



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:50 am BST

PDB ID : 3S51
Title : Structure of FANCI
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
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 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	:	2.11
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)	:	2.11

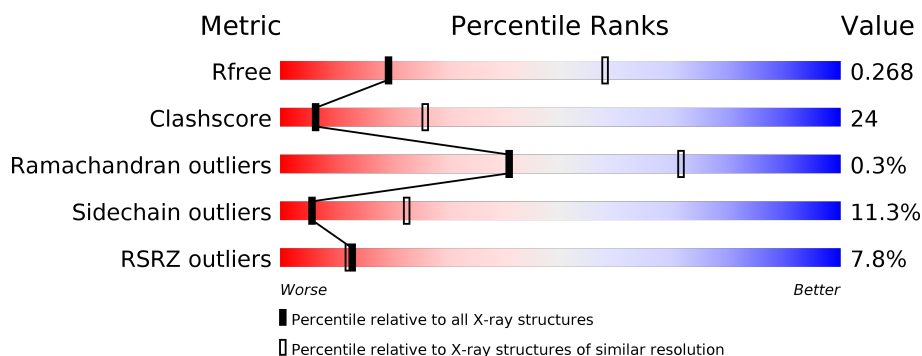
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1308	<div> <div>6%</div> <div>44%</div> <div>37%</div> <div>5%</div> <div>13%</div> </div>
1	B	1308	<div> <div>8%</div> <div>41%</div> <div>36%</div> <div>5%</div> <div>18%</div> </div>
1	C	1308	<div> <div>5%</div> <div>45%</div> <div>37%</div> <div>5%</div> <div>13%</div> </div>
1	D	1308	<div> <div>6%</div> <div>40%</div> <div>34%</div> <div>5%</div> <div>21%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34594 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 Fanconi anemia group I protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	B	1071	Total	C	N	O	S	0	0	0
			8487	5468	1409	1559	51			
1	C	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	D	1034	Total	C	N	O	S	0	0	0
			8187	5277	1358	1504	48			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1305	HIS	-	EXPRESSION TAG	UNP Q8K368

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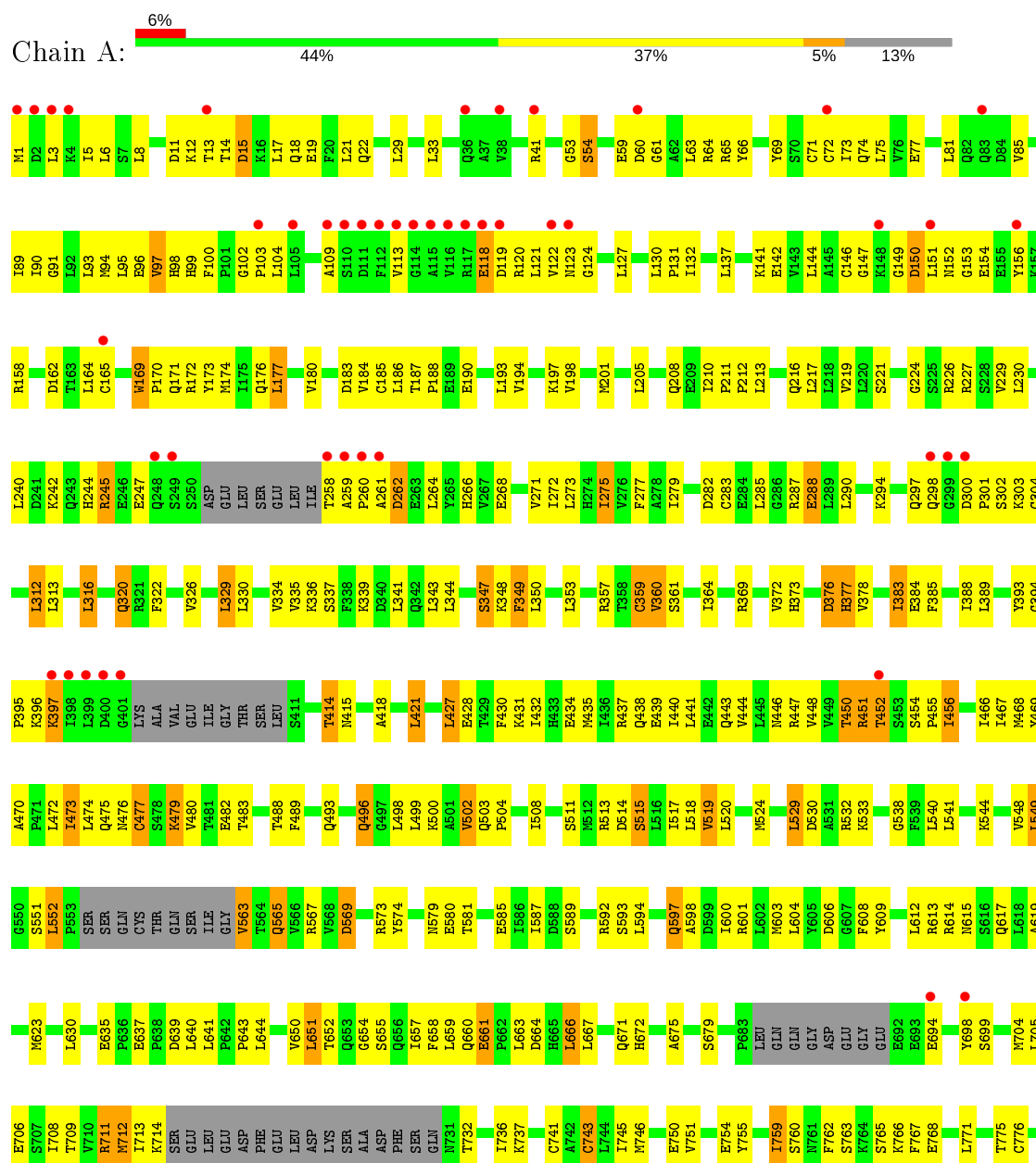
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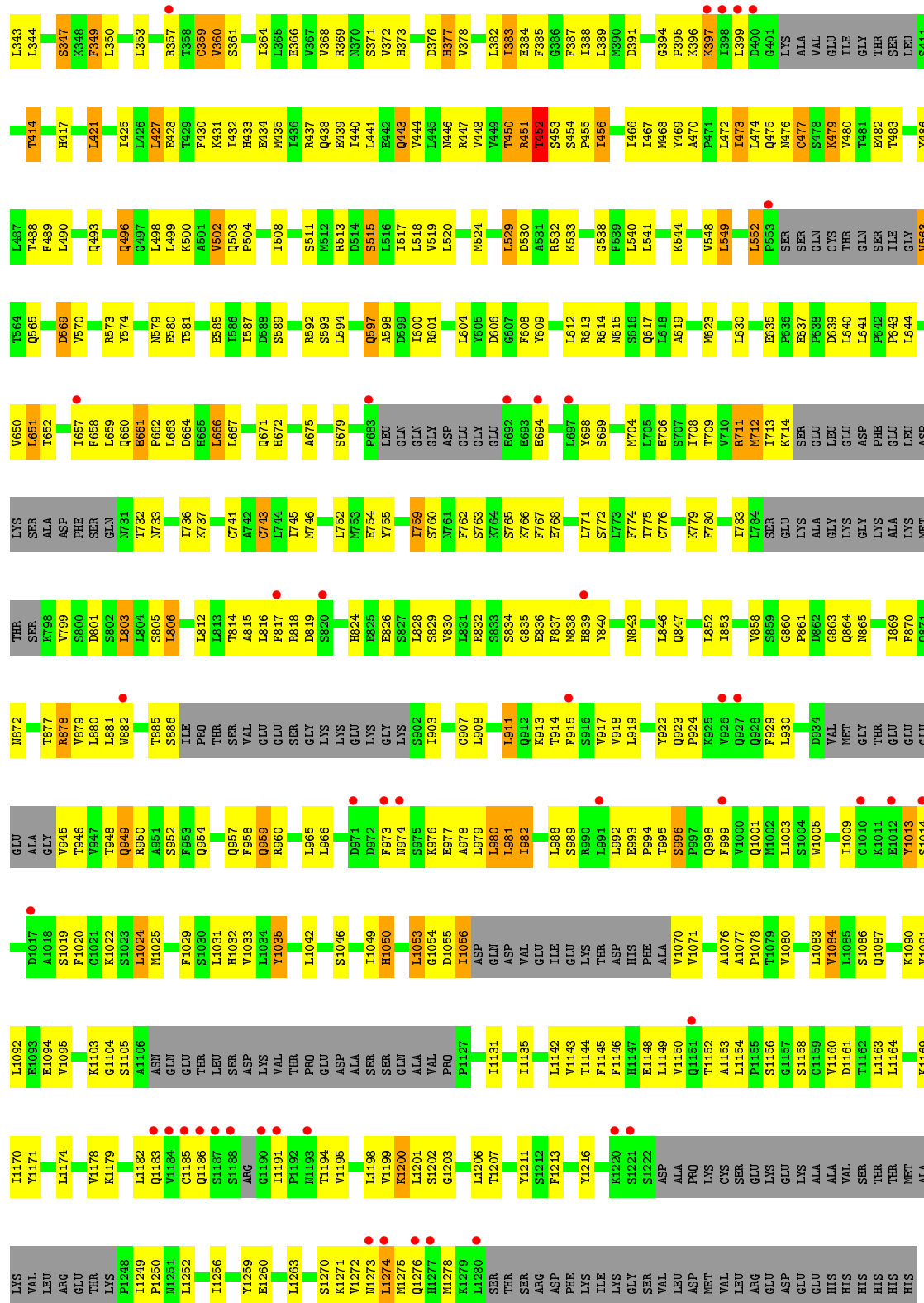
Chain	Residue	Modelled	Actual	Comment	Reference
D	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1308	HIS	-	EXPRESSION TAG	UNP Q8K368

3 Residue-property plots

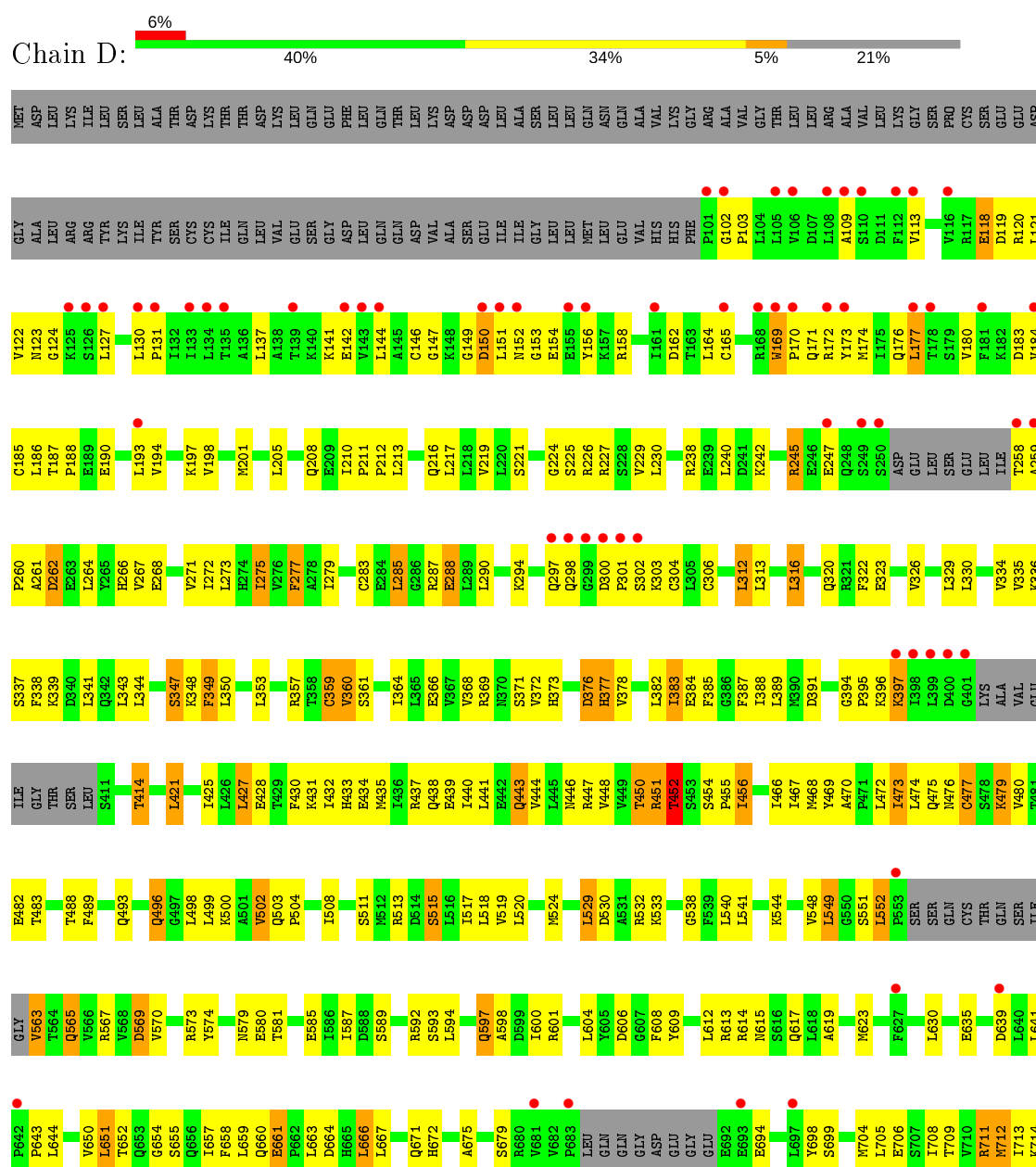
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

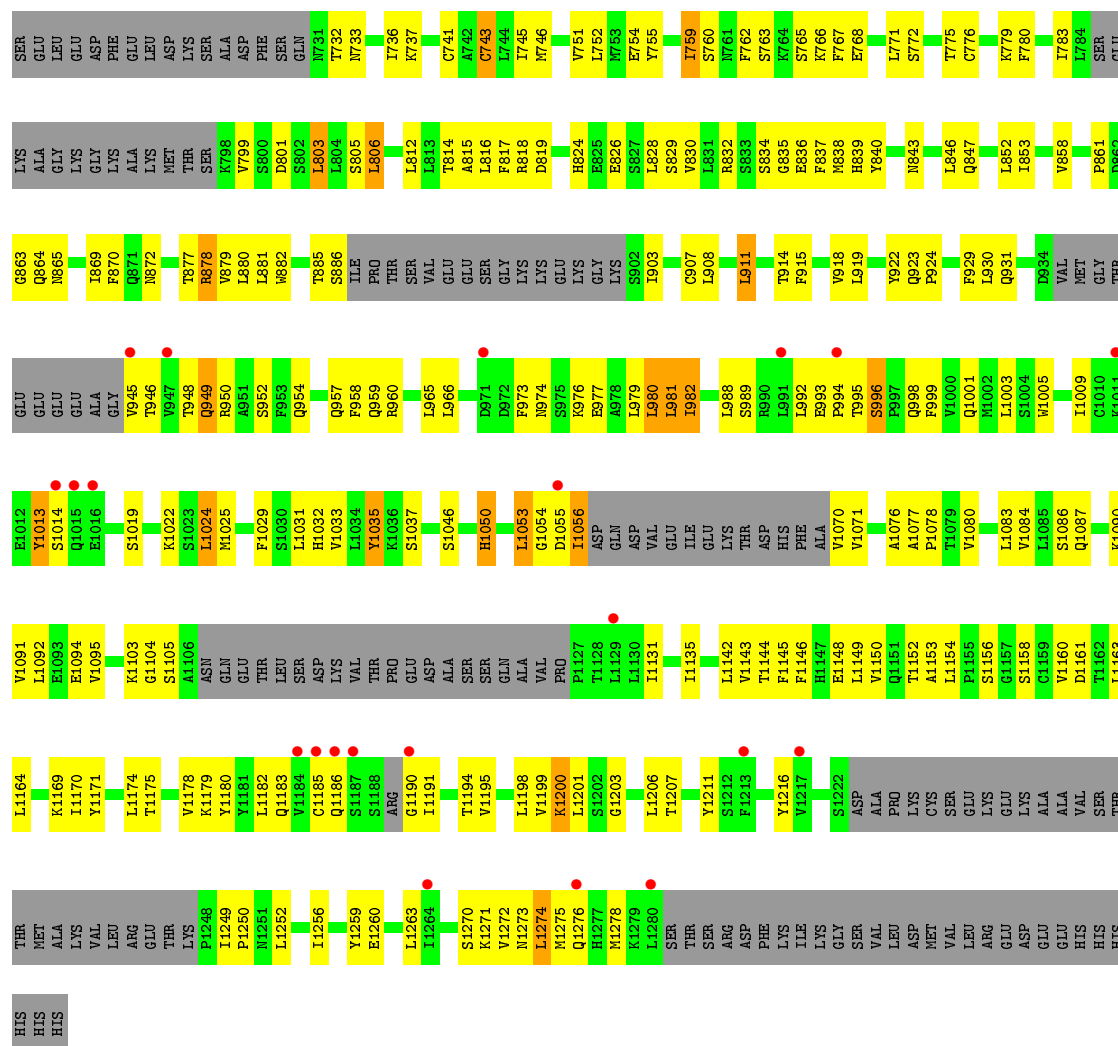
- Molecule 1: Fanconi anemia group I protein homolog





T995	F915	F837	S765	GLU	R613	P539	S454	I388	P301	G224	G149	E77	M1
S996	V918	M638	K766	E892	R614	L540	P456	M389	S302	G224	D150	L81	D2
Q998	L919	H839	F767	E694	R615	L541	I456	M390	K303	R226	N152	L81	K3
F999	L919	Y840	E768	E694	S616	K544	I466	D391	C304	R226	G153	D84	I5
V1000	Y922	N843	L771	Y698	L618	K544	I467	G384	L312	V229	E154	R85	L6
Q1001	Q923	Q923	S772	S699	A619	V543	M468	P395	L313	L230	E155	S7	S7
H1002	P924	L846	T775	M704	M623	L549	M468	P396	L316	L240	Y156	L89	L8
S1003	C776	Q847	C776	L705	M623	S551	Y469	K396	L316	L240	R158	I90	A9
W1005	L930	L852	C776	E706	F627	S551	M471	K397	Q320	K242	R158	G91	T10
I1009	Q931	I853	K779	S707	L630	P563	I473	L399	R321	R345	D162	L93	K12
E934	V858	F780	F780	I708	L630	SER	I474	D400	F322	E246	G165	L94	T13
Y1013	S859	I783	I783	I709	K631	SER	Q475	G401	E323	E247	G165	L95	T14
S1014	NET	L784	L784	V710	K631	GLN	M476	LYS	V326	E247	R168	E96	D15
G1019	GLY	SER	SER	R711	E635	CYS	C477	ALA	L329	ASP	K16	V97	K16
F1020	THR	GLU	GLU	M712	P636	THR	S478	VAL	L329	ASP	M169	H98	L17
C1021	GLU	LYS	LYS	I713	E637	GLN	K479	GLU	L330	GLU	P170	H99	Q18
K1022	GLU	ALA	ALA	K714	P638	SER	V480	ILE	L330	LEU	Q171	F100	E19
S1023	GLU	GLY	GLY	SER	D639	ILE	T481	GLY	V334	SER	R172	P101	F20
L1024	ALA	GLY	GLY	LEU	L640	V563	E482	THR	V335	GLU	M174	P103	L21
F1029	GLY	ASP	GLY	P642	L641	T564	T483	LEU	K336	LEU	I175	L104	Q22
S1030	V945	PHE	ALA	P643	L644	Q565	T488	S411	S337	ILE	Q176	L105	D28
L1031	T946	GLU	LYS	GLU	L644	D569	F489	T444	K339	A259	L177	L106	L29
H1032	V947	LEU	THR	LEU	V650	V570	Q493	H417	K339	A259	L177	L106	L29
V1033	R878	ASP	THR	ASP	L651	V570	Q493	H417	L341	A261	Y180	A109	L33
L1034	R879	SER	SER	LRS	T652	R573	Q496	G497	L341	A261	D183	S110	L33
Y1035	L880	ALA	G654	ALA	G653	Y574	G497	G497	Q342	E263	V184	D111	Q36
S952	S800	ASP	S655	ASP	G654	N579	L499	L421	L343	E263	C185	F112	A37
F953	D801	PHE	S655	PHE	G656	E580	L499	L421	L343	E263	C185	V113	V38
Q954	S802	SER	S655	SER	G656	T581	A501	L425	S347	H266	L186	G114	R41
S1046	L803	GLN	L667	GLN	L667	T581	F658	L425	K348	H266	L186	V116	A42
I1049	L806	ILE	L667	ILE	L667	E585	V502	L425	F349	E268	P188	R117	R41
H1050	L812	THR	L667	THR	L667	T587	P504	L425	L350	E268	E189	L118	A42
L1053	L813	SER	L667	SER	L667	D588	I508	L425	L350	E268	E189	E118	L47
G1054	T814	VAL	L667	VAL	L667	S589	I508	L425	L350	E268	E189	D119	R48
D1055	A815	GLU	L667	GLU	L667	S589	I508	L425	L350	E268	E189	R120	R48
I1056	L816	GLU	L667	GLU	L667	R592	S511	L425	L350	E268	E189	L121	L51
ASP	F817	SER	L667	SER	L667	S593	S511	L425	L350	E268	E189	V122	R52
GLN	R818	GLY	L667	GLN	L667	L594	S511	L425	L350	E268	E189	N123	G53
ASP	D819	THR	L667	ASP	L667	Q597	S511	L425	L350	E268	E189	G124	S54
ASP	H824	THR	L667	ASP	L667	A598	S511	L425	L350	E268	E189	K125	S54
VAL	E825	VAL	L667	VAL	L667	L600	S511	L425	L350	E268	E189	S126	B59
GLU	E826	GLU	L667	GLU	L667	B601	S511	L425	L350	E268	E189	L127	D60
GLY	S827	SER	L667	GLY	L667	L603	S511	L425	L350	E268	E189	L130	A62
LYS	S828	LYS	L667	LYS	L667	L603	S511	L425	L350	E268	E189	P131	L63
THR	S829	THR	L667	THR	L667	L603	S511	L425	L350	E268	E189	I132	R64
ASP	S830	ASP	L667	ASP	L667	L603	S511	L425	L350	E268	E189	L137	R65
HIS	S831	HIS	L667	HIS	L667	L603	S511	L425	L350	E268	E189	K141	Y66
PHE	S832	PHE	L667	PHE	L667	L603	S511	L425	L350	E268	E189	K141	Y66
ALA	S833	ALA	L667	ALA	L667	L603	S511	L425	L350	E268	E189	K141	Y66
V1070	V1071	V1070	L667	V1070	L667	L603	S511	L425	L350	E268	E189	K141	Y66
V1071	V1071	V1071	L667	V1071	L667	L603	S511	L425	L350	E268	E189	K141	Y66
A1076	A1076	A1076	L667	A1076	L667	L603	S511	L425	L350	E268	E189	K141	Y66





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	114.70 Å 136.50 Å 149.70 Å 115.90° 106.00° 95.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.82 – 3.28	Depositor EDS
% Data completeness (in resolution range)	82.8 (39.82-3.30) 83.1 (39.82-3.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.25 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.259 , 0.278 0.245 , 0.268	Depositor DCC
R_{free} test set	2199 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 117.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34594	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.26	2/9099 (0.0%)	0.46	0/12286
1	B	0.29	4/8624 (0.0%)	0.46	0/11646
1	C	0.26	2/9099 (0.0%)	0.46	0/12286
1	D	0.26	2/8319 (0.0%)	0.46	0/11234
All	All	0.27	10/35141 (0.0%)	0.46	0/47452

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	959	GLN	CD-NE2	-9.98	1.07	1.32
1	B	959	GLN	CD-OE1	-7.80	1.06	1.24
1	C	320	GLN	CD-NE2	-6.76	1.16	1.32
1	D	320	GLN	CD-NE2	-6.59	1.16	1.32
1	A	320	GLN	CD-NE2	-6.15	1.17	1.32
1	D	320	GLN	CD-OE1	-6.15	1.10	1.24
1	B	320	GLN	CD-NE2	-6.14	1.17	1.32
1	C	320	GLN	CD-OE1	-6.06	1.10	1.24
1	A	320	GLN	CD-OE1	-6.06	1.10	1.24
1	B	320	GLN	CD-OE1	-6.00	1.10	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	LEU	Peptide
1	B	1053	LEU	Peptide
1	C	1053	LEU	Peptide
1	D	1053	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8960	0	9275	454	0
1	B	8487	0	8776	449	0
1	C	8960	0	9275	435	0
1	D	8187	0	8476	411	0
All	All	34594	0	35802	1705	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 (1705) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:VAL:O	1:C:847:GLN:NE2	1.87	1.07
1:A:799:VAL:O	1:A:847:GLN:NE2	1.88	1.07
1:B:799:VAL:O	1:B:847:GLN:NE2	1.88	1.06
1:D:799:VAL:O	1:D:847:GLN:NE2	1.88	1.05
1:A:489:PHE:HB3	1:C:450:THR:HG21	1.35	1.04
1:A:450:THR:HG21	1:C:489:PHE:HB3	1.38	1.01
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.43	1.01
1:B:77:GLU:HB2	1:B:121:LEU:HA	1.43	1.00
1:D:259:ALA:HB3	1:D:260:PRO:HD3	1.44	0.99
1:C:259:ALA:HB3	1:C:260:PRO:HD3	1.43	0.99
1:B:259:ALA:HB3	1:B:260:PRO:HD3	1.43	0.97
1:A:376:ASP:HB2	1:B:570:VAL:HG21	1.45	0.96
1:B:672:HIS:ND1	1:B:861:PRO:HG3	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:MET:HA	1:B:129:LEU:HD21	1.48	0.93
1:A:671:GLN:HE21	1:A:755:TYR:HA	1.35	0.92
1:D:713:ILE:O	1:D:714:LYS:HG2	1.71	0.91
1:C:713:ILE:O	1:C:714:LYS:HG2	1.70	0.91
1:B:713:ILE:O	1:B:714:LYS:HG2	1.72	0.90
1:A:1055:ASP:H	1:A:1152:THR:HA	1.36	0.90
1:A:713:ILE:O	1:A:714:LYS:HG2	1.71	0.89
1:A:335:VAL:HG13	1:A:414:THR:HG21	1.54	0.89
1:A:29:LEU:O	1:A:33:LEU:HG	1.73	0.86
1:D:672:HIS:ND1	1:D:861:PRO:HG3	1.90	0.86
1:C:29:LEU:O	1:C:33:LEU:HG	1.74	0.86
1:B:452:THR:HA	1:D:452:THR:HA	1.58	0.85
1:C:598:ALA:HB2	1:C:660:GLN:HA	1.59	0.85
1:A:598:ALA:HB2	1:A:660:GLN:HA	1.59	0.85
1:A:641:LEU:O	1:A:643:PRO:HD3	1.78	0.84
1:B:1055:ASP:H	1:B:1152:THR:HA	1.43	0.83
1:B:598:ALA:HB2	1:B:660:GLN:HA	1.59	0.83
1:B:77:GLU:OE1	1:B:121:LEU:HD23	1.78	0.83
1:C:1055:ASP:H	1:C:1152:THR:HA	1.42	0.83
1:B:100:PHE:HD2	1:B:104:LEU:HB3	1.43	0.83
1:B:301:PRO:HA	1:B:304:CYS:HB2	1.60	0.83
1:D:1077:ALA:HB3	1:D:1078:PRO:HD3	1.61	0.83
1:C:1077:ALA:HB3	1:C:1078:PRO:HD3	1.61	0.83
1:C:301:PRO:HA	1:C:304:CYS:HB2	1.60	0.83
1:A:1077:ALA:HB3	1:A:1078:PRO:HD3	1.61	0.83
1:B:227:ARG:HG3	1:B:288:GLU:HG3	1.61	0.83
1:A:301:PRO:HA	1:A:304:CYS:HB2	1.60	0.82
1:D:598:ALA:HB2	1:D:660:GLN:HA	1.59	0.82
1:C:641:LEU:O	1:C:643:PRO:HD3	1.78	0.82
1:A:672:HIS:ND1	1:A:861:PRO:HG3	1.95	0.81
1:B:258:THR:N	1:B:261:ALA:HB3	1.95	0.81
1:D:1055:ASP:H	1:D:1152:THR:HA	1.45	0.81
1:A:258:THR:N	1:A:261:ALA:HB3	1.95	0.81
1:B:1077:ALA:HB3	1:B:1078:PRO:HD3	1.61	0.81
1:B:641:LEU:O	1:B:643:PRO:HD3	1.79	0.81
1:B:450:THR:HG21	1:D:489:PHE:HB3	1.63	0.81
1:D:301:PRO:HA	1:D:304:CYS:HB2	1.60	0.81
1:D:641:LEU:O	1:D:643:PRO:HD3	1.80	0.81
1:D:258:THR:N	1:D:261:ALA:HB3	1.96	0.80
1:C:1056:ILE:HG12	1:C:1153:ALA:HB2	1.64	0.80
1:D:217:LEU:HD22	1:D:229:VAL:HG13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:THR:N	1:C:261:ALA:HB3	1.96	0.79
1:C:217:LEU:HD22	1:C:229:VAL:HG13	1.63	0.79
1:C:65:ARG:HB3	1:C:100:PHE:HZ	1.48	0.79
1:A:217:LEU:HD22	1:A:229:VAL:HG13	1.63	0.78
1:C:427:LEU:HD22	1:C:431:LYS:HD2	1.65	0.78
1:A:302:SER:HB2	1:A:357:ARG:HG2	1.66	0.78
1:A:65:ARG:HB3	1:A:100:PHE:HZ	1.47	0.78
1:B:302:SER:HB2	1:B:357:ARG:HG2	1.66	0.78
1:D:302:SER:HB2	1:D:357:ARG:HG2	1.66	0.78
1:B:165:CYS:HB3	1:B:197:LYS:HG3	1.66	0.77
1:A:1054:GLY:HA3	1:A:1153:ALA:H	1.48	0.77
