Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 11:51 PM EST

PDB ID	:	3EI4
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:

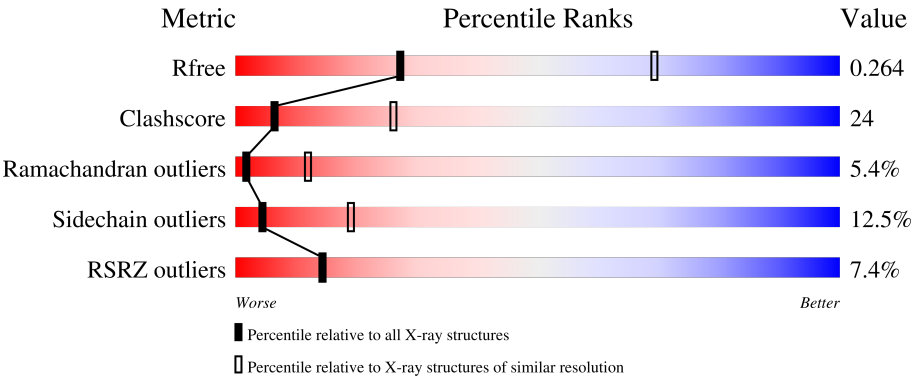
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1158	8% 55% 36% 7%
1	C	1158	7% 56% 36% 7%
1	E	1158	9% 54% 37% 6%
2	B	436	3% 38% 37% 8% 16%
2	D	436	4% 40% 34% 9% 16%

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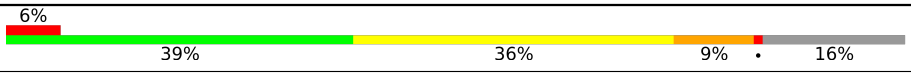
Mol	Chain	Length	Quality of chain
2	F	436	

2 Entry composition (i)

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	C	N	O	S	0	0	0
			2886	1841	513	515	17			
2	D	368	Total	C	N	O	S	0	0	0
			2886	1841	513	515	17			
2	F	368	Total	C	N	O	S	0	0	0
			2886	1841	513	515	17			

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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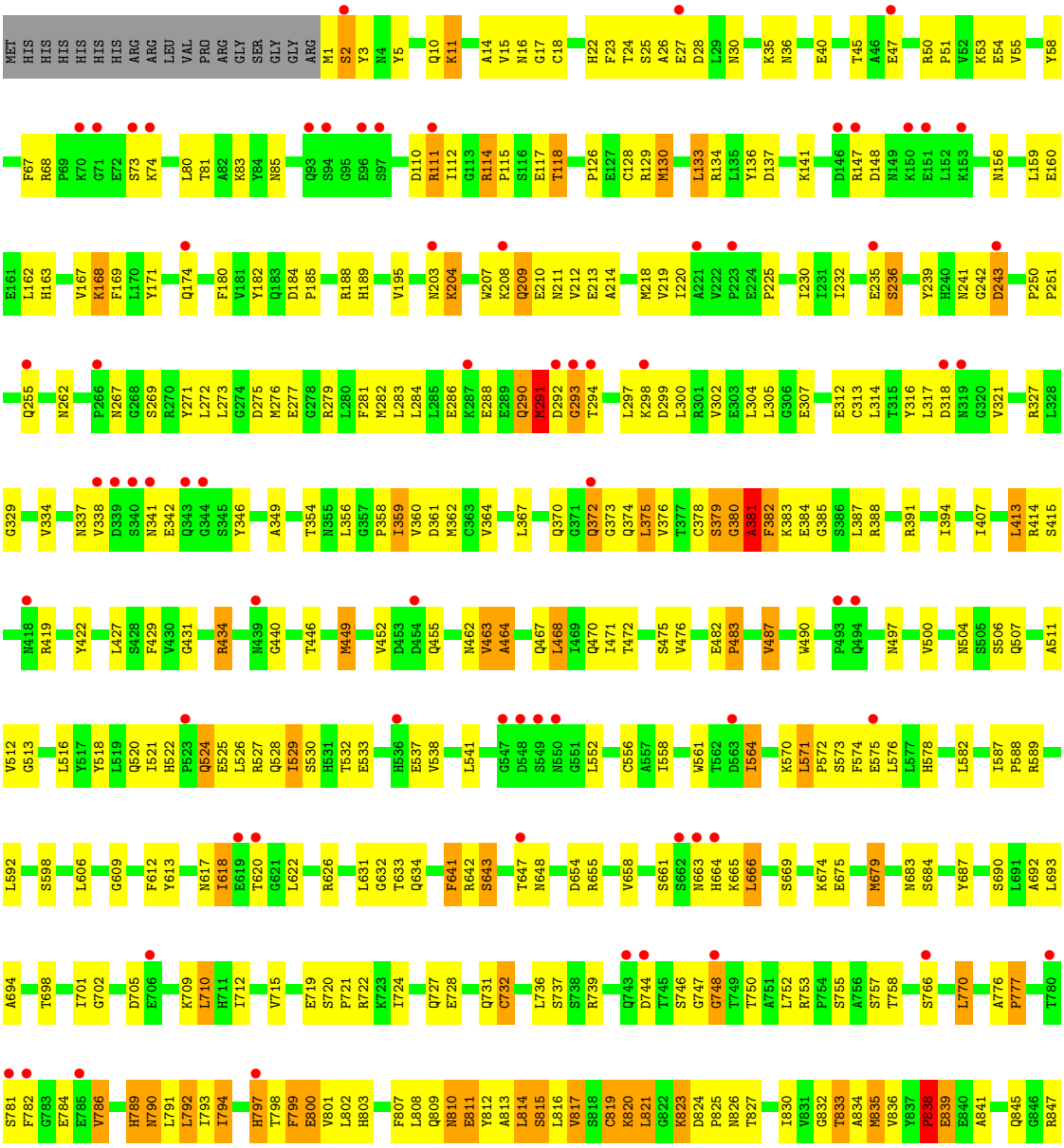
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	GLY	-	expression tag	UNP Q92466
D	8	GLY	-	expression tag	UNP Q92466
D	9	ARG	-	expression tag	UNP Q92466
F	-8	MET	-	expression tag	UNP Q92466
F	-7	HIS	-	expression tag	UNP Q92466
F	-6	HIS	-	expression tag	UNP Q92466
F	-5	HIS	-	expression tag	UNP Q92466
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

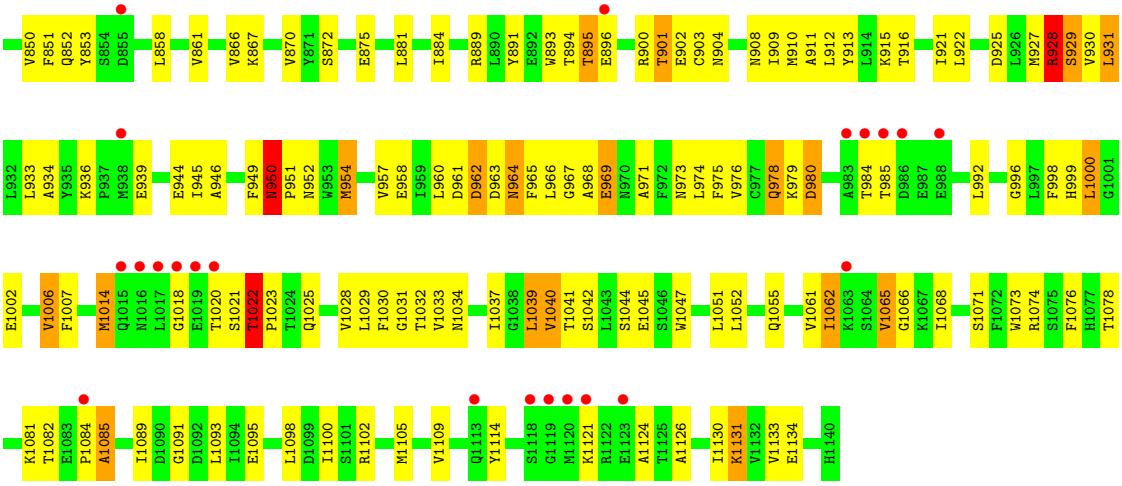
3 Residue-property plots (i)

