
2	B	277	GLY	2.1
1	C	554	PRO	2.1
1	A	815	SER	2.1
1	E	1063	LYS	2.1
1	C	297	LEU	2.1
1	C	148	ASP	2.1
1	A	1015	GLN	2.1
1	E	21	GLY	2.1
1	A	1123	GLU	2.1
1	C	612	PHE	2.1
1	C	785	GLU	2.1
1	E	777	PRO	2.1
1	A	347	VAL	2.0
1	C	1104	LYS	2.0
1	A	768	SER	2.0
1	C	379	SER	2.0
1	C	392	ASN	2.0
1	E	300	LEU	2.0
1	E	546	LEU	2.0
2	F	207	LEU	2.0
1	E	1140	HIS	2.0
2	B	66	CYS	2.0
2	D	66	CYS	2.0
1	A	1113	GLN	2.0
1	C	242	GLY	2.0
1	C	747	GLY	2.0
1	A	1084	PRO	2.0
2	F	204	PHE	2.0
1	E	194	GLU	2.0
1	A	295	VAL	2.0
1	C	858	LEU	2.0
1	C	981	SER	2.0
1	E	248	ILE	2.0
1	A	1	MET	2.0
1	E	58	TYR	2.0
1	A	227	GLY	2.0
1	A	329	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	380	GLY	2.0
1	E	940	GLY	2.0
1	E	1055	GLN	2.0
2	D	278	LYS	2.0
1	A	1079	GLU	2.0
1	C	111	ARG	2.0
1	C	443	VAL	2.0
1	E	160	GLU	2.0
1	E	201	GLU	2.0
1	E	360	VAL	2.0
2	B	207	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.