1:B:217:LEU:HD22	1:B:229:VAL:HG13	1.65	0.77
1:A:452:THR:HA	1:C:452:THR:HA	1.67	0.77
1:D:371:SER:OG	1:D:433:HIS:CE1	2.38	0.77
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.66	0.77
1:C:302:SER:HB2	1:C:357:ARG:HG2	1.66	0.77
1:C:671:GLN:HE21	1:C:755:TYR:HA	1.50	0.77
1:C:349:PHE:HD2	1:C:349:PHE:H	1.33	0.77
1:B:489:PHE:HB3	1:D:450:THR:HG21	1.66	0.77
1:B:1056:ILE:HG12	1:B:1153:ALA:HB2	1.67	0.76
1:A:470:ALA:O	1:A:473:ILE:HG13	1.86	0.76
1:C:470:ALA:O	1:C:473:ILE:HG13	1.86	0.76
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.67	0.76
1:D:377:HIS:CD2	1:D:377:HIS:H	2.05	0.75
1:B:149:GLY:O	1:B:151:LEU:N	2.19	0.75
1:B:65:ARG:HB3	1:B:100:PHE:HZ	1.51	0.75
1:C:377:HIS:H	1:C:377:HIS:CD2	2.04	0.75
1:B:470:ALA:O	1:B:473:ILE:HG13	1.86	0.75
1:D:371:SER:OG	1:D:433:HIS:HE1	1.70	0.75
1:C:1054:GLY:O	1:C:1055:ASP:HB2	1.87	0.75
1:D:165:CYS:HB3	1:D:197:LYS:HG3	1.66	0.75
1:D:259:ALA:CB	1:D:260:PRO:HD3	2.17	0.75
1:B:377:HIS:H	1:B:377:HIS:CD2	2.05	0.75
1:C:259:ALA:CB	1:C:260:PRO:HD3	2.16	0.75
1:B:94:MET:HA	1:B:129:LEU:CD2	2.16	0.75
1:B:349:PHE:H	1:B:349:PHE:HD2	1.33	0.75
1:A:349:PHE:H	1:A:349:PHE:HD2	1.33	0.75
1:A:377:HIS:H	1:A:377:HIS:CD2	2.04	0.75
1:B:338:PHE:CD2	1:B:414:THR:HG23	2.22	0.74
1:D:1054:GLY:O	1:D:1055:ASP:HB2	1.87	0.74
1:B:259:ALA:CB	1:B:260:PRO:HD3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:THR:HB	1:B:454:SER:H	1.51	0.74
1:D:427:LEU:HD22	1:D:431:LYS:HD2	1.69	0.74
1:D:452:THR:HB	1:D:454:SER:H	1.51	0.74
1:C:165:CYS:HB3	1:C:197:LYS:HG3	1.67	0.74
1:A:1054:GLY:O	1:A:1055:ASP:HB2	1.87	0.74
1:C:452:THR:HB	1:C:454:SER:H	1.51	0.74
1:D:1056:ILE:HG12	1:D:1153:ALA:HB2	1.68	0.74
1:D:470:ALA:O	1:D:473:ILE:HG13	1.87	0.74
1:B:1014:SER:HB3	1:B:1070:VAL:HG12	1.70	0.73
1:D:149:GLY:O	1:D:151:LEU:N	2.21	0.73
1:A:946:THR:O	1:A:950:ARG:HG2	1.88	0.73
1:A:1056:ILE:HG12	1:A:1153:ALA:HB2	1.70	0.73
1:A:1146:PHE:CD1	1:A:1170:ILE:HD11	2.23	0.73
1:B:474:LEU:O	1:B:477:CYS:HB2	1.89	0.73
1:A:149:GLY:O	1:A:151:LEU:N	2.20	0.73
1:B:1054:GLY:O	1:B:1055:ASP:HB2	1.87	0.73
1:B:1146:PHE:CD1	1:B:1170:ILE:HD11	2.23	0.73
1:B:1203:GLY:HA3	1:B:1278:MET:CG	2.19	0.73
1:A:1014:SER:HB3	1:A:1070:VAL:HG12	1.70	0.73
1:A:452:THR:HB	1:A:454:SER:H	1.51	0.73
1:C:1146:PHE:CD1	1:C:1170:ILE:HD11	2.23	0.73
1:B:297:GLN:HG3	1:B:1104:GLY:HA2	1.71	0.73
1:D:474:LEU:O	1:D:477:CYS:HB2	1.89	0.73
1:A:474:LEU:O	1:A:477:CYS:HB2	1.88	0.73
1:B:427:LEU:HD22	1:B:431:LYS:HD2	1.69	0.73
1:D:1014:SER:HB3	1:D:1070:VAL:HG12	1.70	0.73
1:B:946:THR:O	1:B:950:ARG:HG2	1.89	0.73
1:C:474:LEU:O	1:C:477:CYS:HB2	1.88	0.72
1:C:946:THR:O	1:C:950:ARG:HG2	1.88	0.72
1:A:548:VAL:O	1:A:549:LEU:HB3	1.89	0.72
1:D:1146:PHE:CD1	1:D:1170:ILE:HD11	2.23	0.72
1:B:297:GLN:HG3	1:B:1104:GLY:CA	2.19	0.72
1:B:548:VAL:O	1:B:549:LEU:HB3	1.88	0.72
1:D:349:PHE:HD2	1:D:349:PHE:H	1.33	0.72
1:C:1014:SER:HB3	1:C:1070:VAL:HG12	1.70	0.72
1:C:544:LYS:O	1:C:614:ARG:HD2	1.90	0.72
1:D:946:THR:O	1:D:950:ARG:HG2	1.89	0.72
1:A:931:GLN:HG2	1:A:950:ARG:NH1	2.05	0.71
1:C:389:LEU:HD13	1:C:421:LEU:HD23	1.73	0.71
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.17	0.71
1:A:335:VAL:HG13	1:A:414:THR:CG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:GLY:N	1:A:1271:LYS:HZ2	1.89	0.71
1:A:448:VAL:HA	1:A:456:ILE:HD13	1.73	0.71
1:B:451:ARG:HB3	1:B:456:ILE:HD11	1.73	0.71
1:D:372:VAL:HG22	1:D:432:ILE:CG2	2.21	0.70
1:C:1054:GLY:HA3	1:C:1153:ALA:H	1.56	0.70
1:A:94:MET:HG2	1:A:132:ILE:HD13	1.74	0.70
1:A:451:ARG:HB3	1:A:456:ILE:HD11	1.73	0.70
1:C:149:GLY:O	1:C:151:LEU:N	2.24	0.70
1:C:483:THR:HG21	1:C:498:LEU:HD21	1.73	0.70
1:A:389:LEU:HD13	1:A:421:LEU:HD23	1.72	0.70
1:D:548:VAL:O	1:D:549:LEU:HB3	1.90	0.70
1:A:483:THR:HG21	1:A:498:LEU:HD21	1.71	0.70
1:B:483:THR:HG21	1:B:498:LEU:HD21	1.72	0.70
1:B:227:ARG:HG3	1:B:288:GLU:CG	2.21	0.70
1:C:574:TYR:CE1	1:D:439:GLU:HG2	2.26	0.70
1:B:371:SER:OG	1:B:433:HIS:HE1	1.75	0.69
1:C:448:VAL:HA	1:C:456:ILE:HD13	1.74	0.69
1:C:548:VAL:O	1:C:549:LEU:HB3	1.89	0.69
1:D:448:VAL:HA	1:D:456:ILE:HD13	1.74	0.69
1:B:946:THR:HG22	1:B:950:ARG:HE	1.57	0.69
1:B:760:SER:HB2	1:B:766:LYS:HE2	1.75	0.69
1:C:946:THR:HG22	1:C:950:ARG:HE	1.57	0.69
1:C:1143:VAL:HG13	1:C:1206:LEU:HG	1.73	0.69
1:D:451:ARG:HB3	1:D:456:ILE:HD11	1.73	0.69
1:B:100:PHE:CD2	1:B:104:LEU:HB3	2.28	0.69
1:C:451:ARG:HB3	1:C:456:ILE:HD11	1.73	0.69
1:A:946:THR:HG22	1:A:950:ARG:HE	1.57	0.69
1:C:1190:GLY:N	1:C:1271:LYS:HZ2	1.91	0.69
1:C:672:HIS:ND1	1:C:861:PRO:HG3	2.07	0.69
1:D:428:GLU:O	1:D:432:ILE:HG12	1.93	0.69
1:B:94:MET:HG2	1:B:129:LEU:HG	1.74	0.69
1:D:483:THR:HG21	1:D:498:LEU:HD21	1.74	0.68
1:D:760:SER:HB2	1:D:766:LYS:HE2	1.75	0.68
1:B:672:HIS:CE1	1:B:861:PRO:HG3	2.29	0.68
1:A:369:ARG:O	1:A:372:VAL:HG23	1.94	0.68
1:B:1200:LYS:HB3	1:B:1274:LEU:HD21	1.74	0.68
1:B:371:SER:OG	1:B:433:HIS:CE1	2.46	0.68
1:B:428:GLU:O	1:B:432:ILE:HG12	1.94	0.68
1:B:448:VAL:HA	1:B:456:ILE:HD13	1.75	0.68
1:B:369:ARG:O	1:B:372:VAL:HG23	1.94	0.68
1:D:946:THR:HG22	1:D:950:ARG:HE	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1054:GLY:HA3	1:D:1153:ALA:H	1.58	0.67
1:A:1055:ASP:N	1:A:1152:THR:HA	2.07	0.67
1:A:760:SER:HB2	1:A:766:LYS:HE2	1.75	0.67
1:B:1143:VAL:HG13	1:B:1206:LEU:HG	1.75	0.67
1:C:760:SER:HB2	1:C:766:LYS:HE2	1.75	0.67
1:A:65:ARG:HB3	1:A:100:PHE:CZ	2.30	0.67
1:A:1154:LEU:HD11	1:A:1163:LEU:HD12	1.76	0.67
1:B:1200:LYS:HB3	1:B:1274:LEU:CD2	2.25	0.67
1:D:759:ILE:HG22	1:D:760:SER:N	2.09	0.67
1:B:1154:LEU:HD11	1:B:1163:LEU:HD12	1.76	0.67
1:B:275:ILE:HD11	1:B:312:LEU:HD11	1.76	0.67
1:D:275:ILE:HD11	1:D:312:LEU:HD11	1.75	0.67
1:B:713:ILE:HG21	1:B:772:SER:HB3	1.77	0.67
1:C:330:LEU:O	1:C:334:VAL:HG23	1.95	0.67
1:D:1154:LEU:HD11	1:D:1163:LEU:HD12	1.76	0.67
1:A:908:LEU:HD22	1:A:980:LEU:HG	1.77	0.67
1:B:452:THR:HG22	1:D:452:THR:HG22	1.77	0.67
1:A:470:ALA:HB3	1:A:473:ILE:HD11	1.77	0.67
1:A:759:ILE:HG22	1:A:760:SER:N	2.10	0.67
1:A:863:GLY:O	1:A:869:ILE:HD11	1.94	0.67
1:D:330:LEU:O	1:D:334:VAL:HG23	1.95	0.67
1:A:347:SER:HB2	1:A:349:PHE:CE2	2.31	0.66
1:B:1259:TYR:CZ	1:B:1263:LEU:HD11	2.30	0.66
1:C:1195:VAL:O	1:C:1199:VAL:HG23	1.95	0.66
1:A:428:GLU:O	1:A:432:ILE:HG12	1.95	0.66
1:C:759:ILE:HG22	1:C:760:SER:N	2.09	0.66
1:D:369:ARG:O	1:D:372:VAL:HG23	1.95	0.66
1:A:959:GLN:HB2	1:A:1005:TRP:CZ2	2.30	0.66
1:A:275:ILE:HD11	1:A:312:LEU:HD11	1.77	0.66
1:C:65:ARG:HB3	1:C:100:PHE:CZ	2.30	0.66
1:C:863:GLY:O	1:C:869:ILE:HD11	1.94	0.66
1:D:347:SER:HB2	1:D:349:PHE:CE2	2.31	0.66
1:B:1054:GLY:HA3	1:B:1153:ALA:H	1.58	0.66
1:B:759:ILE:HG22	1:B:760:SER:N	2.09	0.66
1:C:1154:LEU:HD11	1:C:1163:LEU:HD12	1.76	0.66
1:C:470:ALA:HB3	1:C:473:ILE:HD11	1.77	0.66
1:C:959:GLN:HB2	1:C:1005:TRP:CZ2	2.30	0.66
1:A:1259:TYR:CZ	1:A:1263:LEU:HD11	2.30	0.66
1:B:863:GLY:O	1:B:869:ILE:HD11	1.95	0.66
1:D:1203:GLY:HA3	1:D:1278:MET:CG	2.26	0.66
1:A:475:GLN:HG3	1:A:476:ASN:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLN:CB	1:B:1104:GLY:HA3	2.26	0.66
1:D:227:ARG:HG3	1:D:288:GLU:HG3	1.77	0.66
1:A:330:LEU:O	1:A:334:VAL:HG23	1.94	0.66
1:B:1203:GLY:HA3	1:B:1278:MET:HG2	1.78	0.66
1:D:1195:VAL:O	1:D:1199:VAL:HG23	1.96	0.66
1:A:1195:VAL:O	1:A:1199:VAL:HG23	1.96	0.66
1:B:1195:VAL:O	1:B:1199:VAL:HG23	1.96	0.66
1:C:369:ARG:O	1:C:372:VAL:HG23	1.95	0.66
1:C:428:GLU:O	1:C:432:ILE:HG12	1.94	0.66
1:D:959:GLN:HB2	1:D:1005:TRP:CZ2	2.31	0.66
1:C:275:ILE:HD11	1:C:312:LEU:HD11	1.77	0.65
1:C:33:LEU:HD23	1:C:75:LEU:HD11	1.78	0.65
1:D:863:GLY:O	1:D:869:ILE:HD11	1.95	0.65
1:B:475:GLN:HG3	1:B:476:ASN:H	1.62	0.65
1:B:347:SER:HB2	1:B:349:PHE:CE2	2.30	0.65
1:C:347:SER:HB2	1:C:349:PHE:CE2	2.30	0.65
1:D:650:VAL:HG21	1:D:737:LYS:HG3	1.78	0.65
1:D:907:CYS:O	1:D:911:LEU:HB2	1.96	0.65
1:D:475:GLN:HG3	1:D:476:ASN:H	1.62	0.65
1:C:335:VAL:HG13	1:C:414:THR:HG21	1.79	0.65
1:D:1259:TYR:CZ	1:D:1263:LEU:HD11	2.31	0.65
1:B:290:LEU:O	1:B:294:LYS:HG3	1.97	0.65
1:C:1259:TYR:CZ	1:C:1263:LEU:HD11	2.32	0.65
1:A:226:ARG:HB2	1:A:288:GLU:HG2	1.77	0.65
1:A:377:HIS:HD2	1:A:377:HIS:H	1.45	0.65
1:C:1164:LEU:HB3	1:C:1252:LEU:HD21	1.79	0.65
1:C:475:GLN:HG3	1:C:476:ASN:H	1.61	0.65
1:B:330:LEU:O	1:B:334:VAL:HG23	1.96	0.64
1:C:907:CYS:O	1:C:911:LEU:HB2	1.97	0.64
1:A:907:CYS:O	1:A:911:LEU:HB2	1.96	0.64
1:B:470:ALA:HB3	1:B:473:ILE:HD11	1.78	0.64
1:D:120:ARG:HG2	1:D:172:ARG:NH1	2.13	0.64
1:B:361:SER:HG	1:B:417:HIS:CE1	2.16	0.64
1:D:470:ALA:HB3	1:D:473:ILE:HD11	1.80	0.64
1:B:959:GLN:HB2	1:B:1005:TRP:CZ2	2.32	0.64
1:C:298:GLN:HE21	1:C:336:LYS:HG2	1.63	0.64
1:B:548:VAL:HG11	1:B:580:GLU:O	1.97	0.64
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.12	0.64
1:A:290:LEU:O	1:A:294:LYS:HG3	1.97	0.64
1:A:434:GLU:HG2	1:B:472:LEU:HD21	1.79	0.64
1:A:431:LYS:HE3	1:A:469:TYR:CE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLN:HE21	1:B:336:LYS:HG2	1.62	0.64
1:B:907:CYS:O	1:B:911:LEU:HB2	1.96	0.64
1:D:431:LYS:HE3	1:D:469:TYR:CE1	2.32	0.64
1:D:1160:VAL:O	1:D:1164:LEU:HG	1.98	0.64
1:B:377:HIS:H	1:B:377:HIS:HD2	1.46	0.64
1:D:548:VAL:HG11	1:D:580:GLU:O	1.96	0.64
1:B:671:GLN:OE1	1:B:672:HIS:CD2	2.50	0.63
1:D:1200:LYS:HB3	1:D:1274:LEU:HD21	1.79	0.63
1:D:1203:GLY:HA3	1:D:1278:MET:HG2	1.80	0.63
1:C:712:MET:HA	1:C:712:MET:HE2	1.80	0.63
1:A:169:TRP:CD1	1:A:169:TRP:N	2.66	0.63
1:A:298:GLN:HE21	1:A:336:LYS:HG2	1.63	0.63
1:C:1160:VAL:O	1:C:1164:LEU:HG	1.98	0.63
1:D:245:ARG:NH1	1:D:366:GLU:OE2	2.31	0.63
1:B:1160:VAL:O	1:B:1164:LEU:HG	1.98	0.63
1:B:169:TRP:H	1:B:169:TRP:HD1	1.47	0.63
1:B:372:VAL:HG22	1:B:432:ILE:CG2	2.28	0.63
1:C:120:ARG:HG2	1:C:172:ARG:NH1	2.13	0.63
1:C:431:LYS:HE3	1:C:469:TYR:CE1	2.33	0.63
1:A:931:GLN:HG2	1:A:950:ARG:HH12	1.64	0.63
1:B:431:LYS:HE3	1:B:469:TYR:CE1	2.33	0.63
1:D:290:LEU:O	1:D:294:LYS:HG3	1.98	0.63
1:C:708:ILE:O	1:C:712:MET:HB2	1.99	0.63
1:A:1056:ILE:HD12	1:A:1216:TYR:CD1	2.34	0.62
1:C:551:SER:C	1:D:277:PHE:HZ	2.02	0.62
1:C:290:LEU:O	1:C:294:LYS:HG3	1.99	0.62
1:C:377:HIS:H	1:C:377:HIS:HD2	1.45	0.62
1:A:1198:LEU:HD22	1:A:1201:LEU:HD13	1.81	0.62
1:A:712:MET:HA	1:A:712:MET:HE2	1.80	0.62
1:B:120:ARG:HG2	1:B:172:ARG:NH1	2.13	0.62