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

• Molecule 1: DNA damage-binding protein 1

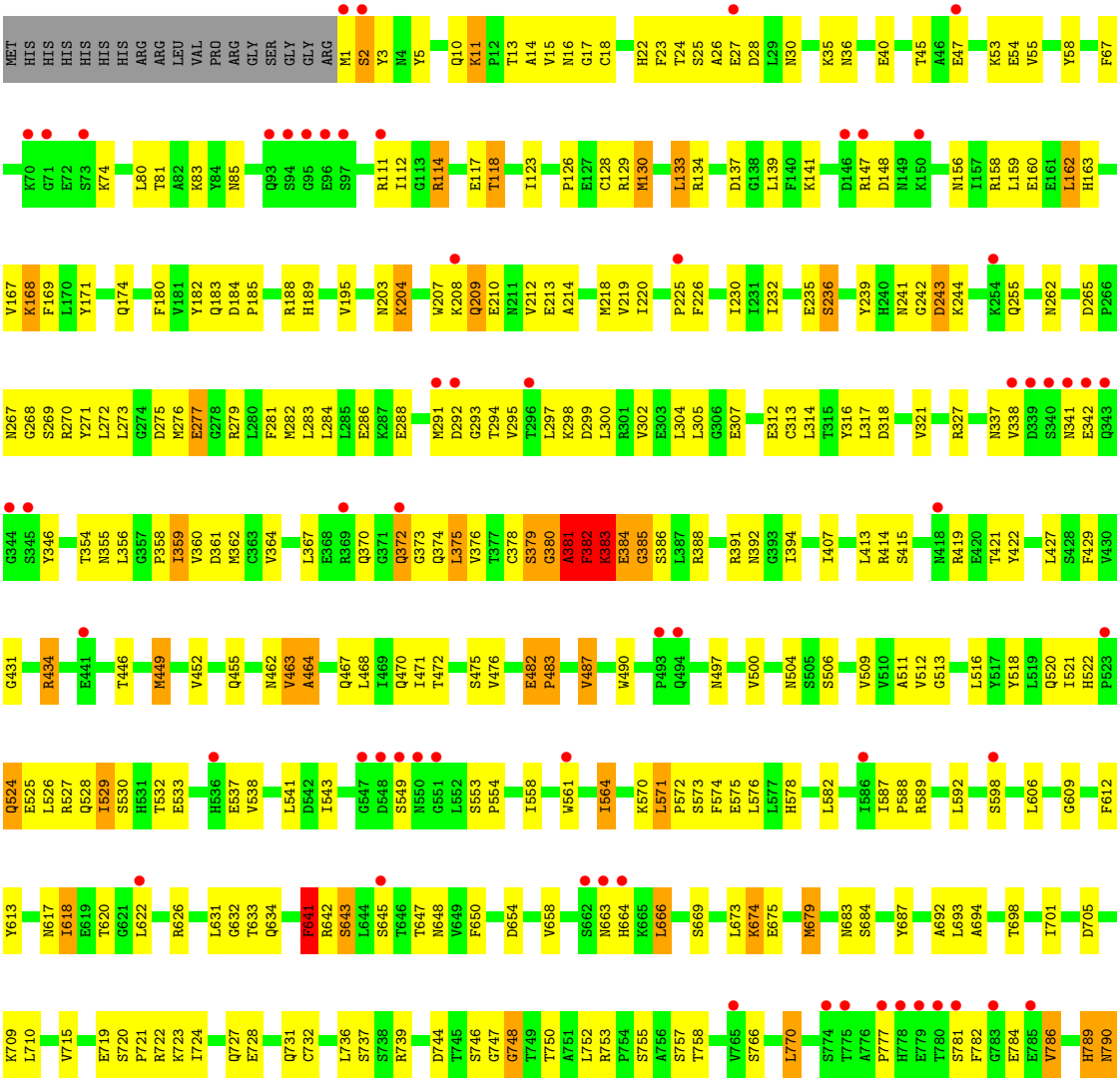
Chain A:

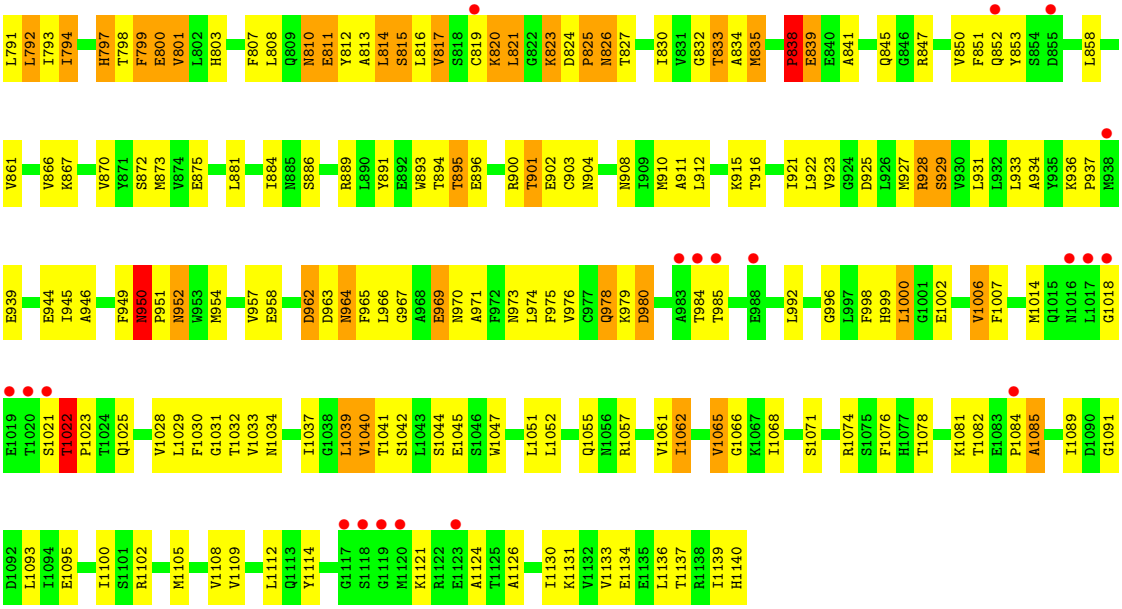




• Molecule 1: DNA damage-binding protein 1

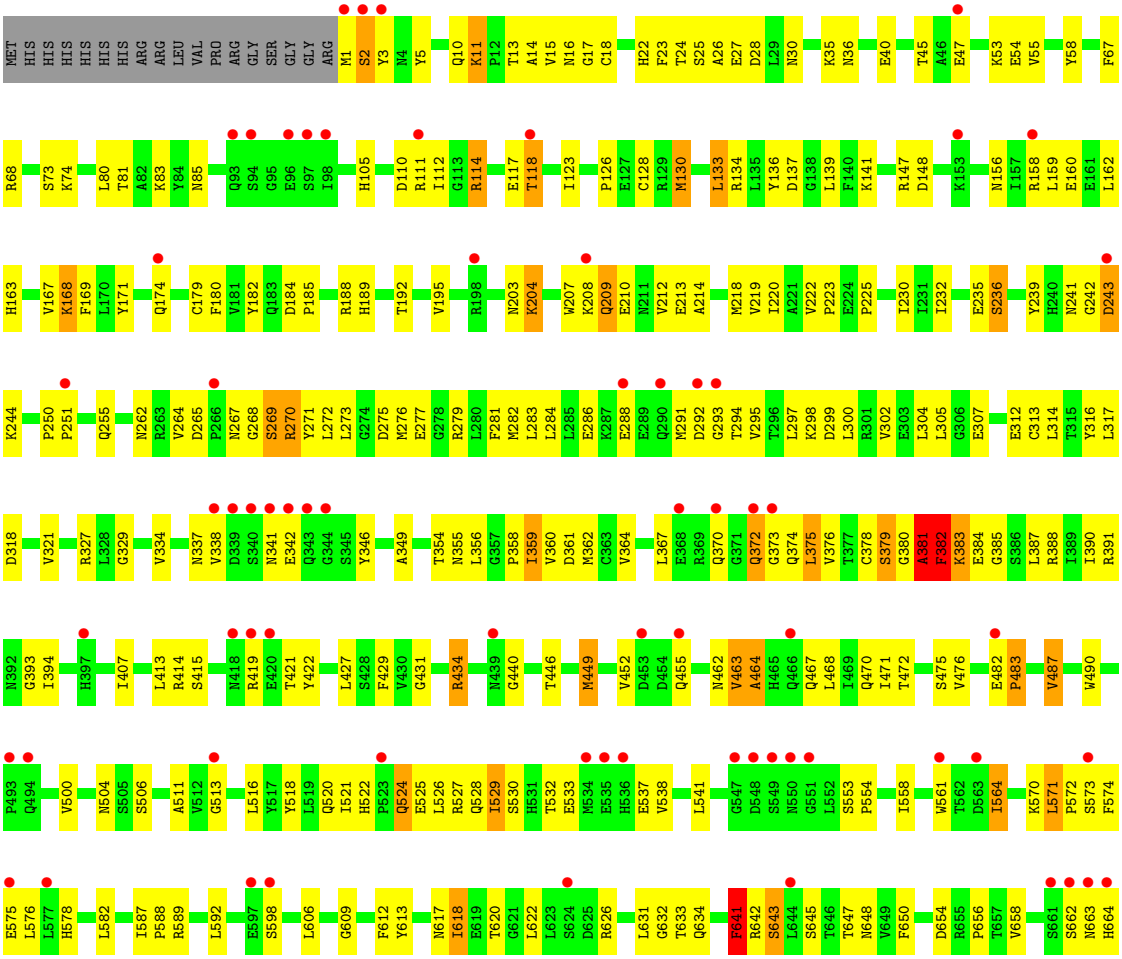
Chain C:

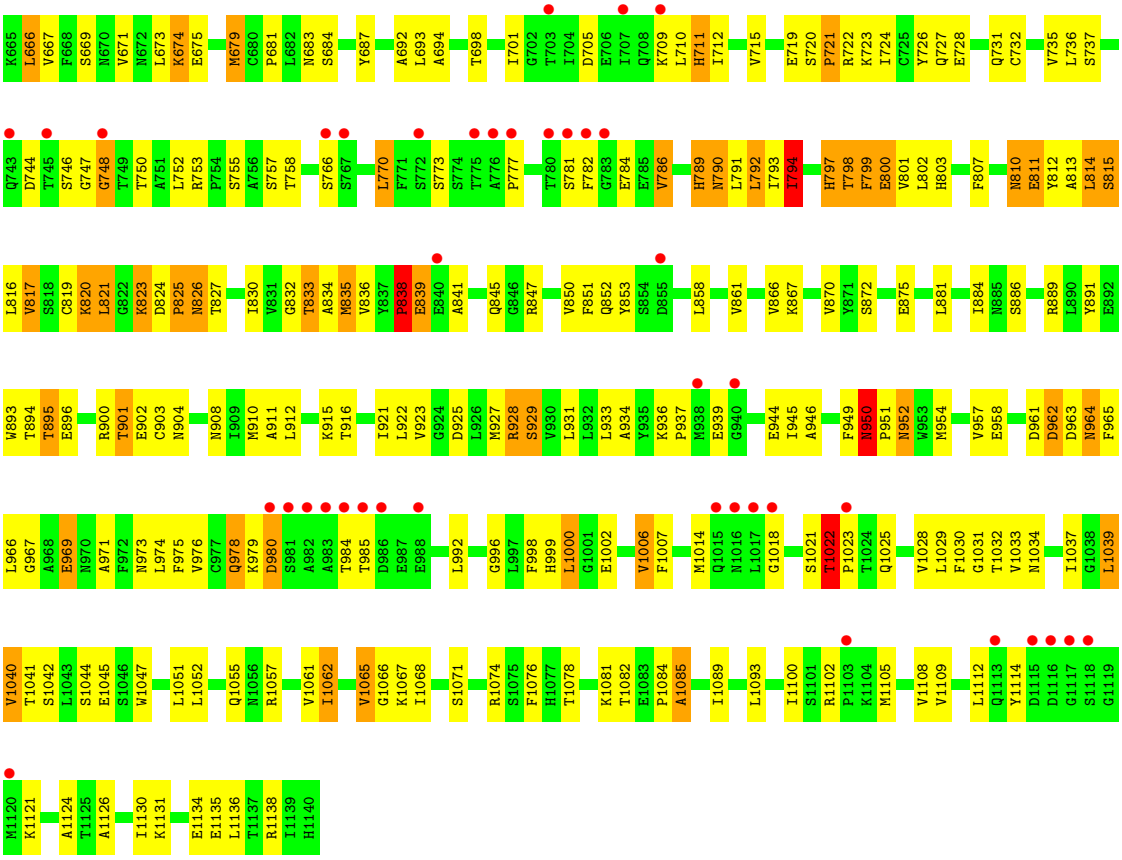




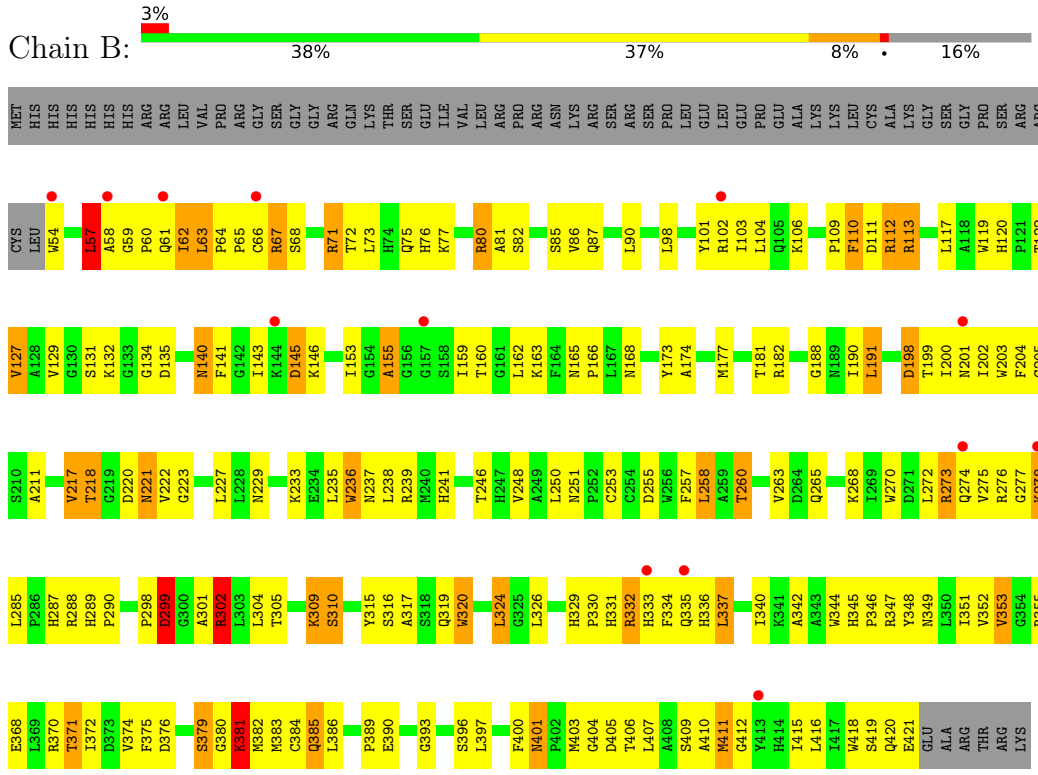
• Molecule 1: DNA damage-binding protein 1

Chain E:



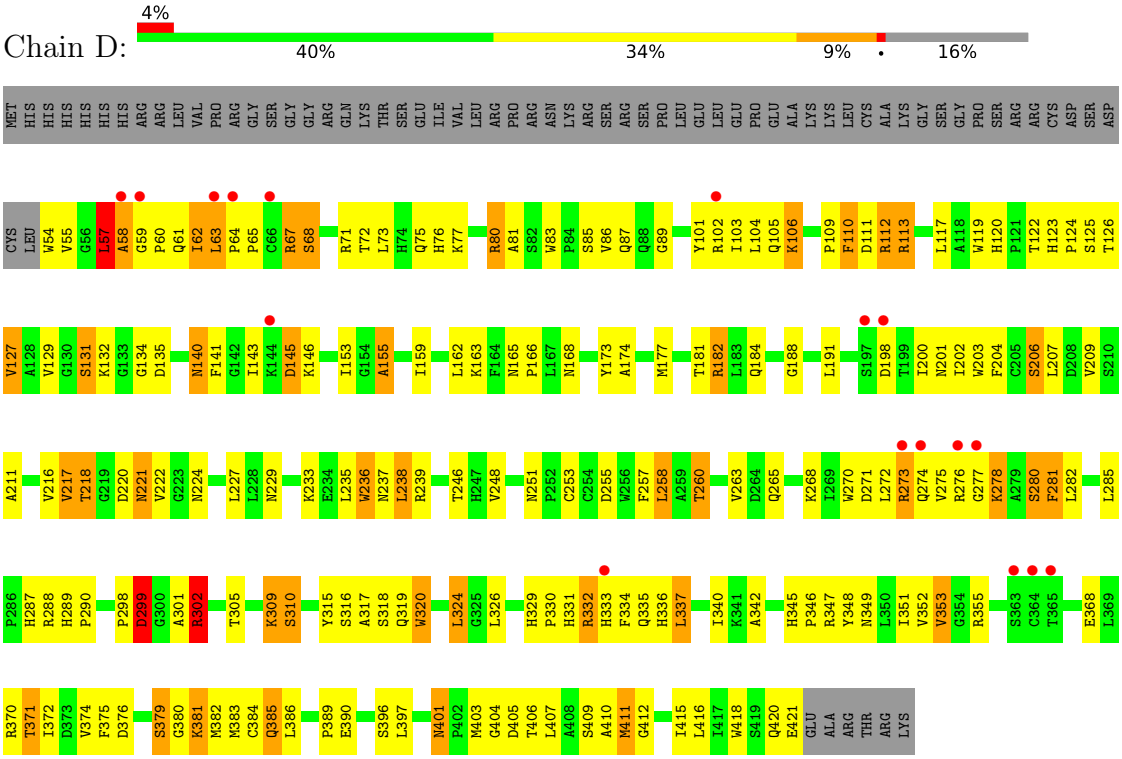


• Molecule 2: DNA damage-binding protein 2



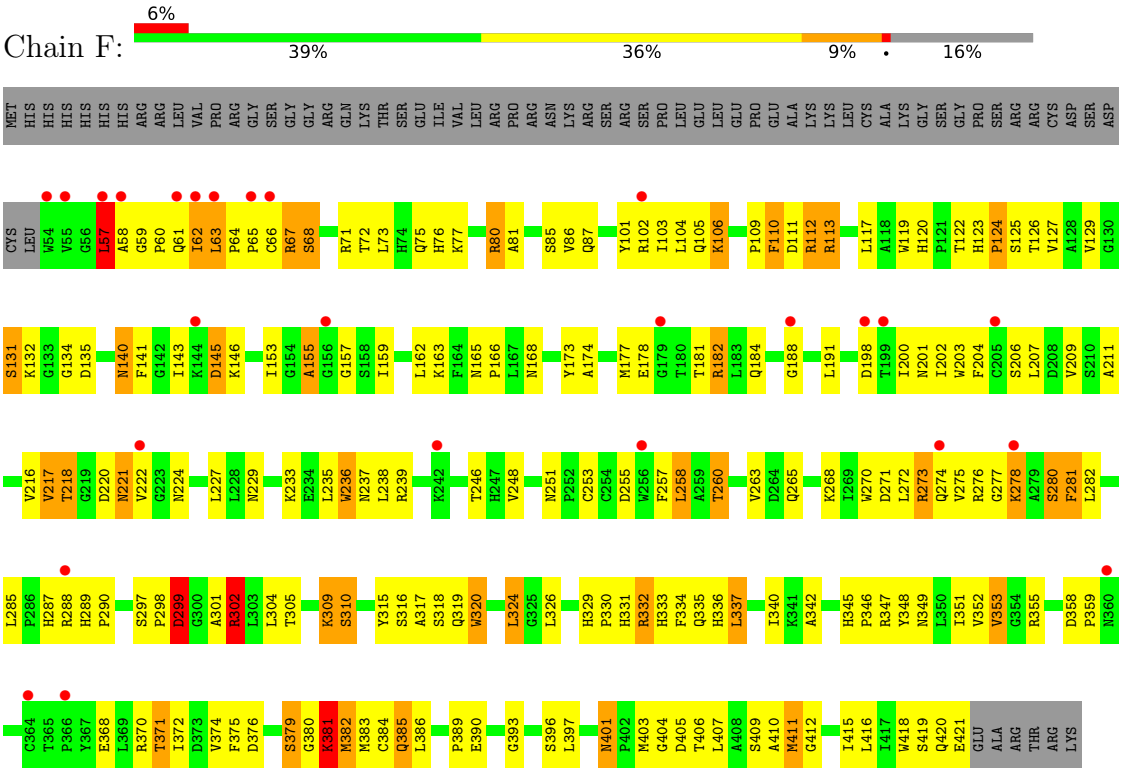
• Molecule 2: DNA damage-binding protein 2

Chain D:



• Molecule 2: DNA damage-binding protein 2

Chain F:



4 Data and refinement statistics (i)

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 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	80.2 (25.00-3.30) 86.8 (19.98-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.254 , 0.288 0.266 , 0.264	Depositor DCC
R_{free} test set	1368 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 83.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	35241	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.59	2/9026 (0.0%)	0.72	2/12239 (0.0%)
1	C	0.50	1/9026 (0.0%)	0.68	2/12239 (0.0%)
1	E	0.51	2/9026 (0.0%)	0.69	5/12239 (0.0%)
2	B	0.65	0/2970	0.78	4/4042 (0.1%)
2	D	0.57	0/2970	0.74	2/4042 (0.0%)
2	F	0.55	0/2970	0.73	2/4042 (0.0%)
All	All	0.55	5/35988 (0.0%)	0.71	17/48843 (0.0%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	381	ALA	CA-CB	-5.83	1.40	1.52
1	A	819	CYS	CB-SG	-5.80	1.72	1.81
1	C	384	GLU	C-O	-5.73	1.12	1.23
1	E	711	HIS	N-CA	-5.17	1.36	1.46
1	A	732	CYS	CB-SG	-5.08	1.73	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	794	ILE	CG1-CB-CG2	-5.98	98.24	111.40
1	E	802	LEU	CA-CB-CG	5.92	128.91	115.30
2	D	57	LEU	CA-CB-CG	5.89	128.84	115.30
2	B	57	LEU	CA-CB-CG	5.88	128.81	115.30
2	F	57	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	641	PHE	CB-CA-C	-5.52	99.36	110.40
2	D	206	SER	C-N-CA	5.51	135.48	121.70
1	E	641	PHE	CB-CA-C	-5.43	99.54	110.40
2	B	207	LEU	CB-CG-CD2	-5.27	102.05	111.00
2	B	207	LEU	CB-CA-C	-5.27	100.19	110.20
1	E	381	ALA	N-CA-C	5.21	125.06	111.00
2	F	393	GLY	N-CA-C	-5.19	100.13	113.10
2	B	393	GLY	N-CA-C	-5.14	100.26	113.10
1	A	838	PRO	C-N-CA	5.10	134.46	121.70
1	E	838	PRO	C-N-CA	5.10	134.44	121.70
1	C	838	PRO	C-N-CA	5.05	134.32	121.70
1	A	712	ILE	CB-CA-C	-5.05	101.51	111.60