1:B:169:TRP:CD1	1:B:169:TRP:N	2.66	0.62
1:D:169:TRP:N	1:D:169:TRP:CD1	2.67	0.62
1:C:499:LEU:HB3	1:C:541:LEU:HD13	1.82	0.62
1:B:245:ARG:NH1	1:B:366:GLU:OE2	2.32	0.62
1:B:1046:SER:O	1:B:1050:HIS:HB3	1.99	0.62
1:B:708:ILE:O	1:B:712:MET:HB2	2.00	0.62
1:C:1046:SER:O	1:C:1050:HIS:HB3	1.99	0.62
1:D:708:ILE:O	1:D:712:MET:HB2	1.99	0.62
1:A:94:MET:HG2	1:A:132:ILE:CD1	2.29	0.62
1:B:1198:LEU:HD22	1:B:1201:LEU:HD13	1.81	0.62
1:B:609:TYR:CZ	1:B:613:ARG:HD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:HIS:N	1:C:377:HIS:CD2	2.67	0.62
1:D:1046:SER:O	1:D:1050:HIS:HB3	1.99	0.62
1:D:372:VAL:HG22	1:D:432:ILE:HG21	1.82	0.62
1:A:574:TYR:CE1	1:B:439:GLU:HG2	2.35	0.62
1:A:948:THR:HG23	1:A:992:LEU:HA	1.81	0.62
1:B:230:LEU:HD21	1:B:285:LEU:HD21	1.81	0.62
1:C:397:LYS:H	1:C:397:LYS:HD3	1.65	0.62
1:D:348:LYS:HG2	1:D:1035:TYR:O	2.00	0.62
1:D:298:GLN:HE21	1:D:336:LYS:HG2	1.63	0.62
1:A:190:GLU:O	1:A:194:VAL:HG23	2.00	0.62
1:A:377:HIS:N	1:A:377:HIS:CD2	2.67	0.62
1:B:65:ARG:HB3	1:B:100:PHE:CZ	2.31	0.62
1:B:650:VAL:HG21	1:B:737:LYS:HG3	1.82	0.62
1:D:245:ARG:HD2	1:D:366:GLU:OE1	2.00	0.62
1:D:609:TYR:CZ	1:D:613:ARG:HD2	2.34	0.62
1:A:708:ILE:O	1:A:712:MET:HB2	1.99	0.61
1:C:190:GLU:O	1:C:194:VAL:HG23	2.00	0.61
1:C:877:THR:OG1	1:C:914:THR:HG21	2.00	0.61
1:D:397:LYS:HD3	1:D:397:LYS:H	1.65	0.61
1:C:434:GLU:HG2	1:D:472:LEU:HD21	1.81	0.61
1:C:609:TYR:CZ	1:C:613:ARG:HD2	2.35	0.61
1:A:1179:LYS:HA	1:A:1182:LEU:HD12	1.82	0.61
1:A:397:LYS:HD3	1:A:397:LYS:H	1.65	0.61
1:B:948:THR:HG23	1:B:992:LEU:HA	1.81	0.61
1:D:1200:LYS:HB3	1:D:1274:LEU:CD2	2.31	0.61
1:D:190:GLU:O	1:D:194:VAL:HG23	2.00	0.61
1:D:948:THR:HG23	1:D:992:LEU:HA	1.82	0.61
1:B:877:THR:OG1	1:B:914:THR:HG21	2.00	0.61
1:C:1198:LEU:HD22	1:C:1201:LEU:HD13	1.81	0.61
1:C:169:TRP:N	1:C:169:TRP:CD1	2.67	0.61
1:C:472:LEU:HD21	1:D:434:GLU:HG2	1.82	0.61
1:C:713:ILE:HG21	1:C:772:SER:HB3	1.81	0.61
1:C:948:THR:HG23	1:C:992:LEU:HA	1.81	0.61
1:D:377:HIS:CD2	1:D:377:HIS:N	2.68	0.61
1:A:1160:VAL:O	1:A:1164:LEU:HG	1.99	0.61
1:A:475:GLN:HG3	1:A:476:ASN:N	2.16	0.61
1:B:190:GLU:O	1:B:194:VAL:HG23	2.00	0.61
1:B:377:HIS:N	1:B:377:HIS:CD2	2.68	0.61
1:C:33:LEU:HD22	1:C:75:LEU:HD21	1.81	0.61
1:A:348:LYS:HG2	1:A:1035:TYR:O	2.00	0.61
1:D:169:TRP:H	1:D:169:TRP:HD1	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:TYR:CZ	1:A:613:ARG:HD2	2.35	0.61
1:B:779:LYS:O	1:B:783:ILE:HG13	2.01	0.61
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.82	0.61
1:D:338:PHE:CD2	1:D:414:THR:HG23	2.36	0.61
1:A:11:ASP:O	1:A:12:LYS:HG2	2.01	0.61
1:B:1179:LYS:HA	1:B:1182:LEU:HD12	1.82	0.61
1:C:475:GLN:HG3	1:C:476:ASN:N	2.15	0.61
1:D:187:THR:HG22	1:D:188:PRO:HD2	1.83	0.61
1:A:877:THR:OG1	1:A:914:THR:HG21	2.01	0.60
1:B:397:LYS:HD3	1:B:397:LYS:H	1.66	0.60
1:C:349:PHE:N	1:C:349:PHE:CD2	2.68	0.60
1:D:779:LYS:O	1:D:783:ILE:HG13	2.01	0.60
1:A:1046:SER:O	1:A:1050:HIS:HB3	1.99	0.60
1:C:13:THR:HA	1:C:17:LEU:HD12	1.83	0.60
1:B:1076:ALA:HA	1:B:1080:VAL:HB	1.83	0.60
1:B:499:LEU:HB3	1:B:541:LEU:HD13	1.82	0.60
1:C:1203:GLY:HA3	1:C:1278:MET:CG	2.30	0.60
1:D:1249:ILE:N	1:D:1250:PRO:HD2	2.16	0.60
1:B:100:PHE:O	1:B:105:LEU:HG	2.00	0.60
1:B:1249:ILE:N	1:B:1250:PRO:HD2	2.16	0.60
1:C:1076:ALA:HA	1:C:1080:VAL:HB	1.83	0.60
1:C:1249:ILE:N	1:C:1250:PRO:HD2	2.16	0.60
1:D:1198:LEU:HD22	1:D:1201:LEU:HD13	1.81	0.60
1:D:1076:ALA:HA	1:D:1080:VAL:HB	1.83	0.60
1:A:779:LYS:O	1:A:783:ILE:HG13	2.02	0.60
1:B:338:PHE:HD2	1:B:414:THR:HG23	1.65	0.60
1:A:499:LEU:HB3	1:A:541:LEU:HD13	1.83	0.60
1:B:121:LEU:C	1:B:123:ASN:H	2.05	0.60
1:B:475:GLN:HG3	1:B:476:ASN:N	2.16	0.60
1:C:1179:LYS:HA	1:C:1182:LEU:HD12	1.82	0.60
1:C:11:ASP:O	1:C:12:LYS:HG2	2.01	0.60
1:C:548:VAL:HG11	1:C:580:GLU:O	2.01	0.60
1:D:529:LEU:HG	1:D:597:GLN:HG3	1.83	0.60
1:D:877:THR:OG1	1:D:914:THR:HG21	2.01	0.60
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.82	0.60
1:A:21:LEU:HD13	1:A:64:ARG:HD3	1.82	0.60
1:C:779:LYS:O	1:C:783:ILE:HG13	2.01	0.60
1:A:169:TRP:HD1	1:A:169:TRP:H	1.47	0.60
1:C:169:TRP:HD1	1:C:169:TRP:H	1.47	0.60
1:C:480:VAL:O	1:C:483:THR:HB	2.02	0.60
1:D:1179:LYS:HA	1:D:1182:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:PHE:N	1:D:349:PHE:CD2	2.68	0.60
1:B:1022:LYS:HA	1:B:1083:LEU:HD11	1.84	0.59
1:D:1022:LYS:HA	1:D:1083:LEU:HD11	1.84	0.59
1:D:1055:ASP:N	1:D:1152:THR:HA	2.17	0.59
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.16	0.59
1:A:124:GLY:O	1:A:127:LEU:N	2.36	0.59
1:A:72:CYS:HB2	1:A:93:LEU:HD11	1.84	0.59
1:A:930:LEU:HD13	1:A:950:ARG:HB2	1.84	0.59
1:D:1190:GLY:N	1:D:1271:LYS:HZ1	2.00	0.59
1:A:529:LEU:HG	1:A:597:GLN:HG3	1.84	0.59
1:B:187:THR:HG22	1:B:188:PRO:HD2	1.83	0.59
1:C:989:SER:HB2	1:C:1031:LEU:HD21	1.83	0.59
1:C:1055:ASP:N	1:C:1152:THR:HA	2.13	0.59
1:C:121:LEU:C	1:C:123:ASN:H	2.06	0.59
1:C:187:THR:HG22	1:C:188:PRO:HD2	1.83	0.59
1:D:480:VAL:O	1:D:483:THR:HB	2.03	0.59
1:A:13:THR:HA	1:A:17:LEU:HD12	1.84	0.59
1:C:570:VAL:HG21	1:D:376:ASP:HB2	1.83	0.59
1:D:230:LEU:HD21	1:D:285:LEU:HD21	1.83	0.59
1:D:741:CYS:O	1:D:745:ILE:HG13	2.03	0.59
1:A:480:VAL:O	1:A:483:THR:HB	2.03	0.59
1:D:499:LEU:HB3	1:D:541:LEU:HD13	1.82	0.59
1:A:672:HIS:HE1	1:A:805:SER:HB3	1.67	0.59
1:B:102:GLY:HA3	1:B:144:LEU:HD22	1.83	0.59
1:B:372:VAL:HG22	1:B:432:ILE:HG21	1.83	0.59
1:C:982:ILE:HD11	1:C:1024:LEU:HG	1.84	0.59
1:C:102:GLY:HA3	1:C:144:LEU:HD22	1.85	0.59
1:A:18:GLN:HG2	1:A:53:GLY:O	2.03	0.59
1:A:518:LEU:HD11	1:D:518:LEU:HD11	1.85	0.58
1:B:671:GLN:OE1	1:B:672:HIS:HD2	1.85	0.58
1:D:1143:VAL:HG13	1:D:1206:LEU:HG	1.84	0.58
1:D:475:GLN:HG3	1:D:476:ASN:N	2.17	0.58
1:D:671:GLN:HE21	1:D:755:TYR:HA	1.68	0.58
1:A:1087:GLN:O	1:A:1091:VAL:HG23	2.03	0.58
1:B:349:PHE:CD2	1:B:349:PHE:N	2.68	0.58
1:C:1022:LYS:HA	1:C:1083:LEU:HD11	1.85	0.58
1:D:102:GLY:HA3	1:D:144:LEU:HD22	1.85	0.58
1:D:227:ARG:HG3	1:D:288:GLU:CG	2.33	0.58
1:B:275:ILE:CD1	1:B:312:LEU:HD11	2.34	0.58
1:A:472:LEU:HD21	1:B:434:GLU:HG2	1.85	0.58
1:C:1200:LYS:HB3	1:C:1274:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:O	1:A:614:ARG:HD2	2.02	0.58
1:C:124:GLY:O	1:C:127:LEU:N	2.35	0.58
1:C:741:CYS:O	1:C:745:ILE:HG13	2.03	0.58
1:A:372:VAL:HG22	1:A:432:ILE:CG2	2.33	0.58
1:B:245:ARG:HD2	1:B:366:GLU:OE1	2.03	0.58
1:D:121:LEU:C	1:D:123:ASN:H	2.06	0.58
1:B:102:GLY:N	1:B:103:PRO:HD2	2.18	0.58
1:B:1164:LEU:HB3	1:B:1252:LEU:HD21	1.85	0.58
1:B:395:PRO:O	1:B:455:PRO:HG2	2.03	0.58
1:B:480:VAL:O	1:B:483:THR:HB	2.03	0.58
1:B:72:CYS:HB2	1:B:93:LEU:HD11	1.85	0.58
1:B:1055:ASP:N	1:B:1152:THR:HA	2.15	0.58
1:C:72:CYS:HB2	1:C:93:LEU:HD11	1.85	0.58
1:C:18:GLN:HG2	1:C:53:GLY:O	2.03	0.58
1:D:275:ILE:CD1	1:D:312:LEU:HD11	2.33	0.58
1:D:377:HIS:HD2	1:D:377:HIS:H	1.46	0.58
1:A:496:GLN:O	1:A:500:LYS:HG2	2.03	0.58
1:B:297:GLN:CG	1:B:1104:GLY:HA3	2.34	0.58
1:A:121:LEU:C	1:A:123:ASN:H	2.05	0.58
1:A:349:PHE:N	1:A:349:PHE:CD2	2.68	0.58
1:B:1087:GLN:O	1:B:1091:VAL:HG23	2.04	0.58
1:B:741:CYS:O	1:B:745:ILE:HG13	2.04	0.58
1:C:529:LEU:HG	1:C:597:GLN:HG3	1.85	0.58
1:A:1022:LYS:HA	1:A:1083:LEU:HD11	1.84	0.57
1:A:102:GLY:HA3	1:A:144:LEU:HD22	1.85	0.57
1:B:518:LEU:HD11	1:C:518:LEU:HD11	1.85	0.57
1:B:313:LEU:HB3	1:B:326:VAL:HG13	1.86	0.57
1:C:300:ASP:O	1:C:304:CYS:N	2.38	0.57
1:C:760:SER:HB2	1:C:766:LYS:HZ1	1.68	0.57
1:D:496:GLN:O	1:D:500:LYS:HG2	2.04	0.57
1:D:835:GLY:HA2	1:D:838:MET:HB2	1.87	0.57
1:A:131:PRO:HA	1:A:184:VAL:HG22	1.87	0.57
1:A:1203:GLY:HA3	1:A:1278:MET:HG2	1.86	0.57
1:D:1087:GLN:O	1:D:1091:VAL:HG23	2.03	0.57
1:D:118:GLU:HA	1:D:118:GLU:OE1	2.05	0.57
1:C:1203:GLY:HA3	1:C:1278:MET:HG2	1.86	0.57
1:C:21:LEU:HD13	1:C:64:ARG:HD3	1.87	0.57
1:C:977:GLU:O	1:C:981:LEU:HB2	2.05	0.57
1:A:102:GLY:N	1:A:103:PRO:HD2	2.20	0.57
1:A:671:GLN:CG	1:A:755:TYR:HB2	2.34	0.57
1:C:713:ILE:C	1:C:714:LYS:HG2	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:PHE:HD1	1:C:922:TYR:HD2	1.53	0.57
1:D:300:ASP:O	1:D:304:CYS:N	2.38	0.57
1:A:741:CYS:O	1:A:745:ILE:HG13	2.05	0.57
1:C:496:GLN:O	1:C:500:LYS:HG2	2.05	0.57
1:C:650:VAL:HG21	1:C:737:LYS:HG3	1.85	0.57
1:D:131:PRO:HA	1:D:184:VAL:HG22	1.87	0.57
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.05	0.56
1:B:131:PRO:HA	1:B:184:VAL:HG22	1.86	0.56
1:B:297:GLN:HG3	1:B:1104:GLY:HA3	1.87	0.56
1:B:977:GLU:O	1:B:981:LEU:HB2	2.04	0.56
1:C:1087:GLN:O	1:C:1091:VAL:HG23	2.05	0.56
1:C:430:PHE:CE2	1:C:466:ILE:HG23	2.40	0.56
1:D:259:ALA:HB3	1:D:260:PRO:CD	2.29	0.56
1:D:313:LEU:HB3	1:D:326:VAL:HG13	1.86	0.56
1:A:300:ASP:O	1:A:304:CYS:N	2.38	0.56
1:A:593:SER:HB2	1:A:600:ILE:HG21	1.87	0.56
1:A:439:GLU:HG2	1:B:574:TYR:CE1	2.39	0.56
1:B:713:ILE:C	1:B:714:LYS:HG2	2.25	0.56
1:D:977:GLU:O	1:D:981:LEU:HB2	2.05	0.56
1:B:300:ASP:O	1:B:304:CYS:N	2.38	0.56
1:C:313:LEU:HB3	1:C:326:VAL:HG13	1.87	0.56
1:C:835:GLY:HA2	1:C:838:MET:HB2	1.87	0.56
1:D:102:GLY:N	1:D:103:PRO:HD2	2.20	0.56
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.05	0.56
1:A:430:PHE:CE2	1:A:466:ILE:HG23	2.40	0.56
1:B:496:GLN:O	1:B:500:LYS:HG2	2.05	0.56
1:C:1146:PHE:CE1	1:C:1170:ILE:HD11	2.41	0.56
1:D:1146:PHE:O	1:D:1150:VAL:HG23	2.06	0.56
1:B:870:PHE:HD1	1:B:922:TYR:HD2	1.53	0.56
1:C:275:ILE:CD1	1:C:312:LEU:HD11	2.35	0.56
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.36	0.56
1:A:389:LEU:CD1	1:A:421:LEU:HD23	2.36	0.56
1:A:870:PHE:HD1	1:A:922:TYR:HD2	1.53	0.56
1:B:150:ASP:OD1	1:B:151:LEU:HG	2.06	0.56
1:B:593:SER:HB2	1:B:600:ILE:HG21	1.88	0.56
1:C:150:ASP:OD1	1:C:151:LEU:HG	2.06	0.56
1:D:870:PHE:HD1	1:D:922:TYR:HD2	1.53	0.56
1:B:103:PRO:HA	1:B:146:CYS:SG	2.45	0.56
1:C:102:GLY:N	1:C:103:PRO:HD2	2.21	0.56
1:C:1146:PHE:O	1:C:1150:VAL:HG23	2.06	0.56
1:C:194:VAL:O	1:C:198:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:PRO:HA	1:D:146:CYS:SG	2.46	0.56
1:A:313:LEU:HB3	1:A:326:VAL:HG13	1.87	0.56
1:B:124:GLY:O	1:B:127:LEU:N	2.37	0.56
1:D:713:ILE:C	1:D:714:LYS:HG2	2.25	0.56
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.06	0.56
1:B:1146:PHE:O	1:B:1150:VAL:HG23	2.06	0.56
1:B:194:VAL:O	1:B:198:VAL:HG23	2.06	0.56
1:B:712:MET:HE2	1:B:712:MET:HA	1.88	0.56
1:C:451:ARG:HB3	1:C:456:ILE:CD1	2.36	0.56