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

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Mol	Chain	Res	Type	Group
2	F	380	GLY	Peptide
2	F	381	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8861	0	8781	397	0
1	C	8861	0	8781	386	0
1	E	8861	0	8781	400	0
2	B	2886	0	2836	195	0
2	D	2886	0	2836	181	0
2	F	2886	0	2836	188	0
All	All	35241	0	34851	1677	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 (1677) 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
2:F:375:PHE:CE2	2:F:382:MET:HE2	1.83	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:B:208:ASP:C	2:B:209:VAL:CG1	2.21	1.03
1:A:380:GLY:HA3	1:A:721:PRO:HG2	1.40	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
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
2:F:287:HIS:HE1	2:F:305:THR:HG21	1.20	0.95
2:B:208:ASP:C	2:B:209:VAL:HG13	1.84	0.95
2:B:63:LEU:HB3	2:B:64:PRO:HD3	0.97	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
2:F:381:LYS:HB2	2:F:381:LYS:HZ2	1.23	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:A:927:MET:HE2	2:B:90:LEU:HD22	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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
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:422:TYR:HD1	1:A:683:ASN:H	1.25	0.84
1:C:382:PHE:C	1:C:384:GLU:H	1.81	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:E:168:LYS:HE2	1:E:219:VAL:O	1.78	0.83
1:C:117:GLU:OE2	2:D:60:PRO:HB3	1.78	0.83
2:B:208:ASP:O	2:B:209:VAL:HG13	1.76	0.82
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:810:ASN:CG	1:A:813:ALA:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLY:O	1:A:243:ASP:HB2	1.79	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
1:E:810:ASN:CG	1:E:813:ALA:HB2	2.01	0.80
2:B:198:ASP:HA	2:F:112:ARG:NH2	1.96	0.80
1:C:810:ASN:CG	1:C:813:ALA:HB2	2.01	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
2:F:375:PHE:CZ	2:F:382:MET:HE1	2.15	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:A:293:GLY:C	1:A:294:THR:HG22	2.03	0.79
1:A:929:SER:OG	1:A:951:PRO:C	2.20	0.79
1:C:810:ASN:ND2	1:C:813:ALA:HB2	1.96	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
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: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:A:449:MET:HA	1:A:449:MET:CE	2.12	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:F:376:ASP:CG	2:F:379:SER:OG	2.22	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
2:F:381:LYS:HB2	2:F:381:LYS:HZ3	1.49	0.78
1:E:487:VAL:HG13	1:E:524:GLN:HA	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:C:449:MET:HA	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
2:D:110:PHE:HD2	2:D:111:ASP:H	0.85	0.75
2:F:375:PHE:CD2	2:F:382:MET:HE2	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:375:PHE:CZ	2:F:382:MET:CE	2.72	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
2:B:375:PHE:CE2	2:B:382:MET:HE2	2.24	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:376:ASP:CG	2:B:379:SER:OG	2.31	0.69
1:C:382:PHE:C	1:C:384:GLU:N	2.46	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: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
1:E:449:MET:HA	1:E:449:MET:HE2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:384:GLU:C	1:C:385:GLY:O	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:VAL:HG13	2:D:227:LEU:HD23	1.78	0.66
2:D:381:LYS:O	2:D:382:MET:C	2.30	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:A:449:MET:HA	1:A:449:MET:HE3	1.78	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
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:927:MET:CE	2:B:90:LEU:CD2	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1021:SER:C	1:A:1023:PRO:HD2	2.17	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:C:1021:SER:C	1:C:1023:PRO:HD2	2.18	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:E:1021:SER:C	1:E:1023:PRO:HD2	2.18	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
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:A:930:VAL:HG23	1:A:931:LEU:N	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1084:PRO:O	1:E:1085:ALA:HB3	1.99	0.63
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:A:1084:PRO:O	1:A:1085:ALA:HB3	1.99	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:810:ASN:HB2	1:A:835:MET:HE1	1.81	0.62
1:C:382:PHE:HD1	1:C:720:SER:HG	1.47	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
2:D:298:PRO:O	2:D:299:ASP:HB3	1.99	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
2:F:381:LYS:CB	2:F:381:LYS:HZ3	2.05	0.62
1:A:383:LYS:NZ	1:A:384:GLU:OE2	2.32	0.62
1:E:929:SER:HB3	1:E:952:ASN:HB2	1.80	0.62
1:E:810:ASN:HB2	1:E:835:MET:HE1	1.81	0.61
2:B:198:ASP:HB2	2:F:112:ARG:HH22	1.65	0.61
1:C:889:ARG:HE	1:C:904:ASN:HD21	1.48	0.61
1:A:810:ASN:CG	1:A:813:ALA:CB	2.68	0.61
1:A:951:PRO:HB2	2:B:347:ARG:CZ	2.31	0.61
2:B:345:HIS:CD2	2:B:348:TYR:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:573:SER:O	1:C:574:PHE:HB2	2.01	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
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: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:810:ASN:HB2	1:C:835:MET:HE1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:810:ASN:CG	1:C:813:ALA:CB	2.71	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:537:GLU:HB2	1:A:561:TRP:HB2	1.83	0.59
1:C:203:ASN:O	1:C:204:LYS:HB2	2.02	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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:PHE:HD2	1:E:720:SER:HG	1.50	0.58
1:E:709:LYS:O	1:E:710:LEU:HB3	2.04	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:449:MET:HA	1:C:449:MET:HE2	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:317:ALA:HA	2:F:320:TRP:CE2	2.40	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
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:384:GLU:O	1:C:385:GLY:C	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLY:C	1:A:294:THR:CG2	2.73	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: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
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:CG	2:F:381:LYS:O	2.49	0.56
1:E:810:ASN:CG	1:E:813:ALA:CB	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
2:D:375:PHE:CE2	2:D:382:MET:HE2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:E:792:LEU:HB3	1:E:807:PHE:C	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:3:TYR:HE1	1:C:1045:GLU:HG2	1.73	0.54
1:C:449:MET:HA	1:C:449:MET:HE3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:ASP:HA	2:F:112:ARG:HH22	1.71	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:A:791:LEU:C	1:A:792:LEU:HD12	2.23	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:F:111:ASP:CG	2:F:112:ARG:N	2.62	0.53
1:C:118:THR:HB	1:C:134:ARG:NH2	2.23	0.53
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
2:F:209:VAL:HG12	2:F:216:VAL:HG22	1.90	0.53
1:A:727:GLN:HE21	1:A:820:LYS:HB2	1.74	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:853:TYR:HB2	1:E:858:LEU:HD23	1.91	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:927:MET:HE3	2:B:90:LEU:CD2	2.39	0.52
1:A:969:GLU:OE2	1:A:973:ASN:HB2	2.09	0.52
1:C:791:LEU:C	1:C:792:LEU:HD12	2.26	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HD12	1:A:694:ALA:CB	2.40	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
1:C:356:LEU:HD23	1:C:388:ARG:HG3	1.92	0.51
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
2:B:381:LYS:HG3	2:B:381:LYS:O	2.10	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:449:MET:HA	1:A:449:MET:HE2	1.92	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
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:A:663:ASN:CG	1:A:664:HIS:H	2.13	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:A:134:ARG:HD2	1:A:134:ARG:C	2.31	0.51
2:D:63:LEU:HG	2:D:85:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:617:ASN:ND2	1:C:620:THR:H	2.09	0.51
2:D:310:SER:HB3	2:D:330:PRO:HA	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
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:571:LEU:O	1:A:572:PRO:C	2.49	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:E:571:LEU:O	1:E:572:PRO:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:111:ASP:CG	2:B:112:ARG:N	2.64	0.50
1:C:571:LEU:O	1:C:572:PRO:C	2.50	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: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:18:CYS:HG	1:E:313:CYS:HG	1.59	0.50
1:E:130:MET:HE1	1:E:195:VAL:HG11	1.94	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:63:LEU:HD11	2:B:81:ALA:HB1	1.94	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:790:ASN:C	1:A:790:ASN:HD22	2.16	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:757:SER:CB	1:A:792:LEU:CD2	2.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:838:PRO:CA	1:E:839:GLU:HB2	2.43	0.49
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:E:790:ASN:HD22	1:E:790:ASN:C	2.17	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:299:ASP:OD1	2:B:299:ASP:C	2.52	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
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
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:134:ARG:HD2	1:E:134:ARG:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:C:663:ASN:CG	1:C:664:HIS:H	2.17	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
2:F:420:GLN:O	2:F:421:GLU:C	2.52	0.48
1:A:312:GLU:HG3	1:A:327:ARG:HB2	1.95	0.48
2:D:376:ASP:CG	2:D:379:SER:OG	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:E:1022:THR:N	1:E:1023:PRO:HD2	2.30	0.47
2:B:420:GLN:O	2:B:421:GLU:C	2.53	0.47
2:F:273:ARG:HE	2:F:274:GLN:HB2	1.80	0.47
2:B:375:PHE:CZ	2:B:382:MET:HE1	2.49	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:111:ASP:CG	2:D:112:ARG:N	2.67	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
1:A:792:LEU:HB3	1:A:807:PHE:C	2.34	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
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
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:663:ASN:CG	1:E:664:HIS:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:372:ILE:HB	2:F:386:LEU:HB2	1.96	0.47
1:A:1022:THR:N	1:A:1023:PRO:HD2	2.30	0.46
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
1:C:414:ARG:H	1:C:462:ASN:HD21	1.63	0.46
1:C:792:LEU:HB3	1:C:807:PHE:C	2.36	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:C:790:ASN:C	1:C:790:ASN:HD22	2.19	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: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
2:B:381:LYS:O	2:B:381:LYS:CG	2.61	0.46
1:C:134:ARG:HD2	1:C:134:ARG:C	2.35	0.46
1:C:373:GLY:N	1:C:374:GLN:HB3	2.30	0.46
2:D:177:MET:HA	2:D:203:TRP:CD1	2.50	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
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
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
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
2:B:382:MET:HE2	2:B:382:MET:CA	2.46	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
2:F:376:ASP:OD1	2:F:379:SER:OG	2.34	0.46
1:A:967:GLY:O	1:A:974:LEU:HA	2.15	0.46
1:C:538:VAL:HG13	1:C:558:ILE:HD11	1.97	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:B:375:PHE:CE2	2:B:382:MET:HE1	2.51	0.45
2:B:382:MET:HE2	2:B:382:MET:HA	1.98	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:292:ASP:C	1:A:294:THR:N	2.69	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: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
1:E:390:ILE:HG23	1:E:712:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:684:SER:HB3	1:A:687:TYR:HB2	1.98	0.45
2:B:140:ASN:C	2:B:140:ASN:HD22	2.20	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:E:963:ASP:C	1:E:964:ASN:HD22	2.20	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: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:C:383:LYS:CG	1:C:384:GLU:HG3	2.39	0.45
2:D:420:GLN:O	2:D:421:GLU:C	2.55	0.45
1:E:167:VAL:CG1	1:E:180:PHE:HB3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:273:ARG:HE	2:B:274:GLN:HB2	1.82	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: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: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: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:960:LEU:HD12	1:A:964:ASN:HB3	1.99	0.44
2:B:112:ARG:HD2	2:B:132:LYS:HB3	1.98	0.44
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:A:790:ASN:C	1:A:790:ASN:ND2	2.71	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
2:D:299:ASP:C	2:D:299:ASP:OD1	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:819:CYS:SG	1:C:873:MET:HE3	2.57	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: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
2:B:263:VAL:C	2:B:265:GLN:H	2.21	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
2:B:227:LEU:HB3	2:B:236:TRP:HB2	1.99	0.44
2:B:382:MET:HB2	2:B:382:MET:HE3	1.15	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
2:F:382:MET:HE3	2:F:382:MET:HB2	1.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:140:ASN:HD22	2:D:140:ASN:C	2.20	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: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:A:18:CYS:SG	1:A:313:CYS:SG	3.08	0.43
1:C:141:LYS:HD2	1:C:156:ASN:ND2	2.33	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:MET:HE3	2:B:90:LEU:HD22	1.92	0.43
1:A:964:ASN:ND2	1:A:978:GLN:NE2	2.66	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:101:TYR:C	2:D:103:ILE:N	2.72	0.43
2:D:227:LEU:HB3	2:D:236:TRP:HB2	2.01	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
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
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:212:VAL:O	1:A:213:GLU:C	2.57	0.42
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: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:790:ASN:C	1:E:790:ASN:ND2	2.73	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:E:1100:ILE:O	1:E:1105:MET:HE3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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:C:1100:ILE:O	1:C:1105:MET:HE3	2.19	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:265:ASP:N	1:E:265:ASP:OD1	2.52	0.42
1:E:378:CYS:HG	1:E:388:ARG:HB2	1.83	0.42
1:E:383:LYS:HG3	1:E:384:GLU:N	2.35	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:792:LEU:CB	1:C:807:PHE:O	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:208:ASP:CG	2:B:209:VAL:H	2.23	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:101:TYR:C	2:F:103:ILE:N	2.73	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
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:819:CYS:SG	1:C:873:MET:CE	3.08	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:130:MET:CE	1:A:195:VAL:HG11	2.50	0.42
1:A:766:SER:N	1:A:807:PHE:HE2	2.17	0.42
1:A:1100:ILE:O	1:A:1105:MET:HE3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:998:PHE:CE1	1:E:1074:ARG:HD2	2.55	0.42
2:F:140:ASN:C	2:F:140:ASN:HD22	2.22	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
2:D:263:VAL:C	2:D:265:GLN:H	2.23	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
1:E:673:LEU:C	1:E:674:LYS:O	2.57	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
1:A:961:ASP:C	1:A:963:ASP:H	2.23	0.41
2:B:304:LEU:HD21	2:B:351:ILE:HG23	2.02	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:449:MET:HA	1:E:449:MET:HE3	1.96	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:E:937:PRO:C	1:E:939:GLU:N	2.73	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
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
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:C:963:ASP:C	1:C:964:ASN:HD22	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:220:ASP:OD2	2:D:220:ASP:C	2.59	0.41
2:D:235:LEU:C	2:D:236:TRP:HE3	2.24	0.41
2:D:376:ASP:HB2	2:D:383:MET:HE2	2.01	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
2:F:301:ALA:C	2:F:302:ARG:HD2	2.41	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
2:F:235:LEU:C	2:F:236:TRP:HE3	2.24	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:673:LEU:C	1:C:674:LYS:O	2.59	0.41
1:C:852:GLN:HB2	1:C:861:VAL:CG2	2.50	0.41
2:D:301:ALA:C	2:D:302:ARG:HD2	2.40	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:130:MET:HE1	1:C:195:VAL:HG11	2.03	0.41
1:C:792:LEU:HB3	1:C:808:LEU:HA	2.03	0.41
1:E:220:ILE:HB	1:E:230:ILE:HB	2.01	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
1:C:212:VAL:O	1:C:213:GLU:C	2.58	0.41
1:C:927:MET:O	1:C:928:ARG:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:189:HIS:HD1	1:A:211:ASN:HA	1.86	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
2:B:301:ALA:C	2:B:302:ARG:HD2	2.41	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:130:MET:HE1	1:A:195:VAL:HG11	2.02	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:790:ASN:C	1:C:790:ASN:ND2	2.74	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:206:SER:HB3	2:F:246:THR:O	2.21	0.41
1:A:220:ILE:HB	1:A:230:ILE:HB	2.02	0.41
1:C:18:CYS:HG	1:C:313:CYS:HG	1.51	0.41
1:C:744:ASP:HB3	1:C:747:GLY:O	2.20	0.41
2:D:101:TYR:C	2:D:103:ILE:H	2.24	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
2:F:263:VAL:C	2:F:265:GLN:H	2.24	0.41
2:F:299:ASP:OD1	2:F:299:ASP:C	2.59	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:A:372:GLN:HA	1:A:373:GLY:HA2	1.46	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: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:C:937:PRO:C	1:C:939:GLU:N	2.74	0.40
1:E:382:PHE:HD2	1:E:382:PHE:HA	1.69	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:961:ASP:C	1:E:963:ASP:H	2.25	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:968:ALA:HA	1:A:973:ASN:O	2.21	0.40
2:B:101:TYR:C	2:B:103:ILE:N	2.73	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
2:D:105:GLN:O	2:D:106:LYS:CB	2.69	0.40
1:E:212:VAL:O	1:E:213:GLU:C	2.59	0.40
1:E:679:MET:HE1	1:E:681:PRO:HD3	2.04	0.40
1:E:791:LEU:C	1:E:792:LEU:HD12	2.30	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1138/1158 (98%)	953 (84%)	130 (11%)	55 (5%)	2	14
1	C	1138/1158 (98%)	944 (83%)	135 (12%)	59 (5%)	2	13
1	E	1138/1158 (98%)	949 (83%)	131 (12%)	58 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	366/436 (84%)	303 (83%)	39 (11%)	24 (7%)	1 8
2	D	366/436 (84%)	303 (83%)	40 (11%)	23 (6%)	1 9
2	F	366/436 (84%)	308 (84%)	35 (10%)	23 (6%)	1 9
All	All	4512/4782 (94%)	3760 (83%)	510 (11%)	242 (5%)	2 12

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	984/1014 (97%)	868 (88%)	116 (12%)	5 21
1	C	984/1014 (97%)	876 (89%)	108 (11%)	6 24
1	E	984/1014 (97%)	875 (89%)	109 (11%)	6 23
2	B	315/378 (83%)	264 (84%)	51 (16%)	2 10
2	D	315/378 (83%)	265 (84%)	50 (16%)	2 11
2	F	315/378 (83%)	262 (83%)	53 (17%)	2 9
All	All	3897/4176 (93%)	3410 (88%)	487 (12%)	4 19

All (487) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	47	GLU
1	A	53	LYS
1	A	111	ARG
1	A	112	ILE
1	A	114	ARG
1	A	118	THR
1	A	129	ARG
1	A	130	MET
1	A	133	LEU
1	A	148	ASP
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	236	SER
1	A	269	SER
1	A	277	GLU
1	A	284	LEU
1	A	290	GLN

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Mol	Chain	Res	Type
1	A	291	MET
1	A	302	VAL
1	A	304	LEU
1	A	307	GLU
1	A	314	LEU
1	A	318	ASP
1	A	338	VAL
1	A	342	GLU
1	A	354	THR
1	A	372	GLN
1	A	375	LEU
1	A	382	PHE
1	A	413	LEU
1	A	415	SER
1	A	419	ARG
1	A	427	LEU
1	A	434	ARG
1	A	446	THR
1	A	449	MET
1	A	463	VAL
1	A	468	LEU
1	A	487	VAL
1	A	524	GLN
1	A	529	ILE
1	A	556	CYS
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	641	PHE
1	A	643	SER
1	A	661	SER
1	A	666	LEU
1	A	669	SER
1	A	679	MET
1	A	698	THR
1	A	701	ILE
1	A	724	ILE
1	A	728	GLU

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Mol	Chain	Res	Type
1	A	731	GLN
1	A	752	LEU
1	A	758	THR
1	A	770	LEU
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
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	875	GLU
1	A	894	THR
1	A	895	THR
1	A	900	ARG
1	A	901	THR
1	A	915	LYS
1	A	922	LEU
1	A	928	ARG
1	A	931	LEU
1	A	950	ASN
1	A	954	MET
1	A	957	VAL
1	A	962	ASP
1	A	964	ASN
1	A	966	LEU
1	A	969	GLU
1	A	978	GLN
1	A	984	THR
1	A	1000	LEU

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Mol	Chain	Res	Type
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	1071	SER
1	A	1093	LEU
1	A	1121	LYS
1	A	1131	LYS
2	B	57	LEU
2	B	61	GLN
2	B	62	ILE
2	B	71	ARG
2	B	80	ARG
2	B	82	SER
2	B	87	GLN
2	B	110	PHE
2	B	112	ARG
2	B	117	LEU
2	B	125	SER
2	B	127	VAL
2	B	140	ASN
2	B	145	ASP
2	B	162	LEU
2	B	163	LYS
2	B	182	ARG
2	B	191	LEU
2	B	198	ASP
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

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Mol	Chain	Res	Type
2	B	288	ARG
2	B	299	ASP
2	B	302	ARG
2	B	309	LYS
2	B	310	SER
2	B	324	LEU
2	B	326	LEU
2	B	336	HIS
2	B	337	LEU
2	B	352	VAL
2	B	353	VAL
2	B	370	ARG
2	B	371	THR
2	B	379	SER
2	B	381	LYS
2	B	385	GLN
2	B	401	ASN
2	B	411	MET
2	B	419	SER
1	C	45	THR
1	C	47	GLU
1	C	53	LYS
1	C	111	ARG
1	C	112	ILE
1	C	114	ARG
1	C	118	THR
1	C	129	ARG
1	C	130	MET
1	C	133	LEU
1	C	148	ASP
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	236	SER
1	C	269	SER
1	C	277	GLU
1	C	284	LEU
1	C	302	VAL
1	C	304	LEU

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Mol	Chain	Res	Type
1	C	307	GLU
1	C	314	LEU
1	C	318	ASP
1	C	338	VAL
1	C	342	GLU
1	C	354	THR
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	446	THR
1	C	449	MET
1	C	463	VAL
1	C	468	LEU
1	C	487	VAL
1	C	524	GLN
1	C	529	ILE
1	C	549	SER
1	C	571	LEU
1	C	589	ARG
1	C	592	LEU
1	C	598	SER
1	C	618	ILE
1	C	631	LEU
1	C	633	THR
1	C	666	LEU
1	C	669	SER
1	C	679	MET
1	C	698	THR
1	C	701	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	786	VAL

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Mol	Chain	Res	Type
1	C	789	HIS
1	C	790	ASN
1	C	792	LEU
1	C	794	ILE
1	C	799	PHE
1	C	800	GLU
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	875	GLU
1	C	894	THR
1	C	895	THR
1	C	900	ARG
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	964	ASN
1	C	966	LEU
1	C	969	GLU
1	C	978	GLN
1	C	984	THR
1	C	1000	LEU
1	C	1014	MET
1	C	1022	THR
1	C	1039	LEU
1	C	1040	VAL
1	C	1041	THR
1	C	1052	LEU
1	C	1071	SER
1	C	1093	LEU
1	C	1121	LYS