1:D:760:SER:HB2	1:D:766:LYS:HZ1	1.70	0.56
1:D:930:LEU:HD13	1:D:950:ARG:HB2	1.88	0.56
1:A:150:ASP:OD1	1:A:151:LEU:HG	2.06	0.55
1:A:194:VAL:O	1:A:198:VAL:HG23	2.06	0.55
1:B:908:LEU:HD11	1:B:981:LEU:HG	1.88	0.55
1:C:439:GLU:HG2	1:D:574:TYR:CE1	2.41	0.55
1:D:372:VAL:HG22	1:D:432:ILE:HG23	1.88	0.55
1:C:376:ASP:HB2	1:D:570:VAL:HG21	1.87	0.55
1:D:672:HIS:CE1	1:D:861:PRO:HG3	2.39	0.55
1:A:1146:PHE:CE1	1:A:1170:ILE:HD11	2.41	0.55
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.87	0.55
1:A:977:GLU:O	1:A:981:LEU:HB2	2.05	0.55
1:B:982:ILE:HD11	1:B:1024:LEU:HG	1.88	0.55
1:B:544:LYS:O	1:B:614:ARG:HD2	2.06	0.55
1:C:760:SER:HB2	1:C:766:LYS:CE	2.36	0.55
1:D:1146:PHE:CE1	1:D:1170:ILE:HD11	2.41	0.55
1:D:187:THR:CG2	1:D:188:PRO:HD2	2.37	0.55
1:D:451:ARG:HB3	1:D:456:ILE:CD1	2.35	0.55
1:A:65:ARG:HD3	1:A:100:PHE:CE1	2.41	0.55
1:A:384:GLU:O	1:A:388:ILE:HG13	2.07	0.55
1:A:395:PRO:O	1:A:455:PRO:HG2	2.05	0.55
1:A:661:GLU:OE1	1:A:666:LEU:HD12	2.06	0.55
1:A:713:ILE:C	1:A:714:LYS:HG2	2.26	0.55
1:B:664:ASP:HB2	1:B:803:LEU:CD1	2.37	0.55
1:C:661:GLU:OE1	1:C:666:LEU:HD12	2.06	0.55
1:C:979:LEU:HD11	1:C:1019:SER:HB2	1.87	0.55
1:A:103:PRO:HA	1:A:146:CYS:SG	2.47	0.55
1:B:1146:PHE:CE1	1:B:1170:ILE:HD11	2.41	0.55
1:C:131:PRO:HA	1:C:184:VAL:HG22	1.87	0.55
1:C:615:ASN:OD1	1:C:617:GLN:HG2	2.06	0.55
1:C:65:ARG:HD3	1:C:100:PHE:CE1	2.42	0.55
1:D:704:MET:O	1:D:708:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:760:SER:HB2	1:D:766:LYS:CE	2.36	0.55
1:C:277:PHE:HZ	1:D:551:SER:C	2.10	0.55
1:A:479:LYS:HE2	1:A:482:GLU:OE1	2.07	0.55
1:A:760:SER:HB2	1:A:766:LYS:CE	2.36	0.55
1:B:187:THR:CG2	1:B:188:PRO:HD2	2.37	0.55
1:B:391:ASP:OD2	1:B:447:ARG:NH1	2.39	0.55
1:B:835:GLY:HA2	1:B:838:MET:HB2	1.87	0.55
1:D:124:GLY:O	1:D:127:LEU:N	2.38	0.55
1:B:451:ARG:HB3	1:B:456:ILE:CD1	2.35	0.55
1:D:479:LYS:HE2	1:D:482:GLU:OE1	2.07	0.55
1:D:593:SER:OG	1:D:604:LEU:HD22	2.07	0.55
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.88	0.55
1:B:479:LYS:HE2	1:B:482:GLU:OE1	2.06	0.55
1:B:593:SER:OG	1:B:604:LEU:HD22	2.07	0.55
1:C:103:PRO:HA	1:C:146:CYS:SG	2.46	0.55
1:D:194:VAL:O	1:D:198:VAL:HG23	2.06	0.55
1:D:826:GLU:O	1:D:830:VAL:HG23	2.07	0.55
1:B:661:GLU:OE1	1:B:666:LEU:HD12	2.07	0.55
1:D:1029:PHE:O	1:D:1033:VAL:HG23	2.07	0.55
1:D:150:ASP:OD1	1:D:151:LEU:HG	2.06	0.55
1:A:1054:GLY:CA	1:A:1152:THR:HG23	2.37	0.55
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.36	0.55
1:A:372:VAL:HG22	1:A:432:ILE:HG21	1.88	0.55
1:A:483:THR:CG2	1:A:498:LEU:HD21	2.37	0.55
1:C:118:GLU:HA	1:C:118:GLU:OE1	2.07	0.55
1:D:176:GLN:O	1:D:180:VAL:HG23	2.07	0.55
1:D:430:PHE:CE2	1:D:466:ILE:HG23	2.42	0.55
1:A:451:ARG:HB3	1:A:456:ILE:CD1	2.36	0.54
1:B:176:GLN:O	1:B:180:VAL:HG23	2.07	0.54
1:B:826:GLU:O	1:B:830:VAL:HG23	2.07	0.54
1:C:1185:CYS:SG	1:C:1191:ILE:HG12	2.47	0.54
1:C:187:THR:CG2	1:C:188:PRO:HD2	2.36	0.54
1:C:479:LYS:HE2	1:C:482:GLU:OE1	2.08	0.54
1:D:337:SER:OG	1:D:359:CYS:HB2	2.07	0.54
1:A:176:GLN:O	1:A:180:VAL:HG23	2.08	0.54
1:A:671:GLN:OE1	1:A:672:HIS:HD2	1.91	0.54
1:A:760:SER:HB2	1:A:766:LYS:HZ1	1.72	0.54
1:B:430:PHE:CE2	1:B:466:ILE:HG23	2.42	0.54
1:C:150:ASP:O	1:C:151:LEU:HD23	2.07	0.54
1:C:551:SER:C	1:D:277:PHE:CZ	2.81	0.54
1:D:353:LEU:HB3	1:D:1131:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:671:GLN:OE1	1:D:672:HIS:HD2	1.89	0.54
1:B:704:MET:O	1:B:708:ILE:HG13	2.07	0.54
1:B:760:SER:HB2	1:B:766:LYS:CE	2.36	0.54
1:B:99:HIS:O	1:B:101:PRO:HD3	2.07	0.54
1:A:1203:GLY:HA3	1:A:1278:MET:CG	2.37	0.54
1:D:661:GLU:OE1	1:D:666:LEU:HD12	2.08	0.54
1:D:713:ILE:HG21	1:D:772:SER:HB3	1.88	0.54
1:A:434:GLU:HA	1:A:437:ARG:HG3	1.90	0.54
1:A:593:SER:OG	1:A:604:LEU:HD22	2.08	0.54
1:B:337:SER:OG	1:B:359:CYS:HB2	2.08	0.54
1:C:1029:PHE:O	1:C:1033:VAL:HG23	2.08	0.54
1:C:574:TYR:OH	1:D:383:ILE:HD11	2.07	0.54
1:A:650:VAL:HG21	1:A:737:LYS:HG3	1.89	0.54
1:C:826:GLU:O	1:C:830:VAL:HG23	2.08	0.54
1:D:446:ASN:O	1:D:450:THR:HB	2.08	0.54
1:D:548:VAL:O	1:D:569:ASP:HB3	2.08	0.54
1:A:966:LEU:O	1:A:1013:TYR:OH	2.26	0.54
1:B:766:LYS:NZ	1:B:766:LYS:HB2	2.23	0.54
1:C:593:SER:HB2	1:C:600:ILE:HG21	1.88	0.54
1:C:704:MET:O	1:C:708:ILE:HG13	2.07	0.54
1:C:383:ILE:HD11	1:D:574:TYR:OH	2.07	0.54
1:A:1029:PHE:O	1:A:1033:VAL:HG23	2.07	0.54
1:A:826:GLU:O	1:A:830:VAL:HG23	2.07	0.54
1:A:85:VAL:O	1:A:89:ILE:HG13	2.08	0.54
1:B:1029:PHE:O	1:B:1033:VAL:HG23	2.07	0.54
1:B:297:GLN:HB2	1:B:1104:GLY:HA3	1.90	0.54
1:B:513:ARG:O	1:B:517:ILE:HD12	2.08	0.54
1:B:499:LEU:HD13	1:B:538:GLY:HA2	1.90	0.54
1:C:176:GLN:O	1:C:180:VAL:HG23	2.07	0.54
1:C:533:LYS:HA	1:C:603:MET:HE1	1.89	0.54
1:D:499:LEU:HD13	1:D:538:GLY:HA2	1.90	0.54
1:B:384:GLU:O	1:B:388:ILE:HG13	2.09	0.53
1:B:615:ASN:OD1	1:B:617:GLN:HG2	2.08	0.53
1:B:713:ILE:CG2	1:B:772:SER:HB3	2.38	0.53
1:C:434:GLU:HA	1:C:437:ARG:HG3	1.89	0.53
1:A:760:SER:HB3	1:A:762:PHE:HD1	1.73	0.53
1:D:593:SER:HB2	1:D:600:ILE:HG21	1.89	0.53
1:D:667:LEU:HB3	1:D:751:VAL:HG11	1.90	0.53
1:A:1164:LEU:HB3	1:A:1252:LEU:HD21	1.90	0.53
1:D:544:LYS:O	1:D:614:ARG:HD2	2.08	0.53
1:D:524:MET:CB	1:D:592:ARG:HH21	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:SER:OG	1:C:359:CYS:HB2	2.08	0.53
1:C:389:LEU:CD1	1:C:421:LEU:HD23	2.38	0.53
1:D:815:ALA:O	1:D:819:ASP:HB3	2.09	0.53
1:A:671:GLN:OE1	1:A:672:HIS:CD2	2.62	0.53
1:A:815:ALA:O	1:A:819:ASP:HB3	2.09	0.53
1:B:529:LEU:HG	1:B:597:GLN:HG3	1.91	0.53
1:B:763:SER:O	1:B:767:PHE:HD1	1.92	0.53
1:D:391:ASP:OD2	1:D:447:ARG:NH1	2.42	0.53
1:D:671:GLN:OE1	1:D:672:HIS:CD2	2.62	0.53
1:D:766:LYS:NZ	1:D:766:LYS:HB2	2.23	0.53
1:D:908:LEU:HD22	1:D:980:LEU:HG	1.89	0.53
1:D:946:THR:HA	1:D:949:GLN:HB2	1.91	0.53
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.43	0.53
1:B:238:ARG:HE	1:B:306:CYS:HB3	1.74	0.53
1:B:368:VAL:HG11	1:B:428:GLU:HB3	1.91	0.53
1:B:446:ASN:O	1:B:450:THR:HB	2.07	0.53
1:C:384:GLU:O	1:C:388:ILE:HG13	2.08	0.53
1:C:593:SER:OG	1:C:604:LEU:HD22	2.08	0.53
1:D:832:ARG:HA	1:D:838:MET:HG2	1.91	0.53
1:B:989:SER:HB2	1:B:1031:LEU:HD21	1.90	0.53
1:B:434:GLU:HA	1:B:437:ARG:HG3	1.90	0.53
1:B:467:ILE:HG12	1:B:474:LEU:HD12	1.90	0.53
1:B:483:THR:CG2	1:B:498:LEU:HD21	2.38	0.53
1:B:65:ARG:HD3	1:B:100:PHE:CE1	2.43	0.53
1:B:815:ALA:O	1:B:819:ASP:HB3	2.09	0.53
1:D:574:TYR:N	1:D:574:TYR:CD2	2.74	0.53
1:D:760:SER:HB3	1:D:762:PHE:HD1	1.74	0.53
1:A:615:ASN:OD1	1:A:617:GLN:HG2	2.08	0.53
1:B:210:ILE:N	1:B:211:PRO:HD2	2.24	0.53
1:C:815:ALA:O	1:C:819:ASP:HB3	2.09	0.53
1:D:434:GLU:HA	1:D:437:ARG:HG3	1.90	0.53
1:B:548:VAL:O	1:B:569:ASP:HB3	2.09	0.53
1:C:654:GLY:O	1:C:655:SER:OG	2.22	0.53
1:D:712:MET:HA	1:D:712:MET:HE2	1.91	0.53
1:A:704:MET:O	1:A:708:ILE:HG13	2.08	0.52
1:C:766:LYS:NZ	1:C:766:LYS:HB2	2.23	0.52
1:A:446:ASN:O	1:A:450:THR:HB	2.09	0.52
1:A:467:ILE:HG12	1:A:474:LEU:HD12	1.90	0.52
1:B:755:TYR:CZ	1:B:759:ILE:HD11	2.45	0.52
1:B:946:THR:HA	1:B:949:GLN:HB2	1.91	0.52
1:C:446:ASN:O	1:C:450:THR:HB	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ILE:HG12	1:C:474:LEU:HD12	1.90	0.52
1:C:946:THR:HA	1:C:949:GLN:HB2	1.91	0.52
1:D:513:ARG:O	1:D:517:ILE:HD12	2.09	0.52
1:D:908:LEU:HD11	1:D:981:LEU:HG	1.92	0.52
1:A:456:ILE:HG23	1:A:456:ILE:O	2.09	0.52
1:A:499:LEU:HD13	1:A:538:GLY:HA2	1.91	0.52
1:B:651:LEU:HD23	1:B:658:PHE:HB2	1.92	0.52
1:B:865:ASN:O	1:B:869:ILE:HG13	2.08	0.52
1:C:1032:HIS:O	1:C:1035:TYR:N	2.37	0.52
1:C:483:THR:CG2	1:C:498:LEU:HD21	2.38	0.52
1:C:499:LEU:HD13	1:C:538:GLY:HA2	1.91	0.52
1:D:923:GLN:HB3	1:D:924:PRO:HD3	1.92	0.52
1:A:828:LEU:HB3	1:A:832:ARG:HD3	1.91	0.52
1:B:100:PHE:CD2	1:B:104:LEU:HD13	2.45	0.52
1:C:763:SER:O	1:C:767:PHE:HD1	1.92	0.52
1:D:389:LEU:HD13	1:D:421:LEU:HD23	1.91	0.52
1:A:94:MET:HE2	1:A:132:ILE:HD11	1.92	0.52
1:A:210:ILE:N	1:A:211:PRO:HD2	2.25	0.52
1:A:259:ALA:HB3	1:A:260:PRO:CD	2.29	0.52
1:C:1200:LYS:HB3	1:C:1274:LEU:CD2	2.39	0.52
1:D:1164:LEU:HB3	1:D:1252:LEU:HD21	1.90	0.52
1:D:865:ASN:O	1:D:869:ILE:HG13	2.09	0.52
1:A:1032:HIS:O	1:A:1035:TYR:N	2.36	0.52
1:A:766:LYS:HB2	1:A:766:LYS:NZ	2.23	0.52
1:B:1149:LEU:HB3	1:B:1163:LEU:HD11	1.92	0.52
1:B:832:ARG:HA	1:B:838:MET:HG2	1.92	0.52
1:C:85:VAL:O	1:C:89:ILE:HG13	2.09	0.52
1:D:210:ILE:N	1:D:211:PRO:HD2	2.24	0.52
1:A:337:SER:OG	1:A:359:CYS:HB2	2.08	0.52
1:A:54:SER:HB2	1:A:61:GLY:O	2.10	0.52
1:B:85:VAL:O	1:B:89:ILE:HG13	2.08	0.52
1:C:54:SER:HB2	1:C:61:GLY:O	2.10	0.52
1:C:760:SER:HB3	1:C:762:PHE:HD1	1.73	0.52
1:C:923:GLN:HB3	1:C:924:PRO:HD3	1.92	0.52
1:D:1095:VAL:HG13	1:D:1135:ILE:HG23	1.90	0.52
1:A:865:ASN:O	1:A:869:ILE:HG13	2.10	0.52
1:C:383:ILE:HG22	1:C:429:THR:HG21	1.91	0.52
1:C:755:TYR:CZ	1:C:759:ILE:HD11	2.44	0.52
1:C:832:ARG:HA	1:C:838:MET:HG2	1.91	0.52
1:C:865:ASN:O	1:C:869:ILE:HG13	2.09	0.52
1:D:959:GLN:HB2	1:D:1005:TRP:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:SER:O	1:A:767:PHE:HD1	1.91	0.52
1:A:923:GLN:HB3	1:A:924:PRO:HD3	1.91	0.52
1:C:574:TYR:CZ	1:D:439:GLU:HG2	2.45	0.52
1:C:828:LEU:HB3	1:C:832:ARG:HD3	1.91	0.52
1:D:467:ILE:HG12	1:D:474:LEU:HD12	1.91	0.52
1:A:21:LEU:HB3	1:A:64:ARG:NE	2.25	0.52
1:B:574:TYR:N	1:B:574:TYR:CD2	2.75	0.52
1:B:760:SER:HB3	1:B:762:PHE:HD1	1.74	0.52
1:C:1149:LEU:HB3	1:C:1163:LEU:HD11	1.92	0.52
1:C:395:PRO:O	1:C:455:PRO:HG2	2.10	0.52
1:C:574:TYR:CD2	1:C:574:TYR:N	2.76	0.52
1:A:671:GLN:HG3	1:A:755:TYR:HB2	1.91	0.51
1:A:832:ARG:HA	1:A:838:MET:HG2	1.90	0.51
1:B:828:LEU:HB3	1:B:832:ARG:HD3	1.92	0.51
1:C:210:ILE:N	1:C:211:PRO:HD2	2.25	0.51
1:A:946:THR:HA	1:A:949:GLN:HB2	1.91	0.51
1:B:303:LYS:HG2	1:B:357:ARG:NH2	2.25	0.51
1:C:348:LYS:HG2	1:C:1035:TYR:O	2.10	0.51
1:C:651:LEU:HD23	1:C:658:PHE:HB2	1.91	0.51
1:C:959:GLN:HB2	1:C:1005:TRP:CE2	2.45	0.51
1:D:763:SER:O	1:D:767:PHE:HD1	1.92	0.51
1:A:672:HIS:CE1	1:A:805:SER:HB3	2.43	0.51
1:A:959:GLN:HB2	1:A:1005:TRP:CE2	2.44	0.51
1:B:456:ILE:O	1:B:456:ILE:HG23	2.10	0.51
1:B:908:LEU:HD22	1:B:980:LEU:HG	1.91	0.51
1:C:1056:ILE:HD12	1:C:1216:TYR:CG	2.45	0.51
1:D:303:LYS:HG2	1:D:357:ARG:NH2	2.26	0.51
1:D:651:LEU:HD23	1:D:658:PHE:HB2	1.92	0.51
1:A:1149:LEU:HB3	1:A:1163:LEU:HD11	1.92	0.51
1:C:1095:VAL:HG13	1:C:1135:ILE:HG23	1.93	0.51
1:D:384:GLU:O	1:D:388:ILE:HG13	2.11	0.51
1:D:615:ASN:OD1	1:D:617:GLN:HG2	2.10	0.51
1:D:652:THR:OG1	1:D:657:ILE:HG12	2.11	0.51
1:A:60:ASP:O	1:A:64:ARG:HB2	2.11	0.51
1:C:652:THR:OG1	1:C:657:ILE:HG12	2.11	0.51
1:C:966:LEU:HB3	1:C:1013:TYR:CZ	2.46	0.51
1:D:931:GLN:HG2	1:D:950:ARG:NH1	2.26	0.51
1:A:303:LYS:HG2	1:A:357:ARG:NH2	2.26	0.51
1:B:297:GLN:CG	1:B:1104:GLY:CA	2.88	0.51
1:B:361:SER:OG	1:B:417:HIS:CE1	2.64	0.51
1:B:639:ASP:H	1:B:711:ARG:HE	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:GLN:HB2	1:B:1005:TRP:CE2	2.46	0.51
1:C:456:ILE:O	1:C:456:ILE:HG23	2.09	0.51
1:D:297:GLN:HG3	1:D:1104:GLY:HA2	1.93	0.51
1:A:72:CYS:CB	1:A:93:LEU:HD11	2.40	0.51
1:B:66:TYR:CE1	1:B:107:ASP:HB3	2.47	0.51
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.29	0.51
1:C:1054:GLY:CA	1:C:1152:THR:HG23	2.41	0.51
1:A:394:GLY:O	1:A:396:LYS:HE3	2.11	0.50
1:A:513:ARG:O	1:A:517:ILE:HD12	2.11	0.50
1:A:799:VAL:O	1:A:847:GLN:CD	2.50	0.50
1:B:979:LEU:HD11	1:B:1019:SER:HB2	1.93	0.50
1:C:743:CYS:HA	1:C:746:MET:HB2	1.94	0.50
1:D:1273:ASN:O	1:D:1276:GLN:N	2.44	0.50
1:D:755:TYR:CZ	1:D:759:ILE:HD11	2.46	0.50
1:A:33:LEU:HD22	1:A:75:LEU:HD21	1.92	0.50
1:A:839:HIS:HB3	1:A:903:ILE:HG13	1.93	0.50
1:D:1056:ILE:HD12	1:D:1216:TYR:CG	2.47	0.50
1:A:1086:SER:O	1:A:1090:LYS:HG2	2.12	0.50
1:A:651:LEU:HD23	1:A:658:PHE:HB2	1.92	0.50
1:A:743:CYS:HA	1:A:746:MET:HB2	1.93	0.50
1:A:995:THR:O	1:A:996:SER:O	2.29	0.50
1:B:72:CYS:CB	1:B:93:LEU:HD11	2.41	0.50
1:C:348:LYS:HD3	1:C:1034:LEU:O	2.10	0.50
1:D:1149:LEU:HB3	1:D:1163:LEU:HD11	1.92	0.50
1:A:1050:HIS:HA	1:A:1152:THR:OG1	2.12	0.50
1:B:382:LEU:HD22	1:B:425:ILE:HG23	1.92	0.50
1:B:652:THR:OG1	1:B:657:ILE:HG12	2.11	0.50
1:B:743:CYS:HA	1:B:746:MET:HB2	1.93	0.50
1:C:216:GLN:O	1:C:219:VAL:HG22	2.12	0.50
1:D:483:THR:CG2	1:D:498:LEU:HD21	2.40	0.50
1:D:839:HIS:HB3	1:D:903:ILE:HG13	1.94	0.50
1:A:652:THR:OG1	1:A:657:ILE:HG12	2.11	0.50
1:B:839:HIS:HB3	1:B:903:ILE:HG13	1.94	0.50
1:B:923:GLN:HB3	1:B:924:PRO:HD3	1.92	0.50
1:C:72:CYS:CB	1:C:93:LEU:HD11	2.41	0.50
1:C:839:HIS:HB3	1:C:903:ILE:HG13	1.93	0.50
1:D:395:PRO:O	1:D:455:PRO:HG2	2.12	0.50
1:D:456:ILE:HG23	1:D:456:ILE:O	2.10	0.50
1:A:1054:GLY:HA3	1:A:1152:THR:HG23	1.93	0.50
1:A:1056:ILE:HD12	1:A:1216:TYR:CG	2.47	0.50
1:B:262:ASP:O	1:B:266:HIS:ND1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LYS:HG2	1:C:357:ARG:NH2	2.26	0.50
1:C:513:ARG:O	1:C:517:ILE:HD12	2.12	0.50
1:C:713:ILE:O	1:C:714:LYS:CG	2.52	0.50
1:D:995:THR:O	1:D:996:SER:O	2.30	0.50
1:A:397:LYS:N	1:A:397:LYS:HD3	2.27	0.50
1:A:511:SER:O	1:A:515:SER:HB2	2.12	0.50
1:B:1032:HIS:O	1:B:1035:TYR:N	2.37	0.50
1:B:1054:GLY:O	1:B:1055:ASP:CB	2.59	0.50
1:B:94:MET:CG	1:B:129:LEU:HG	2.41	0.50
1:B:657:ILE:HD12	1:B:733:ASN:O	2.12	0.50
1:B:760:SER:HB2	1:B:766:LYS:HZ1	1.76	0.50
1:B:995:THR:O	1:B:996:SER:O	2.30	0.50
1:C:275:ILE:O	1:C:279:ILE:HG13	2.11	0.50
1:D:828:LEU:HB3	1:D:832:ARG:HD3	1.91	0.50
1:D:843:ASN:O	1:D:847:GLN:HB2	2.12	0.50
1:A:1252:LEU:O	1:A:1256:ILE:HG13	2.12	0.50
1:A:732:THR:O	1:A:736:ILE:HG13	2.12	0.50
1:B:1054:GLY:CA	1:B:1152:THR:HG23	2.41	0.50
1:B:394:GLY:O	1:B:396:LYS:HE3	2.12	0.50
1:D:639:ASP:H	1:D:711:ARG:HE	1.60	0.50
1:D:973:PHE:CD1	1:D:974:ASN:N	2.72	0.50
1:A:187:THR:HG22	1:A:188:PRO:CD	2.41	0.50
1:A:322:PHE:O	1:A:326:VAL:HG23	2.12	0.50
1:A:393:TYR:HB3	1:A:415:ASN:O	2.11	0.50
1:B:1092:LEU:HD13	1:B:1169:LYS:HG2	1.94	0.50
1:C:1252:LEU:O	1:C:1256:ILE:HG13	2.12	0.50
1:D:1086:SER:O	1:D:1090:LYS:HG2	2.12	0.50
1:D:705:LEU:HB3	1:D:755:TYR:CE2	2.47	0.50
1:A:838:MET:HA	1:A:838:MET:CE	2.42	0.49
1:B:227:ARG:HH21	1:B:291:LYS:HD3	1.77	0.49
1:B:838:MET:HA	1:B:838:MET:CE	2.42	0.49
1:C:1092:LEU:HD13	1:C:1169:LYS:HG2	1.93	0.49
1:C:639:ASP:H	1:C:711:ARG:HE	1.60	0.49
1:C:838:MET:CE	1:C:838:MET:HA	2.42	0.49
1:A:448:VAL:HA	1:A:456:ILE:CD1	2.42	0.49
1:A:654:GLY:O	1:A:655:SER:OG	2.22	0.49
1:B:1086:SER:O	1:B:1090:LYS:HG2	2.12	0.49
1:B:227:ARG:CG	1:B:288:GLU:HG3	2.39	0.49
1:D:511:SER:O	1:D:515:SER:HB2	2.12	0.49
1:A:1002:MET:HG3	1:A:1031:LEU:CD1	2.42	0.49
1:A:216:GLN:O	1:A:219:VAL:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:SER:O	1:A:592:ARG:HG2	2.12	0.49
1:C:187:THR:HG22	1:C:188:PRO:CD	2.41	0.49
1:D:838:MET:HA	1:D:838:MET:CE	2.42	0.49
1:B:1252:LEU:O	1:B:1256:ILE:HG13	2.12	0.49
1:C:1086:SER:O	1:C:1090:LYS:HG2	2.12	0.49
1:D:341:LEU:CD1	1:D:359:CYS:HB3	2.42	0.49
1:A:1054:GLY:HA3	1:A:1153:ALA:N	2.24	0.49
1:A:843:ASN:O	1:A:847:GLN:HB2	2.12	0.49
1:B:275:ILE:O	1:B:279:ILE:HG13	2.12	0.49
1:C:268:GLU:O	1:C:272:ILE:HG13	2.12	0.49
1:A:275:ILE:O	1:A:279:ILE:HG13	2.12	0.49
1:A:435:MET:HG3	1:B:508:ILE:O	2.12	0.49
1:B:524:MET:CB	1:B:592:ARG:HH21	2.26	0.49
1:B:843:ASN:O	1:B:847:GLN:HB2	2.12	0.49
1:C:1050:HIS:HA	1:C:1152:THR:OG1	2.12	0.49
1:C:94:MET:HG2	1:C:132:ILE:HD13	1.94	0.49
1:C:397:LYS:N	1:C:397:LYS:HD3	2.27	0.49
1:C:799:VAL:O	1:C:847:GLN:CD	2.49	0.49
1:C:995:THR:O	1:C:996:SER:O	2.30	0.49
1:D:201:MET:O	1:D:205:LEU:HD12	2.13	0.49
1:D:743:CYS:HA	1:D:746:MET:HB2	1.93	0.49
1:A:915:PHE:CE2	1:A:988:LEU:HD21	2.48	0.49
1:B:1053:LEU:HD21	1:B:1077:ALA:HB2	1.95	0.49
1:B:201:MET:O	1:B:205:LEU:HD12	2.13	0.49
1:C:1273:ASN:O	1:C:1276:GLN:N	2.45	0.49
1:C:230:LEU:HD21	1:C:285:LEU:HD21	1.94	0.49
1:C:322:PHE:O	1:C:326:VAL:HG23	2.13	0.49
1:C:930:LEU:HD13	1:C:950:ARG:HB2	1.94	0.49
1:D:1053:LEU:HD21	1:D:1077:ALA:HB2	1.95	0.49
1:D:238:ARG:HE	1:D:306:CYS:HB3	1.78	0.49
1:D:826:GLU:HA	1:D:829:SER:OG	2.13	0.49
1:D:976:LYS:O	1:D:980:LEU:HD22	2.13	0.49
1:A:1:MET:O	1:A:5:ILE:HG13	2.13	0.49
1:A:33:LEU:HD23	1:A:75:LEU:HD11	1.94	0.49
1:A:524:MET:CB	1:A:592:ARG:HH21	2.26	0.49
1:A:533:LYS:HA	1:A:603:MET:HE1	1.94	0.49
1:A:760:SER:HB2	1:A:766:LYS:NZ	2.28	0.49
1:B:760:SER:HB2	1:B:766:LYS:NZ	2.28	0.49
1:B:77:GLU:OE1	1:B:121:LEU:CD2	2.57	0.49
1:C:1054:GLY:O	1:C:1055:ASP:CB	2.59	0.49
1:C:137:LEU:O	1:C:153:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ALA:HB3	1:C:260:PRO:CD	2.29	0.49
1:C:394:GLY:O	1:C:396:LYS:HE3	2.12	0.49
1:D:1252:LEU:O	1:D:1256:ILE:HG13	2.12	0.49
1:A:1092:LEU:HD13	1:A:1169:LYS:HG2	1.95	0.49
1:A:826:GLU:HA	1:A:829:SER:OG	2.13	0.49
1:B:66:TYR:HE1	1:B:107:ASP:HB3	1.78	0.49
1:B:1273:ASN:O	1:B:1276:GLN:N	2.44	0.49
1:B:732:THR:O	1:B:736:ILE:HG13	2.13	0.49
1:C:826:GLU:HA	1:C:829:SER:OG	2.13	0.49
1:D:216:GLN:O	1:D:219:VAL:HG22	2.13	0.49
1:D:397:LYS:HD3	1:D:397:LYS:N	2.27	0.49
1:A:1156:SER:HB3	1:A:1220:LYS:HE3	1.95	0.49
1:A:639:ASP:H	1:A:711:ARG:HE	1.60	0.49
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.93	0.49
1:B:1054:GLY:HA3	1:B:1152:THR:HG23	1.95	0.49
1:B:187:THR:HG22	1:B:188:PRO:CD	2.42	0.49
1:B:511:SER:O	1:B:515:SER:HB2	2.12	0.49
1:C:341:LEU:CD1	1:C:359:CYS:HB3	2.42	0.49
1:C:21:LEU:HB3	1:C:64:ARG:NE	2.28	0.49
1:B:397:LYS:HD3	1:B:397:LYS:N	2.27	0.48
1:B:713:ILE:O	1:B:714:LYS:CG	2.53	0.48
1:C:201:MET:O	1:C:205:LEU:HD12	2.13	0.48
1:C:775:THR:O	1:C:779:LYS:HB2	2.13	0.48
1:D:1032:HIS:O	1:D:1035:TYR:N	2.37	0.48
1:D:1054:GLY:O	1:D:1055:ASP:CB	2.59	0.48
1:D:275:ILE:O	1:D:279:ILE:HG13	2.13	0.48
1:D:635:GLU:O	1:D:711:ARG:NH2	2.40	0.48
1:A:1273:ASN:O	1:A:1276:GLN:N	2.45	0.48
1:C:74:GLN:HA	1:C:77:GLU:OE2	2.13	0.48
1:A:1200:LYS:HB3	1:A:1274:LEU:HD21	1.96	0.48
1:A:1207:THR:O	1:A:1211:TYR:HD1	1.97	0.48
1:A:548:VAL:HG11	1:A:580:GLU:O	2.14	0.48
1:A:635:GLU:O	1:A:711:ARG:NH2	2.39	0.48
1:A:74:GLN:HA	1:A:77:GLU:OE2	2.14	0.48
1:C:1:MET:O	1:C:5:ILE:HG13	2.13	0.48
1:C:870:PHE:CD1	1:C:922:TYR:HD2	2.32	0.48
1:D:187:THR:HG22	1:D:188:PRO:CD	2.42	0.48
1:A:201:MET:O	1:A:205:LEU:HD12	2.13	0.48
1:A:262:ASP:O	1:A:266:HIS:ND1	2.43	0.48
1:A:383:ILE:HD11	1:B:574:TYR:OH	2.13	0.48
1:A:574:TYR:CZ	1:B:439:GLU:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLN:HA	1:B:77:GLU:OE2	2.14	0.48
1:D:316:LEU:HD22	1:D:316:LEU:O	2.13	0.48
1:D:549:LEU:HD23	1:D:569:ASP:OD1	2.13	0.48
1:D:775:THR:O	1:D:779:LYS:HB2	2.14	0.48
1:A:1091:VAL:HA	1:A:1094:GLU:HG3	1.95	0.48
1:A:818:ARG:NH1	1:A:878:ARG:HD2	2.29	0.48
1:B:216:GLN:O	1:B:219:VAL:HG22	2.13	0.48
1:C:1207:THR:O	1:C:1211:TYR:HD1	1.97	0.48
1:C:511:SER:O	1:C:515:SER:HB2	2.13	0.48
1:C:976:LYS:O	1:C:980:LEU:HD22	2.13	0.48
1:D:1054:GLY:CA	1:D:1152:THR:HG23	2.44	0.48
1:D:1091:VAL:HA	1:D:1094:GLU:HG3	1.95	0.48
1:D:394:GLY:O	1:D:396:LYS:HE3	2.12	0.48
1:D:713:ILE:O	1:D:714:LYS:CG	2.52	0.48
1:A:341:LEU:CD1	1:A:359:CYS:HB3	2.43	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
1:B:503:GLN:HB2	1:B:504:PRO:HD3	1.96	0.48
1:B:828:LEU:O	1:B:832:ARG:HG3	2.14	0.48
1:C:1053:LEU:HD21	1:C:1077:ALA:HB2	1.95	0.48
1:C:141:LYS:O	1:C:142:GLU:HG3	2.13	0.48
1:C:732:THR:O	1:C:736:ILE:HG13	2.14	0.48
1:D:732:THR:O	1:D:736:ILE:HG13	2.13	0.48
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.95	0.48
1:A:94:MET:CE	1:A:132:ILE:HD11	2.44	0.48
1:A:268:GLU:O	1:A:272:ILE:HG13	2.13	0.48
1:B:359:CYS:SG	1:B:361:SER:HB2	2.54	0.48
1:B:776:CYS:O	1:B:780:PHE:HD1	1.97	0.48
1:D:776:CYS:O	1:D:780:PHE:HD1	1.97	0.48
1:D:828:LEU:O	1:D:832:ARG:HG3	2.13	0.48
1:D:931:GLN:HG2	1:D:950:ARG:HH12	1.79	0.48
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.96	0.48
1:A:359:CYS:SG	1:A:361:SER:HB2	2.54	0.48
1:A:801:ASP:OD1	1:A:801:ASP:N	2.47	0.48
1:B:1080:VAL:HG12	1:B:1080:VAL:O	2.14	0.48
1:B:170:PRO:HG2	1:B:173:TYR:HD1	1.79	0.48
1:C:1055:ASP:O	1:C:1056:ILE:C	2.52	0.48
1:C:760:SER:HB2	1:C:766:LYS:NZ	2.28	0.48
1:C:828:LEU:O	1:C:832:ARG:HG3	2.13	0.48
1:C:908:LEU:HD22	1:C:980:LEU:HG	1.96	0.48
1:D:338:PHE:HD2	1:D:414:THR:HG23	1.77	0.48
1:D:589:SER:O	1:D:592:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:818:ARG:NH1	1:D:878:ARG:HD2	2.29	0.48
1:A:775:THR:O	1:A:779:LYS:HB2	2.14	0.48
1:B:137:LEU:O	1:B:153:GLY:HA3	2.14	0.48
1:B:448:VAL:HA	1:B:456:ILE:CD1	2.42	0.48
1:C:8:LEU:HD13	1:C:17:LEU:HA	1.96	0.48
1:C:540:LEU:HD13	1:C:607:GLY:HA3	1.95	0.48
1:A:671:GLN:HG2	1:A:755:TYR:HB2	1.96	0.48
1:B:341:LEU:CD1	1:B:359:CYS:HB3	2.43	0.48
1:B:826:GLU:HA	1:B:829:SER:OG	2.13	0.48
1:C:170:PRO:HG2	1:C:173:TYR:HD1	1.79	0.48