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Mol	Chain	Res	Type
1	C	1131	LYS
2	D	57	LEU
2	D	61	GLN
2	D	62	ILE
2	D	68	SER
2	D	71	ARG
2	D	80	ARG
2	D	87	GLN
2	D	110	PHE
2	D	112	ARG
2	D	117	LEU
2	D	125	SER
2	D	127	VAL
2	D	131	SER
2	D	140	ASN
2	D	145	ASP
2	D	162	LEU
2	D	163	LYS
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	288	ARG
2	D	299	ASP
2	D	302	ARG
2	D	309	LYS
2	D	310	SER
2	D	324	LEU
2	D	326	LEU
2	D	336	HIS
2	D	337	LEU

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Mol	Chain	Res	Type
2	D	352	VAL
2	D	353	VAL
2	D	370	ARG
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	45	THR
1	E	47	GLU
1	E	53	LYS
1	E	111	ARG
1	E	112	ILE
1	E	114	ARG
1	E	118	THR
1	E	130	MET
1	E	133	LEU
1	E	148	ASP
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	236	SER
1	E	269	SER
1	E	270	ARG
1	E	277	GLU
1	E	284	LEU
1	E	302	VAL
1	E	304	LEU
1	E	307	GLU
1	E	314	LEU
1	E	318	ASP
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

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Mol	Chain	Res	Type
1	E	413	LEU
1	E	415	SER
1	E	419	ARG
1	E	427	LEU
1	E	434	ARG
1	E	446	THR
1	E	449	MET
1	E	463	VAL
1	E	468	LEU
1	E	487	VAL
1	E	524	GLN
1	E	529	ILE
1	E	571	LEU
1	E	589	ARG
1	E	592	LEU
1	E	598	SER
1	E	618	ILE
1	E	631	LEU
1	E	633	THR
1	E	666	LEU
1	E	669	SER
1	E	679	MET
1	E	698	THR
1	E	701	ILE
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	786	VAL
1	E	789	HIS
1	E	790	ASN
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

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Mol	Chain	Res	Type
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	875	GLU
1	E	894	THR
1	E	895	THR
1	E	900	ARG
1	E	901	THR
1	E	915	LYS
1	E	922	LEU
1	E	950	ASN
1	E	954	MET
1	E	957	VAL
1	E	962	ASP
1	E	964	ASN
1	E	966	LEU
1	E	969	GLU
1	E	978	GLN
1	E	984	THR
1	E	1000	LEU
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	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	68	SER
2	F	71	ARG
2	F	80	ARG
2	F	87	GLN
2	F	110	PHE

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Mol	Chain	Res	Type
2	F	112	ARG
2	F	117	LEU
2	F	124	PRO
2	F	125	SER
2	F	127	VAL
2	F	131	SER
2	F	140	ASN
2	F	145	ASP
2	F	162	LEU
2	F	163	LYS
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
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	288	ARG
2	F	299	ASP
2	F	302	ARG
2	F	309	LYS
2	F	310	SER
2	F	324	LEU
2	F	326	LEU
2	F	336	HIS
2	F	337	LEU
2	F	352	VAL
2	F	353	VAL
2	F	370	ARG
2	F	371	THR
2	F	379	SER
2	F	381	LYS
2	F	382	MET
2	F	385	GLN

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Mol	Chain	Res	Type
2	F	401	ASN
2	F	411	MET
2	F	419	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) 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	355	ASN
1	A	374	GLN
1	A	462	ASN
1	A	467	GLN
1	A	470	GLN
1	A	504	ASN
1	A	520	GLN
1	A	522	HIS
1	A	528	GLN
1	A	531	HIS
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	885	ASN
1	A	904	ASN
1	A	950	ASN
1	A	964	ASN
1	A	978	GLN
1	A	999	HIS
1	A	1009	HIS
1	A	1034	ASN

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Mol	Chain	Res	Type
1	A	1049	ASN
1	A	1140	HIS
2	B	87	GLN
2	B	92	GLN
2	B	96	HIS
2	B	140	ASN
2	B	184	GLN
2	B	221	ASN
2	B	237	ASN
2	B	251	ASN
2	B	287	HIS
2	B	289	HIS
2	B	319	GLN
2	B	333	HIS
2	B	335	GLN
2	B	345	HIS
2	B	385	GLN
2	B	401	ASN
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	255	GLN
1	C	262	ASN
1	C	355	ASN
1	C	374	GLN
1	C	397	HIS
1	C	462	ASN
1	C	467	GLN
1	C	470	GLN
1	C	504	ASN
1	C	520	GLN
1	C	522	HIS
1	C	528	GLN
1	C	531	HIS
1	C	617	ASN
1	C	677	ASN
1	C	727	GLN
1	C	790	ASN

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Mol	Chain	Res	Type
1	C	796	GLN
1	C	845	GLN
1	C	885	ASN
1	C	904	ASN
1	C	950	ASN
1	C	978	GLN
1	C	999	HIS
1	C	1009	HIS
1	C	1034	ASN
1	C	1049	ASN
1	C	1140	HIS
2	D	87	GLN
2	D	92	GLN
2	D	140	ASN
2	D	184	GLN
2	D	221	ASN
2	D	237	ASN
2	D	247	HIS
2	D	251	ASN
2	D	287	HIS
2	D	289	HIS
2	D	319	GLN
2	D	333	HIS
2	D	345	HIS
2	D	385	GLN
2	D	401	ASN
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	255	GLN
1	E	262	ASN
1	E	355	ASN
1	E	374	GLN
1	E	462	ASN
1	E	467	GLN
1	E	470	GLN
1	E	504	ASN
1	E	520	GLN