1:C:806:LEU:CD2	1:C:872:ASN:HB3	2.44	0.48
1:D:137:LEU:O	1:D:153:GLY:HA3	2.13	0.48
1:D:672:HIS:HE1	1:D:805:SER:HB3	1.79	0.48
1:A:1077:ALA:CB	1:A:1078:PRO:HD3	2.40	0.47
1:A:806:LEU:CD2	1:A:872:ASN:HB3	2.44	0.47
1:A:966:LEU:HB3	1:A:1013:TYR:CZ	2.49	0.47
1:B:1091:VAL:HA	1:B:1094:GLU:HG3	1.95	0.47
1:B:1207:THR:O	1:B:1211:TYR:HD1	1.97	0.47
1:B:818:ARG:NH1	1:B:878:ARG:HD2	2.28	0.47
1:C:1054:GLY:HA3	1:C:1152:THR:HG23	1.95	0.47
1:C:801:ASP:OD1	1:C:801:ASP:N	2.47	0.47
1:C:843:ASN:O	1:C:847:GLN:HB2	2.13	0.47
1:D:268:GLU:O	1:D:272:ILE:HG13	2.14	0.47
1:A:503:GLN:HB2	1:A:504:PRO:HD3	1.96	0.47
1:A:828:LEU:O	1:A:832:ARG:HG3	2.13	0.47
1:B:268:GLU:O	1:B:272:ILE:HG13	2.14	0.47
1:B:806:LEU:CD2	1:B:872:ASN:HB3	2.44	0.47
1:B:976:LYS:O	1:B:980:LEU:HD22	2.13	0.47
1:D:1050:HIS:HA	1:D:1152:THR:OG1	2.14	0.47
1:D:170:PRO:HG2	1:D:173:TYR:HD1	1.79	0.47
1:D:259:ALA:CB	1:D:260:PRO:CD	2.91	0.47
1:D:594:LEU:HG	1:D:604:LEU:HD23	1.96	0.47
1:A:137:LEU:O	1:A:153:GLY:HA3	2.13	0.47
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.49	0.47
1:B:372:VAL:HG22	1:B:432:ILE:HG23	1.96	0.47
1:B:635:GLU:O	1:B:711:ARG:NH2	2.39	0.47
1:B:775:THR:O	1:B:779:LYS:HB2	2.14	0.47
1:C:604:LEU:HG	1:C:608:PHE:CE1	2.50	0.47
1:C:776:CYS:O	1:C:780:PHE:HD1	1.97	0.47
1:C:918:VAL:HG21	1:C:929:PHE:CE2	2.50	0.47
1:D:359:CYS:SG	1:D:361:SER:HB2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LEU:HB3	1:A:755:TYR:CE2	2.49	0.47
1:B:589:SER:O	1:B:592:ARG:HG2	2.13	0.47
1:C:1091:VAL:HA	1:C:1094:GLU:HG3	1.95	0.47
1:D:1207:THR:O	1:D:1211:TYR:HD1	1.97	0.47
1:D:322:PHE:O	1:D:326:VAL:HG23	2.15	0.47
1:C:435:MET:HG3	1:D:508:ILE:O	2.14	0.47
1:A:174:MET:HA	1:A:177:LEU:HB2	1.96	0.47
1:B:581:THR:HB	1:B:585:GLU:HG3	1.97	0.47
1:B:799:VAL:O	1:B:847:GLN:CD	2.50	0.47
1:B:870:PHE:CD1	1:B:922:TYR:HD2	2.32	0.47
1:C:581:THR:HB	1:C:585:GLU:HG3	1.96	0.47
1:D:1054:GLY:HA3	1:D:1152:THR:HG23	1.96	0.47
1:D:1080:VAL:HG12	1:D:1080:VAL:O	2.14	0.47
1:D:630:LEU:HD13	1:D:704:MET:HE1	1.96	0.47
1:A:1055:ASP:O	1:A:1056:ILE:C	2.52	0.47
1:B:1055:ASP:O	1:B:1056:ILE:C	2.52	0.47
1:C:589:SER:O	1:C:592:ARG:HG2	2.13	0.47
1:D:271:VAL:O	1:D:275:ILE:HG23	2.15	0.47
1:B:1095:VAL:HG13	1:B:1135:ILE:HG23	1.97	0.47
1:A:439:GLU:HG2	1:B:574:TYR:CZ	2.49	0.47
1:B:672:HIS:CE1	1:B:861:PRO:CG	2.96	0.47
1:C:360:VAL:O	1:C:364:ILE:HG13	2.15	0.47
1:D:654:GLY:O	1:D:655:SER:OG	2.22	0.47
1:A:1145:PHE:HD2	1:A:1146:PHE:CD1	2.33	0.47
1:A:776:CYS:O	1:A:780:PHE:HD1	1.97	0.47
1:B:966:LEU:HB3	1:B:1013:TYR:CZ	2.50	0.47
1:B:121:LEU:C	1:B:123:ASN:N	2.68	0.47
1:C:1145:PHE:HD2	1:C:1146:PHE:CD1	2.33	0.47
1:D:1145:PHE:HD2	1:D:1146:PHE:CD1	2.33	0.47
1:D:503:GLN:HB2	1:D:504:PRO:HD3	1.97	0.47
1:A:1150:VAL:HG12	1:A:1209:VAL:HG12	1.96	0.47
1:C:503:GLN:HB2	1:C:504:PRO:HD3	1.97	0.47
1:C:922:TYR:N	1:C:922:TYR:CD1	2.83	0.47
1:D:598:ALA:HA	1:D:601:ARG:HD3	1.96	0.47
1:A:1080:VAL:HG12	1:A:1080:VAL:O	2.14	0.47
1:A:918:VAL:HG21	1:A:929:PHE:CE2	2.50	0.47
1:B:922:TYR:N	1:B:922:TYR:CD1	2.83	0.47
1:C:818:ARG:NH1	1:C:878:ARG:HD2	2.29	0.47
1:C:908:LEU:HD11	1:C:981:LEU:HG	1.96	0.47
1:D:262:ASP:O	1:D:266:HIS:ND1	2.43	0.47
1:D:448:VAL:HA	1:D:456:ILE:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:VAL:O	1:D:847:GLN:CD	2.49	0.47
1:D:806:LEU:CD2	1:D:872:ASN:HB3	2.44	0.47
1:D:911:LEU:CD2	1:D:915:PHE:HE1	2.28	0.47
1:A:339:LYS:HD2	1:A:339:LYS:HA	1.67	0.47
1:A:393:TYR:CD1	1:A:418:ALA:HB1	2.49	0.47
1:A:549:LEU:HB2	1:A:567:ARG:CD	2.44	0.47
1:A:598:ALA:HA	1:A:601:ARG:HD3	1.97	0.47
1:B:930:LEU:HD13	1:B:950:ARG:HB2	1.97	0.47
1:D:1055:ASP:O	1:D:1056:ILE:C	2.53	0.47
1:D:1056:ILE:HD12	1:D:1216:TYR:CD1	2.49	0.47
1:D:1249:ILE:N	1:D:1250:PRO:CD	2.78	0.47
1:D:760:SER:HB2	1:D:766:LYS:NZ	2.29	0.47
1:D:870:PHE:CD1	1:D:922:TYR:HD2	2.32	0.47
1:A:271:VAL:O	1:A:275:ILE:HG23	2.15	0.46
1:B:387:PHE:CD1	1:B:447:ARG:CZ	2.99	0.46
1:B:918:VAL:HG21	1:B:929:PHE:CE2	2.49	0.46
1:C:1080:VAL:HG12	1:C:1080:VAL:O	2.14	0.46
1:D:581:THR:HB	1:D:585:GLU:HG3	1.96	0.46
1:A:1002:MET:HG3	1:A:1031:LEU:HD11	1.97	0.46
1:A:170:PRO:HG2	1:A:173:TYR:HD1	1.79	0.46
1:A:581:THR:HB	1:A:585:GLU:HG3	1.97	0.46
1:B:1145:PHE:HD2	1:B:1146:PHE:CD1	2.33	0.46
1:B:664:ASP:HB2	1:B:803:LEU:HD11	1.98	0.46
1:A:551:SER:C	1:B:277:PHE:HZ	2.19	0.46
1:A:713:ILE:O	1:A:714:LYS:CG	2.53	0.46
1:A:870:PHE:CD1	1:A:922:TYR:HD2	2.31	0.46
1:A:922:TYR:CD1	1:A:922:TYR:N	2.83	0.46
1:A:69:TYR:CE2	1:A:97:VAL:HG23	2.51	0.46
1:B:598:ALA:HA	1:B:601:ARG:HD3	1.96	0.46
1:B:664:ASP:HB2	1:B:803:LEU:HD12	1.97	0.46
1:B:99:HIS:O	1:B:101:PRO:CD	2.64	0.46
1:C:262:ASP:O	1:C:266:HIS:ND1	2.44	0.46
1:C:339:LYS:HD2	1:C:339:LYS:HA	1.67	0.46
1:A:1054:GLY:O	1:A:1055:ASP:CB	2.59	0.46
1:A:594:LEU:HG	1:A:604:LEU:HD23	1.96	0.46
1:A:376:ASP:CB	1:B:570:VAL:HG21	2.32	0.46
1:C:174:MET:HA	1:C:177:LEU:HB2	1.97	0.46
1:C:226:ARG:H	1:C:226:ARG:HG2	1.54	0.46
1:D:1171:TYR:O	1:D:1175:THR:OG1	2.24	0.46
1:D:150:ASP:O	1:D:151:LEU:HD23	2.16	0.46
1:A:150:ASP:O	1:A:151:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:LEU:HD13	1:A:704:MET:HE1	1.98	0.46
1:A:911:LEU:CD2	1:A:915:PHE:HE1	2.28	0.46
1:C:121:LEU:C	1:C:123:ASN:N	2.69	0.46
1:C:359:CYS:SG	1:C:361:SER:HB2	2.55	0.46
1:C:448:VAL:HA	1:C:456:ILE:CD1	2.43	0.46
1:A:441:LEU:HD13	1:A:474:LEU:HD22	1.98	0.46
1:A:574:TYR:CD2	1:A:574:TYR:N	2.77	0.46
1:B:322:PHE:O	1:B:326:VAL:HG23	2.15	0.46
1:B:549:LEU:HG	1:B:549:LEU:O	2.16	0.46
1:B:630:LEU:HD13	1:B:704:MET:HE1	1.98	0.46
1:C:594:LEU:HG	1:C:604:LEU:HD23	1.96	0.46
1:D:109:ALA:O	1:D:113:VAL:HG23	2.16	0.46
1:A:230:LEU:HD21	1:A:285:LEU:HD21	1.98	0.46
1:A:316:LEU:O	1:A:316:LEU:HD22	2.15	0.46
1:B:174:MET:HA	1:B:177:LEU:HB2	1.97	0.46
1:B:316:LEU:HD22	1:B:316:LEU:O	2.16	0.46
1:B:440:ILE:O	1:B:444:VAL:HG23	2.16	0.46
1:C:598:ALA:HA	1:C:601:ARG:HD3	1.97	0.46
1:C:630:LEU:HD13	1:C:704:MET:HE1	1.97	0.46
1:D:1053:LEU:HD11	1:D:1077:ALA:HA	1.98	0.46
1:D:121:LEU:C	1:D:123:ASN:N	2.69	0.46
1:D:918:VAL:HG21	1:D:929:PHE:CE2	2.50	0.46
1:A:852:LEU:HD13	1:A:858:VAL:HG23	1.98	0.46
1:B:399:LEU:HD13	1:B:453:SER:O	2.16	0.46
1:C:146:CYS:O	1:C:147:GLY:C	2.54	0.46
1:C:529:LEU:HA	1:C:532:ARG:NH2	2.31	0.46
1:C:973:PHE:HD1	1:C:974:ASN:H	1.57	0.46
1:D:982:ILE:HD11	1:D:1024:LEU:HG	1.98	0.46
1:B:1249:ILE:N	1:B:1250:PRO:CD	2.79	0.46
1:B:158:ARG:O	1:B:162:ASP:HB2	2.16	0.46
1:B:911:LEU:CD2	1:B:915:PHE:HE1	2.28	0.46
1:C:259:ALA:CB	1:C:260:PRO:CD	2.91	0.46
1:C:316:LEU:O	1:C:316:LEU:HD22	2.16	0.46
1:C:361:SER:HG	1:C:417:HIS:CE1	2.34	0.46
1:C:94:MET:HG2	1:C:132:ILE:CD1	2.45	0.46
1:D:298:GLN:HE21	1:D:336:LYS:CG	2.29	0.46
1:D:852:LEU:HD13	1:D:858:VAL:HG23	1.98	0.46
1:D:922:TYR:N	1:D:922:TYR:CD1	2.83	0.46
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.16	0.46
1:B:1164:LEU:HD22	1:B:1252:LEU:CD1	2.46	0.46
1:B:431:LYS:HG2	1:B:469:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:GLN:HE21	1:C:336:LYS:CG	2.28	0.46
1:C:922:TYR:N	1:C:922:TYR:HD1	2.14	0.46
1:D:708:ILE:HG22	1:D:752:LEU:HD11	1.98	0.46
1:D:801:ASP:OD1	1:D:801:ASP:N	2.47	0.46
1:A:109:ALA:O	1:A:113:VAL:HG23	2.16	0.45
1:A:1056:ILE:HB	1:A:1216:TYR:CZ	2.50	0.45
1:A:266:HIS:CE1	1:A:373:HIS:HB3	2.51	0.45
1:A:978:ALA:HB1	1:A:1020:PHE:CE1	2.51	0.45
1:B:1144:THR:O	1:B:1148:GLU:HG2	2.16	0.45
1:B:430:PHE:CZ	1:B:466:ILE:HG23	2.52	0.45
1:B:774:PHE:HE2	1:B:836:GLU:HG3	1.81	0.45
1:C:441:LEU:HD13	1:C:474:LEU:HD22	1.98	0.45
1:C:59:GLU:O	1:C:63:LEU:HG	2.16	0.45
1:D:979:LEU:HD11	1:D:1019:SER:HB2	1.97	0.45
1:A:121:LEU:C	1:A:123:ASN:N	2.68	0.45
1:A:259:ALA:CB	1:A:260:PRO:CD	2.91	0.45
1:A:667:LEU:HA	1:A:667:LEU:HD23	1.80	0.45
1:B:69:TYR:CE2	1:B:97:VAL:HG23	2.51	0.45
1:D:549:LEU:O	1:D:549:LEU:HG	2.16	0.45
1:A:158:ARG:O	1:A:162:ASP:HB2	2.16	0.45
1:B:230:LEU:HD22	1:B:275:ILE:HD12	1.99	0.45
1:B:238:ARG:NH2	1:B:304:CYS:O	2.50	0.45
1:B:227:ARG:NH2	1:B:291:LYS:HD3	2.31	0.45
1:B:993:GLU:CD	1:B:994:PRO:HD2	2.37	0.45
1:C:1144:THR:O	1:C:1148:GLU:HG2	2.17	0.45
1:C:1154:LEU:CD1	1:C:1163:LEU:HD12	2.45	0.45
1:C:911:LEU:CD2	1:C:915:PHE:HE1	2.29	0.45
1:D:1144:THR:O	1:D:1148:GLU:HG2	2.16	0.45
1:D:431:LYS:HG2	1:D:469:TYR:CE1	2.52	0.45
1:A:474:LEU:HB3	1:A:477:CYS:SG	2.57	0.45
1:A:993:GLU:CD	1:A:994:PRO:HD2	2.37	0.45
1:B:1053:LEU:HD11	1:B:1077:ALA:HA	1.99	0.45
1:C:675:ALA:O	1:C:679:SER:HB3	2.17	0.45
1:D:644:LEU:HD21	1:D:708:ILE:HD13	1.98	0.45
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.99	0.45
1:B:109:ALA:O	1:B:113:VAL:HG23	2.16	0.45
1:B:360:VAL:O	1:B:364:ILE:HG13	2.16	0.45
1:B:524:MET:HB3	1:B:592:ARG:HH21	1.80	0.45
1:B:594:LEU:HG	1:B:604:LEU:HD23	1.97	0.45
1:C:266:HIS:CE1	1:C:373:HIS:HB3	2.51	0.45
1:C:372:VAL:HG22	1:C:432:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:GLN:OE1	1:C:672:HIS:CD2	2.70	0.45
1:C:573:ARG:NH2	1:D:323:GLU:OE2	2.50	0.45
1:D:360:VAL:O	1:D:364:ILE:HG13	2.16	0.45
1:D:675:ALA:O	1:D:679:SER:HB3	2.17	0.45
1:A:979:LEU:HD11	1:A:1019:SER:HB2	1.99	0.45
1:A:529:LEU:HD21	1:A:600:ILE:HG13	1.99	0.45
1:B:297:GLN:HG2	1:B:297:GLN:H	1.60	0.45
1:B:644:LEU:HD21	1:B:708:ILE:HD13	1.98	0.45
1:C:109:ALA:O	1:C:113:VAL:HG23	2.16	0.45
1:C:217:LEU:CD2	1:C:229:VAL:HG13	2.43	0.45
1:C:271:VAL:O	1:C:275:ILE:HG23	2.16	0.45
1:C:881:LEU:HG	1:C:911:LEU:HD21	1.99	0.45
1:D:524:MET:HB3	1:D:592:ARG:HH21	1.81	0.45
1:D:881:LEU:HG	1:D:911:LEU:HD21	1.99	0.45
1:A:476:ASN:OD1	1:A:476:ASN:N	2.50	0.45
1:A:59:GLU:O	1:A:63:LEU:HG	2.16	0.45
1:A:881:LEU:HG	1:A:911:LEU:HD21	1.98	0.45
1:A:922:TYR:HD1	1:A:922:TYR:N	2.15	0.45
1:B:922:TYR:N	1:B:922:TYR:HD1	2.15	0.45
1:C:430:PHE:CZ	1:C:466:ILE:HG23	2.52	0.45
1:D:158:ARG:O	1:D:162:ASP:HB2	2.16	0.45
1:D:174:MET:HA	1:D:177:LEU:HB2	1.97	0.45
1:D:368:VAL:HG11	1:D:428:GLU:HB3	1.98	0.45
1:A:151:LEU:HD12	1:A:156:TYR:CZ	2.52	0.45
1:B:672:HIS:HE1	1:B:805:SER:HB3	1.81	0.45
1:C:1171:TYR:O	1:C:1175:THR:OG1	2.23	0.45
1:C:1249:ILE:N	1:C:1250:PRO:CD	2.79	0.45
1:D:1174:LEU:O	1:D:1178:VAL:HG23	2.17	0.45
1:D:146:CYS:O	1:D:147:GLY:C	2.55	0.45
1:D:993:GLU:CD	1:D:994:PRO:HD2	2.37	0.45
1:A:1260:GLU:HA	1:A:1263:LEU:HD12	1.99	0.45
1:A:360:VAL:O	1:A:364:ILE:HG13	2.16	0.45
1:A:376:ASP:HB2	1:B:570:VAL:CG2	2.30	0.45
1:B:146:CYS:O	1:B:147:GLY:C	2.55	0.45
1:B:150:ASP:O	1:B:151:LEU:HD23	2.17	0.45
1:B:266:HIS:CE1	1:B:373:HIS:HB3	2.51	0.45
1:B:706:GLU:O	1:B:709:THR:HB	2.17	0.45
1:C:508:ILE:O	1:D:435:MET:HG3	2.16	0.45
1:C:540:LEU:O	1:C:544:LYS:HG3	2.17	0.45
1:C:623:MET:HE2	1:C:623:MET:HB2	1.84	0.45
1:C:993:GLU:CD	1:C:994:PRO:HD2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:713:ILE:CG2	1:D:772:SER:HB3	2.46	0.45
1:A:552:LEU:C	1:A:552:LEU:HD23	2.38	0.45
1:B:271:VAL:O	1:B:275:ILE:HG23	2.15	0.45
1:B:852:LEU:HD13	1:B:858:VAL:HG23	1.98	0.45
1:C:1174:LEU:O	1:C:1178:VAL:HG23	2.17	0.45
1:C:22:GLN:HG2	1:C:60:ASP:OD2	2.18	0.45
1:D:266:HIS:CE1	1:D:373:HIS:HB3	2.51	0.45
1:A:298:GLN:C	1:A:301:PRO:HD2	2.38	0.44
1:A:349:PHE:O	1:A:353:LEU:HG	2.17	0.44
1:A:945:VAL:O	1:A:949:GLN:HB2	2.17	0.44
1:A:996:SER:HB3	1:A:999:PHE:CB	2.47	0.44
1:B:1150:VAL:O	1:B:1213:PHE:HD1	2.00	0.44
1:B:344:LEU:HD23	1:B:350:LEU:HB3	1.99	0.44
1:B:801:ASP:N	1:B:801:ASP:OD1	2.48	0.44
1:C:1056:ILE:HD12	1:C:1216:TYR:CD1	2.53	0.44
1:C:158:ARG:O	1:C:162:ASP:HB2	2.16	0.44
1:D:349:PHE:O	1:D:353:LEU:HG	2.17	0.44
1:D:474:LEU:HB3	1:D:477:CYS:SG	2.56	0.44
1:A:1249:ILE:N	1:A:1250:PRO:CD	2.79	0.44
1:A:14:THR:O	1:A:15:ASP:C	2.55	0.44
1:A:430:PHE:CZ	1:A:466:ILE:HG23	2.53	0.44
1:A:623:MET:HE2	1:A:623:MET:HB2	1.83	0.44
1:A:973:PHE:CD1	1:A:974:ASN:N	2.72	0.44
1:B:1154:LEU:CD1	1:B:1163:LEU:HD12	2.45	0.44
1:B:259:ALA:CB	1:B:260:PRO:CD	2.91	0.44
1:A:573:ARG:NH2	1:B:323:GLU:OE2	2.51	0.44
1:B:816:LEU:HD13	1:B:838:MET:HE1	2.00	0.44
1:B:945:VAL:O	1:B:949:GLN:HB2	2.17	0.44
1:C:1260:GLU:HA	1:C:1263:LEU:HD12	2.00	0.44
1:C:298:GLN:C	1:C:301:PRO:HD2	2.38	0.44
1:C:41:ARG:N	1:C:41:ARG:HD3	2.32	0.44
1:C:644:LEU:HD21	1:C:708:ILE:HD13	1.98	0.44
1:C:51:LEU:HD13	1:C:96:GLU:HG2	1.98	0.44
1:D:441:LEU:HD13	1:D:474:LEU:HD22	1.99	0.44
1:D:476:ASN:OD1	1:D:476:ASN:N	2.50	0.44
1:D:945:VAL:O	1:D:949:GLN:HB2	2.17	0.44
1:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.98	0.44
1:A:146:CYS:O	1:A:147:GLY:C	2.55	0.44
1:A:344:LEU:HD23	1:A:350:LEU:HB3	1.99	0.44
1:B:441:LEU:HD13	1:B:474:LEU:HD22	1.99	0.44
1:C:513:ARG:NH1	1:C:514:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:LEU:HD13	1:C:858:VAL:HG23	1.98	0.44
1:A:548:VAL:O	1:A:569:ASP:HB3	2.17	0.44
1:A:672:HIS:CE1	1:A:861:PRO:HG3	2.52	0.44
1:B:476:ASN:OD1	1:B:476:ASN:N	2.50	0.44
1:B:996:SER:HB3	1:B:999:PHE:CB	2.48	0.44
1:C:344:LEU:HD23	1:C:350:LEU:HB3	2.00	0.44
1:C:349:PHE:O	1:C:353:LEU:HG	2.17	0.44
1:A:211:PRO:N	1:A:212:PRO:HD2	2.33	0.44
1:A:217:LEU:HD23	1:A:217:LEU:O	2.17	0.44
1:A:529:LEU:HA	1:A:532:ARG:NH2	2.33	0.44
1:B:519:VAL:HG12	1:B:520:LEU:N	2.32	0.44
1:C:1053:LEU:HD11	1:C:1077:ALA:HA	1.99	0.44
1:C:1077:ALA:CB	1:C:1078:PRO:HD3	2.40	0.44
1:C:217:LEU:HD22	1:C:229:VAL:CG1	2.42	0.44
1:C:69:TYR:CE2	1:C:97:VAL:HG23	2.51	0.44
1:D:297:GLN:HG3	1:D:1104:GLY:CA	2.47	0.44
1:D:387:PHE:CD1	1:D:447:ARG:CZ	3.01	0.44
1:D:563:VAL:O	1:D:563:VAL:HG13	2.17	0.44
1:D:973:PHE:HD1	1:D:974:ASN:H	1.57	0.44
1:A:217:LEU:CD2	1:A:229:VAL:HG13	2.41	0.44
1:A:519:VAL:HG12	1:A:520:LEU:N	2.32	0.44
1:B:151:LEU:HD12	1:B:156:TYR:CZ	2.53	0.44
1:B:217:LEU:O	1:B:217:LEU:HD23	2.17	0.44
1:B:474:LEU:HB3	1:B:477:CYS:SG	2.57	0.44
1:B:604:LEU:HG	1:B:608:PHE:CE1	2.52	0.44
1:C:476:ASN:N	1:C:476:ASN:OD1	2.50	0.44
1:C:552:LEU:HD23	1:C:552:LEU:C	2.38	0.44
1:C:671:GLN:CG	1:C:755:TYR:HB2	2.47	0.44
1:C:574:TYR:CD1	1:D:439:GLU:HG2	2.53	0.44
1:D:989:SER:HB2	1:D:1031:LEU:HD21	2.00	0.44
1:A:1174:LEU:O	1:A:1178:VAL:HG23	2.17	0.44
1:A:221:SER:O	1:A:224:GLY:N	2.51	0.44
1:A:540:LEU:O	1:A:544:LYS:HG3	2.17	0.44
1:B:211:PRO:N	1:B:212:PRO:HD2	2.33	0.44
1:B:548:VAL:CG1	1:B:580:GLU:HA	2.48	0.44
1:C:1002:MET:HG3	1:C:1031:LEU:CD1	2.47	0.44
1:C:15:ASP:OD1	1:C:15:ASP:N	2.47	0.44
1:C:396:LYS:HE2	1:C:396:LYS:HB3	1.90	0.44
1:C:996:SER:HB3	1:C:999:PHE:CB	2.48	0.44
1:D:1046:SER:HB2	1:D:1148:GLU:HB2	2.00	0.44
1:D:151:LEU:HD12	1:D:156:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:O	1:D:197:LYS:HG2	2.18	0.44
1:D:211:PRO:N	1:D:212:PRO:HD2	2.33	0.44
1:D:344:LEU:HD23	1:D:350:LEU:HB3	1.99	0.44
1:D:430:PHE:CZ	1:D:466:ILE:HG23	2.52	0.44
1:A:22:GLN:HG2	1:A:60:ASP:OD2	2.18	0.44
1:A:650:VAL:HG13	1:A:657:ILE:HG23	2.00	0.44
1:A:675:ALA:O	1:A:679:SER:HB3	2.17	0.44
1:B:1049:ILE:HG13	1:B:1049:ILE:H	1.57	0.44
1:B:298:GLN:HE21	1:B:336:LYS:CG	2.28	0.44
1:C:221:SER:O	1:C:224:GLY:N	2.51	0.44
1:C:341:LEU:HD11	1:C:359:CYS:HB3	2.00	0.44
1:D:120:ARG:HG2	1:D:172:ARG:HH12	1.82	0.44
1:D:298:GLN:C	1:D:301:PRO:HD2	2.38	0.44
1:D:552:LEU:HD23	1:D:552:LEU:C	2.37	0.44
1:D:604:LEU:HG	1:D:608:PHE:CE1	2.53	0.44
1:A:1049:ILE:H	1:A:1049:ILE:HG13	1.57	0.44
1:A:41:ARG:N	1:A:41:ARG:HD3	2.33	0.44
1:A:447:ARG:O	1:A:456:ILE:HD11	2.18	0.44
1:A:90:ILE:O	1:A:94:MET:HG3	2.18	0.44
1:B:529:LEU:HA	1:B:532:ARG:NH2	2.32	0.44
1:B:667:LEU:HA	1:B:667:LEU:HD23	1.80	0.44
1:C:335:VAL:HG13	1:C:414:THR:CG2	2.46	0.44
1:C:431:LYS:HG2	1:C:469:TYR:CE1	2.53	0.44
1:D:242:LYS:HA	1:D:245:ARG:HE	1.83	0.44
1:D:529:LEU:HD22	1:D:533:LYS:HE3	1.99	0.44
1:D:529:LEU:HA	1:D:532:ARG:NH2	2.33	0.44
1:D:706:GLU:O	1:D:709:THR:HB	2.18	0.44
1:A:297:GLN:H	1:A:297:GLN:HG2	1.62	0.43
1:B:225:SER:O	1:B:226:ARG:C	2.57	0.43
1:B:389:LEU:HD13	1:B:421:LEU:HD23	2.00	0.43
1:B:549:LEU:HD23	1:B:569:ASP:OD1	2.18	0.43
1:B:675:ALA:O	1:B:679:SER:HB3	2.17	0.43
1:C:1046:SER:HB2	1:C:1148:GLU:HB2	2.00	0.43
1:C:211:PRO:N	1:C:212:PRO:HD2	2.33	0.43
1:C:540:LEU:CD1	1:C:607:GLY:HA3	2.48	0.43
1:D:519:VAL:HG12	1:D:520:LEU:N	2.32	0.43
1:D:672:HIS:CE1	1:D:805:SER:HB3	2.53	0.43
1:A:664:ASP:O	1:A:751:VAL:HG21	2.18	0.43
1:B:552:LEU:HD23	1:B:552:LEU:C	2.38	0.43
1:B:563:VAL:O	1:B:563:VAL:HG13	2.17	0.43
1:B:860:GLY:HA3	1:B:861:PRO:HD2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1164:LEU:HD22	1:C:1252:LEU:CD1	2.48	0.43
1:C:563:VAL:O	1:C:563:VAL:HG13	2.17	0.43
1:C:978:ALA:HB1	1:C:1020:PHE:CE1	2.53	0.43
1:D:540:LEU:O	1:D:544:LYS:HG3	2.18	0.43
1:A:431:LYS:HG2	1:A:469:TYR:CE1	2.53	0.43
1:A:619:ALA:O	1:A:623:MET:HB2	2.19	0.43
1:A:821:ILE:H	1:A:821:ILE:HG13	1.53	0.43
1:B:193:LEU:O	1:B:197:LYS:HG2	2.18	0.43
1:B:298:GLN:C	1:B:301:PRO:HD2	2.38	0.43
1:B:540:LEU:O	1:B:544:LYS:HG3	2.18	0.43
1:C:1145:PHE:CD2	1:C:1146:PHE:CD1	3.07	0.43
1:C:1270:SER:OG	1:C:1271:LYS:N	2.51	0.43
1:C:193:LEU:O	1:C:197:LYS:HG2	2.18	0.43
1:C:619:ALA:O	1:C:623:MET:HB2	2.18	0.43
1:C:650:VAL:HG13	1:C:657:ILE:HG23	2.00	0.43
1:C:708:ILE:HG22	1:C:752:LEU:HD11	1.99	0.43
1:C:945:VAL:O	1:C:949:GLN:HB2	2.17	0.43
1:C:952:SER:HB3	1:C:998:GLN:HB3	2.01	0.43
1:D:1260:GLU:HA	1:D:1263:LEU:HD12	1.99	0.43
1:C:439:GLU:HG2	1:D:574:TYR:CZ	2.54	0.43
1:A:563:VAL:HG13	1:A:563:VAL:O	2.17	0.43
1:B:1050:HIS:HA	1:B:1152:THR:OG1	2.18	0.43
1:B:881:LEU:HG	1:B:911:LEU:HD21	1.99	0.43
1:C:151:LEU:HD12	1:C:156:TYR:CZ	2.52	0.43
1:C:283:CYS:O	1:C:287:ARG:HG3	2.18	0.43
1:C:323:GLU:OE2	1:D:573:ARG:NH2	2.51	0.43
1:C:474:LEU:HB3	1:C:477:CYS:SG	2.59	0.43
1:C:667:LEU:HB3	1:C:751:VAL:HG11	2.00	0.43
1:D:922:TYR:HD1	1:D:922:TYR:N	2.14	0.43
1:A:185:CYS:O	1:A:186:LEU:HD23	2.19	0.43
1:B:1260:GLU:HA	1:B:1263:LEU:HD12	1.99	0.43
1:C:466:ILE:O	1:C:469:TYR:HB3	2.18	0.43
1:D:339:LYS:HA	1:D:339:LYS:HD2	1.66	0.43
1:D:382:LEU:HD22	1:D:425:ILE:HG23	2.00	0.43
1:D:502:VAL:O	1:D:502:VAL:HG13	2.18	0.43
1:D:996:SER:HB3	1:D:999:PHE:CB	2.48	0.43
1:A:1003:LEU:HG	1:A:1031:LEU:HB3	2.01	0.43
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.45	0.43
1:B:1174:LEU:O	1:B:1178:VAL:HG23	2.18	0.43
1:B:694:GLU:O	1:B:698:TYR:HD1	2.02	0.43
1:C:957:GLN:HG3	1:C:960:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:SER:O	1:D:226:ARG:C	2.56	0.43
1:A:995:THR:HB	1:A:996:SER:H	1.66	0.43
1:B:242:LYS:HA	1:B:245:ARG:HE	1.83	0.43
1:B:466:ILE:O	1:B:469:TYR:HB3	2.19	0.43
1:C:14:THR:O	1:C:15:ASP:C	2.56	0.43
1:C:382:LEU:HD22	1:C:425:ILE:HG23	2.00	0.43
1:C:502:VAL:HG13	1:C:502:VAL:O	2.19	0.43
1:C:524:MET:CB	1:C:592:ARG:HH21	2.31	0.43
1:D:657:ILE:HD12	1:D:733:ASN:O	2.17	0.43
1:A:1143:VAL:HG13	1:A:1206:LEU:HG	1.99	0.43
1:A:283:CYS:O	1:A:287:ARG:HG3	2.18	0.43
1:A:341:LEU:HD11	1:A:359:CYS:HB3	2.01	0.43
1:B:954:GLN:O	1:B:958:PHE:HD1	2.02	0.43
1:B:952:SER:HB3	1:B:998:GLN:HB3	2.01	0.43
1:C:217:LEU:O	1:C:217:LEU:HD23	2.18	0.43
1:C:549:LEU:HG	1:C:549:LEU:O	2.18	0.43
1:D:447:ARG:O	1:D:456:ILE:HD11	2.19	0.43
1:D:650:VAL:HG13	1:D:657:ILE:HG23	2.00	0.43
1:D:816:LEU:HD13	1:D:838:MET:HE1	2.00	0.43
1:A:298:GLN:HE21	1:A:336:LYS:CG	2.29	0.43
1:A:383:ILE:HG13	1:A:384:GLU:N	2.34	0.43
1:A:549:LEU:HG	1:A:549:LEU:O	2.19	0.43
1:A:952:SER:HB3	1:A:998:GLN:HB3	2.01	0.43
1:B:383:ILE:HG13	1:B:384:GLU:N	2.34	0.43
1:B:762:PHE:CD1	1:B:762:PHE:N	2.86	0.43
1:C:1156:SER:HA	1:C:1160:VAL:HG21	2.01	0.43
1:C:225:SER:O	1:C:226:ARG:C	2.57	0.43
1:D:221:SER:O	1:D:224:GLY:N	2.51	0.43
1:A:1156:SER:HA	1:A:1160:VAL:HG21	2.01	0.43
1:A:1199:VAL:O	1:A:1202:SER:OG	2.30	0.43
1:A:227:ARG:HG3	1:A:288:GLU:HG3	2.00	0.43
1:A:466:ILE:O	1:A:469:TYR:HB3	2.19	0.43
1:A:508:ILE:O	1:B:435:MET:HG3	2.18	0.43
1:A:549:LEU:HB2	1:A:567:ARG:HD2	2.01	0.43
1:B:349:PHE:O	1:B:353:LEU:HG	2.17	0.43
1:B:385:PHE:CE2	1:B:389:LEU:HD11	2.54	0.43
1:B:387:PHE:CZ	1:B:443:GLN:HB3	2.53	0.43
1:B:816:LEU:HD13	1:B:838:MET:CE	2.49	0.43
1:B:973:PHE:CD1	1:B:974:ASN:N	2.72	0.43
1:C:880:LEU:HD22	1:C:907:CYS:HA	2.01	0.43
1:D:694:GLU:O	1:D:698:TYR:HD1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:952:SER:HB3	1:D:998:GLN:HB3	2.00	0.43
1:A:174:MET:HE1	1:A:205:LEU:HD11	2.01	0.42
1:B:1145:PHE:CD2	1:B:1146:PHE:CD1	3.07	0.42
1:C:297:GLN:HG2	1:C:297:GLN:H	1.62	0.42
1:D:1185:CYS:SG	1:D:1191:ILE:HG12	2.59	0.42
1:D:165:CYS:HB3	1:D:197:LYS:HE3	2.01	0.42
1:D:387:PHE:CZ	1:D:443:GLN:HB3	2.54	0.42
1:D:816:LEU:HD13	1:D:838:MET:CE	2.49	0.42
1:A:1005:TRP:O	1:A:1009:ILE:HG13	2.19	0.42
1:A:193:LEU:O	1:A:197:LYS:HG2	2.19	0.42
1:A:513:ARG:NH1	1:A:514:ASP:OD1	2.52	0.42
1:B:165:CYS:HB3	1:B:197:LYS:HE3	2.01	0.42
1:B:221:SER:O	1:B:224:GLY:N	2.52	0.42
1:B:708:ILE:HG22	1:B:752:LEU:HD11	2.01	0.42