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Mol	Chain	Res	Type
1	E	522	HIS
1	E	528	GLN
1	E	617	ASN
1	E	677	ASN
1	E	727	GLN
1	E	731	GLN
1	E	790	ASN
1	E	796	GLN
1	E	845	GLN
1	E	885	ASN
1	E	904	ASN
1	E	950	ASN
1	E	964	ASN
1	E	978	GLN
1	E	999	HIS
1	E	1009	HIS
1	E	1034	ASN
1	E	1049	ASN
1	E	1140	HIS
2	F	87	GLN
2	F	92	GLN
2	F	140	ASN
2	F	184	GLN
2	F	221	ASN
2	F	237	ASN
2	F	251	ASN
2	F	287	HIS
2	F	289	HIS
2	F	319	GLN
2	F	333	HIS
2	F	345	HIS
2	F	385	GLN
2	F	401	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1140/1158 (98%)	0.45	91 (7%)	12	11	23, 63, 97, 120	0
1	C	1140/1158 (98%)	0.45	81 (7%)	16	16	23, 63, 95, 120	0
1	E	1140/1158 (98%)	0.54	108 (9%)	8	8	22, 64, 96, 120	0
2	B	368/436 (84%)	0.14	13 (3%)	44	42	24, 55, 86, 141	0
2	D	368/436 (84%)	0.15	17 (4%)	32	30	24, 55, 88, 136	0
2	F	368/436 (84%)	0.31	26 (7%)	16	16	25, 56, 85, 139	0
All	All	4524/4782 (94%)	0.41	336 (7%)	14	14	22, 62, 94, 141	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	548	ASP	9.5
1	C	780	THR	8.9
1	C	1117	GLY	8.8
1	E	984	THR	8.3
1	A	1120	MET	8.0
1	E	985	THR	7.7
1	E	372	GLN	7.2
1	E	550	ASN	6.8
1	C	1	MET	6.4
1	A	780	THR	6.2
1	C	548	ASP	6.1
1	C	550	ASN	6.0
1	E	1118	SER	6.0
1	C	781	SER	6.0
1	C	338	VAL	5.9
1	A	984	THR	5.9
1	E	341	ASN	5.8
1	C	1020	THR	5.8
1	E	780	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	550	ASN	5.7
1	E	1016	ASN	5.7
1	C	984	THR	5.6
1	E	776	ALA	5.6
1	A	343	GLN	5.5
1	E	1117	GLY	5.5
1	C	94	SER	5.4
1	E	663	ASN	5.4
1	A	293	GLY	5.2
1	A	338	VAL	5.1
1	E	343	GLN	5.1
1	E	549	SER	5.1
1	A	781	SER	5.0
1	E	1120	MET	5.0
1	A	94	SER	5.0
1	C	1021	SER	5.0
1	A	983	ALA	5.0
1	E	782	PHE	5.0
1	A	782	PHE	4.9
1	E	662	SER	4.8
1	E	420	GLU	4.8
1	A	548	ASP	4.7
1	A	547	GLY	4.7
1	E	547	GLY	4.5
1	E	535	GLU	4.5
1	A	71	GLY	4.5
1	C	547	GLY	4.4
1	C	342	GLU	4.4
1	E	781	SER	4.4
1	E	339	ASP	4.4
1	E	1113	GLN	4.4
2	B	58	ALA	4.4
1	A	344	GLY	4.3
1	A	146	ASP	4.2
1	C	341	ASN	4.1
1	A	341	ASN	4.1
1	C	1016	ASN	4.0
1	E	664	HIS	4.0
1	E	344	GLY	4.0
1	E	575	GLU	4.0
1	A	985	THR	4.0
1	E	983	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	536	HIS	3.9
1	C	73	SER	3.9
1	C	985	THR	3.9
1	E	439	ASN	3.9
1	E	455	GLN	3.9
1	A	223	PRO	3.8
1	C	150	LYS	3.8
1	E	767	SER	3.8
1	E	1	MET	3.8
2	F	199	THR	3.8
2	D	333	HIS	3.8
2	D	197	SER	3.7
2	D	58	ALA	3.7
1	A	292	ASP	3.7
1	C	785	GLU	3.7
1	E	494	GLN	3.7
2	F	274	GLN	3.7
1	A	1017	LEU	3.7
1	A	96	GLU	3.7
1	A	1015	GLN	3.7
2	B	278	LYS	3.6
1	A	151	GLU	3.6
1	E	1023	PRO	3.6
1	E	493	PRO	3.6
1	A	748	GLY	3.6
1	E	340	SER	3.6
1	C	1018	GLY	3.6
1	A	340	SER	3.5
1	A	494	GLN	3.5
1	C	988	GLU	3.5
1	A	663	ASN	3.5
1	A	938	MET	3.5
1	C	93	GLN	3.5
2	F	66	CYS	3.5
1	A	70	LYS	3.5
1	A	1020	THR	3.4
1	E	208	LYS	3.4
1	C	551	GLY	3.4
1	A	1016	ASN	3.4
1	E	644	LEU	3.3
1	A	1018	GLY	3.3
1	C	1123	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	174	GLN	3.3
1	A	1119	GLY	3.3
1	E	783	GLY	3.3
1	C	344	GLY	3.3
1	A	418	ASN	3.3
1	C	779	GLU	3.2
1	E	47	GLU	3.2
1	E	624	SER	3.2
2	B	54	TRP	3.2
1	C	1120	MET	3.2
1	E	97	SER	3.2
1	A	266	PRO	3.1
1	E	342	GLU	3.1
1	E	1116	ASP	3.1
2	D	273	ARG	3.1
1	E	986	ASP	3.1
1	E	1103	PRO	3.1
1	C	345	SER	3.1
1	C	340	SER	3.1
1	C	372	GLN	3.1
1	C	494	GLN	3.1
1	E	938	MET	3.1
1	E	292	ASP	3.0
1	A	221	ALA	3.0
2	F	58	ALA	3.0
1	A	372	GLN	3.0
1	E	1115	ASP	3.0
1	C	1019	GLU	3.0
2	F	198	ASP	3.0
1	C	339	ASP	3.0
1	E	766	SER	3.0
1	C	783	GLY	3.0
2	F	222	VAL	3.0
1	A	549	SER	3.0
1	A	1019	GLU	3.0
1	A	339	ASP	2.9
1	A	2	SER	2.9
1	A	208	LYS	2.9
1	C	662	SER	2.9
1	E	597	GLU	2.9
1	E	748	GLY	2.9
1	E	1017	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	493	PRO	2.9
1	E	981	SER	2.9
1	A	662	SER	2.9
1	C	70	LYS	2.9
1	C	774	SER	2.9
1	E	982	ALA	2.9
1	A	706	GLU	2.9
1	A	439	ASN	2.9
2	F	54	TRP	2.8
1	C	27	GLU	2.8
1	A	523	PRO	2.8
1	E	293	GLY	2.8
1	C	765	VAL	2.8
1	C	1084	PRO	2.8
1	E	96	GLU	2.8
1	C	97	SER	2.8
2	B	274	GLN	2.8
1	C	938	MET	2.8
1	E	536	HIS	2.8
1	E	373	GLY	2.8
1	E	338	VAL	2.8
2	D	364	CYS	2.8
1	E	419	ARG	2.8
1	E	777	PRO	2.8
2	D	64	PRO	2.8
2	D	274	GLN	2.7
1	C	645	SER	2.7
2	F	57	LEU	2.7
1	C	96	GLU	2.7
1	A	797	HIS	2.7
1	A	73	SER	2.7
1	A	294	THR	2.7
1	A	855	ASP	2.7
1	A	93	GLN	2.7
1	E	988	GLU	2.7
1	C	254	LYS	2.7
1	E	523	PRO	2.7
1	E	288	GLU	2.6
1	C	777	PRO	2.6
1	E	561	TRP	2.6
1	E	534	MET	2.6
2	F	61	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	296	THR	2.6
1	E	772	SER	2.6
2	D	363	SER	2.6
1	A	150	LYS	2.6
1	E	707	ILE	2.6
1	E	661	SER	2.6
1	A	1084	PRO	2.6
2	F	144	LYS	2.6
2	B	102	ARG	2.6
1	A	1118	SER	2.6
2	D	66	CYS	2.6
1	E	174	GLN	2.5
1	A	287	LYS	2.5
1	C	549	SER	2.5
1	C	983	ALA	2.5
1	C	418	ASN	2.5
1	E	111	ARG	2.5
2	D	102	ARG	2.5
1	C	47	GLU	2.5
2	F	364	CYS	2.5
1	A	153	LYS	2.5
1	E	482	GLU	2.5
1	E	251	PRO	2.5
1	E	93	GLN	2.5
1	E	577	LEU	2.5
1	C	147	ARG	2.5
1	C	1119	GLY	2.5
1	A	743	GLN	2.5
1	C	146	ASP	2.5
2	D	365	THR	2.5
1	E	198	ARG	2.5
1	A	1063	LYS	2.5
1	A	243	ASP	2.5
1	E	418	ASN	2.4
2	D	63	LEU	2.4
1	A	988	GLU	2.4
1	A	1121	LYS	2.4
2	B	157	GLY	2.4
1	A	619	GLU	2.4
1	A	664	HIS	2.4
1	E	743	GLN	2.4
2	F	63	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	536	HIS	2.4
1	E	745	THR	2.4
2	D	277	GLY	2.4
2	B	335	GLN	2.4
1	C	95	GLY	2.4
1	E	370	GLN	2.4
1	A	620	THR	2.4
1	C	111	ARG	2.4
2	B	61	GLN	2.4
1	E	1018	GLY	2.4
2	B	413	TYR	2.4
1	E	243	ASP	2.4
1	A	235	GLU	2.4
1	A	1123	GLU	2.4
1	A	27	GLU	2.3
1	C	775	THR	2.3
2	B	333	HIS	2.3
1	E	290	GLN	2.3
1	E	3	TYR	2.3
1	E	551	GLY	2.3
1	A	255	GLN	2.3
1	A	147	ARG	2.3
1	E	573	SER	2.3
2	D	144	LYS	2.3
1	A	203	ASN	2.3
1	C	561	TRP	2.3
1	A	454	ASP	2.3
2	B	66	CYS	2.3
2	F	360	ASN	2.3
1	E	453	ASP	2.3
2	F	205	CYS	2.3
2	F	366	PRO	2.3
1	E	775	THR	2.3
1	E	1015	GLN	2.3
2	B	144	LYS	2.3
1	E	513	GLY	2.3
1	E	940	GLY	2.3
1	C	225	PRO	2.3
1	C	1017	LEU	2.3
1	C	71	GLY	2.3
2	F	156	GLY	2.3
1	A	744	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	663	ASN	2.3
1	E	153	LYS	2.3
1	E	368	GLU	2.2
1	A	563	ASP	2.2
1	E	703	THR	2.2
1	E	709	LYS	2.2
1	A	647	THR	2.2
2	D	198	ASP	2.2
2	D	276	ARG	2.2
1	A	318	ASP	2.2
2	B	201	ASN	2.2
2	F	102	ARG	2.2
1	C	493	PRO	2.2
1	C	855	ASP	2.2
1	E	855	ASP	2.2
1	A	766	SER	2.2
1	C	291	MET	2.2
1	C	1118	SER	2.2
1	E	158	ARG	2.2
1	E	598	SER	2.2
2	D	59	GLY	2.2
2	F	256	TRP	2.2
1	C	622	LEU	2.2
2	F	179	GLY	2.2
1	E	466	GLN	2.2
1	C	819	CYS	2.2
1	E	94	SER	2.1
1	C	586	ILE	2.1
2	F	65	PRO	2.1
1	A	298	LYS	2.1
1	E	397	HIS	2.1
1	A	111	ARG	2.1
1	C	2	SER	2.1
1	C	369	ARG	2.1
1	A	575	GLU	2.1
1	C	343	GLN	2.1
1	A	986	ASP	2.1
2	F	242	LYS	2.1
2	F	55	VAL	2.1
1	A	97	SER	2.1
1	E	2	SER	2.1
1	C	292	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	441	GLU	2.1
1	E	840	GLU	2.1
1	A	74	LYS	2.1
1	E	98	ILE	2.1
1	E	266	PRO	2.1
1	C	598	SER	2.1
1	C	208	LYS	2.1
2	F	278	LYS	2.1
2	F	62	ILE	2.1
1	E	980	ASP	2.1
1	A	319	ASN	2.1
1	C	778	HIS	2.1
1	C	852	GLN	2.0
1	C	523	PRO	2.0
1	E	118	THR	2.0
2	F	188	GLY	2.0
1	C	664	HIS	2.0
1	E	563	ASP	2.0
2	F	288	ARG	2.0
1	A	785	GLU	2.0
1	A	47	GLU	2.0
1	A	896	GLU	2.0
1	A	1113	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.