1:B:885:THR:O	1:B:886:SER:HB2	2.19	0.42
1:C:185:CYS:O	1:C:186:LEU:HD23	2.19	0.42
1:C:456:ILE:O	1:C:456:ILE:CG2	2.67	0.42
1:C:529:LEU:HD21	1:C:600:ILE:HG13	2.02	0.42
1:D:885:THR:O	1:D:886:SER:HB2	2.19	0.42
1:D:954:GLN:O	1:D:958:PHE:HD1	2.02	0.42
1:A:120:ARG:HG2	1:A:172:ARG:HH12	1.82	0.42
1:A:706:GLU:O	1:A:709:THR:HB	2.19	0.42
1:B:957:GLN:HG3	1:B:960:ARG:NH2	2.33	0.42
1:C:1182:LEU:O	1:C:1186:GLN:HG3	2.19	0.42
1:C:165:CYS:HB3	1:C:197:LYS:HE3	2.01	0.42
1:C:635:GLU:O	1:C:711:ARG:NH2	2.40	0.42
1:D:349:PHE:CD2	1:D:1037:SER:HB3	2.54	0.42
1:D:217:LEU:HD22	1:D:229:VAL:CG1	2.43	0.42
1:D:335:VAL:HG13	1:D:414:THR:HG21	2.00	0.42
1:A:573:ARG:HB2	1:A:573:ARG:HE	1.70	0.42
1:A:524:MET:HB3	1:A:592:ARG:HH21	1.83	0.42
1:A:694:GLU:O	1:A:698:TYR:HD1	2.03	0.42
1:B:227:ARG:HH21	1:B:291:LYS:CD	2.32	0.42
1:B:226:ARG:NH1	1:B:282:ASP:CG	2.73	0.42
1:B:619:ALA:O	1:B:623:MET:HB2	2.18	0.42
1:C:90:ILE:CD1	1:C:125:LYS:HB3	2.49	0.42
1:C:440:ILE:O	1:C:444:VAL:HG23	2.18	0.42
1:C:885:THR:O	1:C:886:SER:HB2	2.20	0.42
1:D:185:CYS:O	1:D:186:LEU:HD23	2.19	0.42
1:D:440:ILE:O	1:D:444:VAL:HG23	2.19	0.42
1:A:165:CYS:HB3	1:A:197:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:GLN:HG2	1:A:947:VAL:HG22	2.00	0.42
1:B:185:CYS:O	1:B:186:LEU:HD23	2.19	0.42
1:B:329:LEU:O	1:B:329:LEU:HD12	2.20	0.42
1:C:65:ARG:HD3	1:C:100:PHE:CZ	2.55	0.42
1:C:242:LYS:HA	1:C:245:ARG:HE	1.84	0.42
1:C:3:LEU:HD23	1:C:6:LEU:HD12	2.01	0.42
1:C:60:ASP:O	1:C:64:ARG:HB2	2.19	0.42
1:C:706:GLU:O	1:C:709:THR:HB	2.19	0.42
1:D:1145:PHE:CD2	1:D:1146:PHE:CD1	3.07	0.42
1:D:396:LYS:HB3	1:D:396:LYS:HE2	1.90	0.42
1:D:473:ILE:HG13	1:D:473:ILE:H	1.61	0.42
1:D:762:PHE:N	1:D:762:PHE:CD1	2.86	0.42
1:A:66:TYR:CD1	1:A:104:LEU:HD22	2.54	0.42
1:A:242:LYS:HA	1:A:245:ARG:HE	1.84	0.42
1:A:474:LEU:HD22	1:A:477:CYS:SG	2.59	0.42
1:A:954:GLN:O	1:A:958:PHE:HD1	2.03	0.42
1:A:957:GLN:HG3	1:A:960:ARG:NH2	2.34	0.42
1:B:1185:CYS:SG	1:B:1191:ILE:HG12	2.59	0.42
1:B:1270:SER:OG	1:B:1271:LYS:N	2.52	0.42
1:C:762:PHE:N	1:C:762:PHE:CD1	2.87	0.42
1:C:954:GLN:O	1:C:958:PHE:HD1	2.03	0.42
1:D:966:LEU:HB3	1:D:1013:TYR:CZ	2.54	0.42
1:A:1103:LYS:HB3	1:A:1103:LYS:HE2	1.79	0.42
1:A:1145:PHE:CD2	1:A:1146:PHE:CD1	3.07	0.42
1:B:1077:ALA:CB	1:B:1078:PRO:HD3	2.40	0.42
1:B:1103:LYS:HE2	1:B:1103:LYS:HB3	1.80	0.42
1:B:502:VAL:O	1:B:502:VAL:HG13	2.19	0.42
1:B:529:LEU:HD22	1:B:533:LYS:HE3	2.00	0.42
1:B:650:VAL:HG13	1:B:657:ILE:HG23	2.00	0.42
1:C:1005:TRP:O	1:C:1009:ILE:HG13	2.19	0.42
1:C:120:ARG:HG2	1:C:172:ARG:HH12	1.82	0.42
1:C:474:LEU:HD22	1:C:477:CYS:SG	2.59	0.42
1:C:694:GLU:O	1:C:698:TYR:HD1	2.03	0.42
1:D:1182:LEU:O	1:D:1186:GLN:HG3	2.19	0.42
1:D:283:CYS:O	1:D:287:ARG:HG3	2.20	0.42
1:D:880:LEU:HD22	1:D:907:CYS:HA	2.02	0.42
1:D:957:GLN:HG3	1:D:960:ARG:NH2	2.34	0.42
1:A:1071:VAL:HG12	1:A:1075:THR:HG21	2.02	0.42
1:A:244:HIS:CD2	1:A:260:PRO:HG2	2.54	0.42
1:A:529:LEU:HD22	1:A:533:LYS:HE3	2.00	0.42
1:A:762:PHE:CD1	1:A:762:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:TRP:O	1:B:1009:ILE:HG13	2.19	0.42
1:B:77:GLU:CB	1:B:121:LEU:HA	2.31	0.42
1:B:353:LEU:HB3	1:B:1131:ILE:HG12	2.02	0.42
1:C:383:ILE:C	1:C:383:ILE:HD12	2.40	0.42
1:C:519:VAL:HG12	1:C:520:LEU:N	2.34	0.42
1:D:597:GLN:HG2	1:D:597:GLN:H	1.50	0.42
1:D:623:MET:HE2	1:D:623:MET:HB2	1.85	0.42
1:A:1053:LEU:HA	1:A:1053:LEU:HD23	1.86	0.42
1:A:1136:VAL:HG11	1:A:1194:THR:HG22	2.02	0.42
1:A:3:LEU:HD23	1:A:6:LEU:HD12	2.01	0.42
1:A:816:LEU:HD22	1:A:838:MET:HE3	2.01	0.42
1:B:1156:SER:HA	1:B:1160:VAL:HG21	2.01	0.42
1:B:113:VAL:HG22	1:B:164:LEU:HG	2.01	0.42
1:B:217:LEU:HD22	1:B:229:VAL:CG1	2.44	0.42
1:B:661:GLU:HA	1:B:662:PRO:HD2	1.92	0.42
1:C:1158:SER:O	1:C:1161:ASP:N	2.53	0.42
1:D:1156:SER:HA	1:D:1160:VAL:HG21	2.01	0.42
1:D:763:SER:O	1:D:767:PHE:CD1	2.72	0.42
1:A:1182:LEU:O	1:A:1186:GLN:HG3	2.19	0.42
1:A:1200:LYS:HB3	1:A:1274:LEU:CD2	2.50	0.42
1:B:1005:TRP:CE2	1:B:1009:ILE:HD11	2.55	0.42
1:C:609:TYR:CE2	1:C:861:PRO:HB3	2.55	0.42
1:C:817:PHE:HB3	1:C:882:TRP:CZ3	2.55	0.42
1:C:995:THR:HB	1:C:996:SER:H	1.66	0.42
1:D:217:LEU:O	1:D:217:LEU:HD23	2.19	0.42
1:D:474:LEU:HD22	1:D:477:CYS:SG	2.60	0.42
1:A:1042:LEU:O	1:A:1145:PHE:HD1	2.03	0.41
1:A:440:ILE:O	1:A:444:VAL:HG23	2.19	0.41
1:A:763:SER:O	1:A:767:PHE:CD1	2.72	0.41
1:A:834:SER:OG	1:A:837:PHE:HB3	2.20	0.41
1:A:814:THR:OG1	1:A:879:VAL:HG21	2.20	0.41
1:B:1158:SER:O	1:B:1161:ASP:N	2.53	0.41
1:B:1199:VAL:O	1:B:1202:SER:OG	2.30	0.41
1:B:226:ARG:HH12	1:B:282:ASP:CG	2.24	0.41
1:C:96:GLU:HA	1:C:96:GLU:OE1	2.20	0.41
1:C:973:PHE:CD1	1:C:974:ASN:N	2.72	0.41
1:D:113:VAL:HG22	1:D:164:LEU:HG	2.01	0.41
1:D:383:ILE:HG13	1:D:384:GLU:N	2.34	0.41
1:D:466:ILE:O	1:D:469:TYR:HB3	2.19	0.41
1:A:169:TRP:CZ3	1:A:177:LEU:HB3	2.56	0.41
1:A:816:LEU:HD13	1:A:838:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:GLY:HA3	1:A:861:PRO:HD2	1.77	0.41
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.20	0.41
1:B:1005:TRP:CZ2	1:B:1009:ILE:HD11	2.55	0.41
1:B:978:ALA:HB1	1:B:1020:PHE:CE1	2.55	0.41
1:B:1182:LEU:O	1:B:1186:GLN:HG3	2.20	0.41
1:B:573:ARG:HE	1:B:573:ARG:HB2	1.71	0.41
1:B:834:SER:OG	1:B:837:PHE:HB3	2.20	0.41
1:C:1150:VAL:O	1:C:1213:PHE:HD1	2.03	0.41
1:C:368:VAL:HG11	1:C:428:GLU:HB3	2.02	0.41
1:C:447:ARG:O	1:C:456:ILE:HD11	2.19	0.41
1:C:763:SER:O	1:C:767:PHE:CD1	2.72	0.41
1:C:816:LEU:HD22	1:C:838:MET:HE3	2.01	0.41
1:D:1270:SER:OG	1:D:1271:LYS:N	2.52	0.41
1:D:127:LEU:HB3	1:D:180:VAL:HG21	2.02	0.41
1:D:297:GLN:HB2	1:D:1104:GLY:HA3	2.02	0.41
1:D:524:MET:HB2	1:D:592:ARG:HH21	1.85	0.41
1:D:664:ASP:N	1:D:664:ASP:OD1	2.54	0.41
1:D:817:PHE:HB3	1:D:882:TRP:CZ3	2.56	0.41
1:A:1050:HIS:HB2	1:A:1148:GLU:O	2.20	0.41
1:C:12:LYS:HA	1:C:12:LYS:HD3	1.93	0.41
1:C:549:LEU:HD13	1:D:273:LEU:HD21	2.02	0.41
1:D:816:LEU:HD22	1:D:838:MET:HE3	2.02	0.41
1:A:226:ARG:NH1	1:A:282:ASP:OD1	2.54	0.41
1:A:502:VAL:HG13	1:A:502:VAL:O	2.20	0.41
1:A:533:LYS:HB2	1:A:533:LYS:HE3	1.91	0.41
1:A:928:GLN:H	1:A:928:GLN:HG2	1.59	0.41
1:B:283:CYS:O	1:B:287:ARG:HG3	2.20	0.41
1:B:503:GLN:HG2	1:B:541:LEU:HD21	2.03	0.41
1:C:1049:ILE:HG13	1:C:1049:ILE:H	1.57	0.41
1:C:529:LEU:HD22	1:C:533:LYS:HE3	2.03	0.41
1:C:667:LEU:HD23	1:C:667:LEU:HA	1.79	0.41
1:C:996:SER:HB3	1:C:999:PHE:HB3	2.03	0.41
1:D:1005:TRP:CZ2	1:D:1009:ILE:HD11	2.55	0.41
1:D:1092:LEU:HD13	1:D:1169:LYS:HG2	2.01	0.41
1:D:341:LEU:HD11	1:D:359:CYS:HB3	2.01	0.41
1:D:474:LEU:O	1:D:475:GLN:C	2.57	0.41
1:D:548:VAL:CG1	1:D:580:GLU:HA	2.50	0.41
1:A:226:ARG:HH12	1:A:282:ASP:CG	2.24	0.41
1:A:637:GLU:HB3	1:A:640:LEU:HG	2.03	0.41
1:A:804:LEU:O	1:A:848:LYS:NZ	2.51	0.41
1:A:817:PHE:HB3	1:A:882:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:180:VAL:HB	2.20	0.41
1:B:341:LEU:HD11	1:B:359:CYS:HB3	2.01	0.41
1:C:169:TRP:CZ3	1:C:177:LEU:HB3	2.56	0.41
1:C:329:LEU:HD12	1:C:329:LEU:O	2.21	0.41
1:C:90:ILE:O	1:C:94:MET:HG3	2.21	0.41
1:D:1005:TRP:CE2	1:D:1009:ILE:HD11	2.55	0.41
1:D:1005:TRP:O	1:D:1009:ILE:HG13	2.20	0.41
1:D:141:LYS:O	1:D:142:GLU:HG3	2.20	0.41
1:D:177:LEU:O	1:D:180:VAL:HB	2.21	0.41
1:D:456:ILE:O	1:D:456:ILE:CG2	2.68	0.41
1:D:834:SER:OG	1:D:837:PHE:HB3	2.20	0.41
1:A:1046:SER:HB2	1:A:1148:GLU:HB2	2.03	0.41
1:A:1270:SER:OG	1:A:1271:LYS:N	2.52	0.41
1:A:113:VAL:HG22	1:A:164:LEU:HG	2.03	0.41
1:A:65:ARG:HD3	1:A:100:PHE:CZ	2.54	0.41
1:B:217:LEU:CD2	1:B:229:VAL:HG13	2.45	0.41
1:C:152:ASN:HB2	1:C:154:GLU:HG2	2.03	0.41
1:C:533:LYS:HG3	1:C:603:MET:HE2	2.01	0.41
1:D:1158:SER:O	1:D:1161:ASP:N	2.53	0.41
1:D:503:GLN:HG2	1:D:541:LEU:HD21	2.02	0.41
1:D:619:ALA:O	1:D:623:MET:HB2	2.19	0.41
1:A:750:GLU:OE2	1:A:802:SER:HA	2.21	0.41
1:A:91:GLY:O	1:A:95:LEU:HG	2.21	0.41
1:B:637:GLU:HB3	1:B:640:LEU:HG	2.03	0.41
1:B:672:HIS:CE1	1:B:805:SER:HB3	2.54	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CZ3	2.55	0.41
1:B:880:LEU:HD22	1:B:907:CYS:HA	2.01	0.41
1:C:1042:LEU:CD2	1:C:1084:VAL:HG12	2.51	0.41
1:C:1249:ILE:H	1:C:1249:ILE:HG13	1.68	0.41
1:C:834:SER:OG	1:C:837:PHE:HB3	2.20	0.41
1:D:1103:LYS:HE2	1:D:1103:LYS:HB3	1.79	0.41
1:D:664:ASP:HB2	1:D:803:LEU:CD1	2.50	0.41
1:A:1103:LYS:HG2	1:A:1180:TYR:HD1	1.86	0.41
1:A:141:LYS:O	1:A:142:GLU:HG3	2.21	0.41
1:A:474:LEU:O	1:A:475:GLN:C	2.57	0.41
1:A:533:LYS:HG3	1:A:603:MET:HE2	2.03	0.41
1:B:1053:LEU:HA	1:B:1053:LEU:HD23	1.86	0.41
1:B:1056:ILE:HD12	1:B:1216:TYR:CG	2.56	0.41
1:B:1272:VAL:HG12	1:B:1273:ASN:N	2.36	0.41
1:C:1272:VAL:HG12	1:C:1273:ASN:N	2.36	0.41
1:C:816:LEU:HD13	1:C:838:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1103:LYS:HG2	1:D:1180:TYR:HD1	1.86	0.41
1:D:297:GLN:CB	1:D:1104:GLY:HA3	2.50	0.41
1:D:915:PHE:CE2	1:D:988:LEU:HD21	2.56	0.41
1:A:1158:SER:O	1:A:1161:ASP:N	2.53	0.41
1:A:21:LEU:HB3	1:A:64:ARG:CZ	2.50	0.41
1:A:95:LEU:HA	1:A:98:HIS:HE1	1.86	0.41
1:A:95:LEU:O	1:A:98:HIS:CE1	2.74	0.41
1:B:1025:MET:CE	1:B:1025:MET:HA	2.51	0.41
1:B:1171:TYR:CE1	1:B:1256:ILE:HG12	2.56	0.41
1:B:141:LYS:O	1:B:142:GLU:HG3	2.20	0.41
1:B:169:TRP:CZ3	1:B:177:LEU:HB3	2.56	0.41
1:B:335:VAL:HG13	1:B:414:THR:HG21	2.02	0.41
1:B:816:LEU:HD22	1:B:838:MET:HE3	2.03	0.41
1:B:915:PHE:CE2	1:B:988:LEU:HD21	2.56	0.41
1:C:1009:ILE:HG13	1:C:1009:ILE:H	1.66	0.41
1:C:503:GLN:HG2	1:C:541:LEU:HD21	2.03	0.41
1:D:565:GLN:H	1:D:565:GLN:HG2	1.53	0.41
1:A:329:LEU:HD12	1:A:329:LEU:O	2.21	0.41
1:A:385:PHE:CE2	1:A:389:LEU:HD11	2.55	0.41
1:A:885:THR:O	1:A:886:SER:HB2	2.20	0.41
1:B:1042:LEU:CD2	1:B:1084:VAL:HG12	2.51	0.41
1:B:1259:TYR:CE1	1:B:1263:LEU:HD11	2.56	0.41
1:B:127:LEU:HB3	1:B:180:VAL:HG21	2.03	0.41
1:B:474:LEU:O	1:B:475:GLN:C	2.57	0.41
1:B:91:GLY:O	1:B:95:LEU:HG	2.21	0.41
1:C:1136:VAL:CG1	1:C:1198:LEU:HD12	2.51	0.41
1:C:664:ASP:N	1:C:664:ASP:OD1	2.54	0.41
1:D:1272:VAL:HG12	1:D:1273:ASN:N	2.36	0.41
1:D:211:PRO:HD3	1:D:267:VAL:HG13	2.03	0.41
1:D:385:PHE:CE2	1:D:389:LEU:HD11	2.55	0.41
1:D:814:THR:OG1	1:D:879:VAL:HG21	2.20	0.41
1:A:273:LEU:HD21	1:B:549:LEU:CD1	2.51	0.41
1:A:473:ILE:H	1:A:473:ILE:HG13	1.61	0.41
1:B:69:TYR:O	1:B:73:ILE:HG13	2.21	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CE3	2.56	0.41
1:C:637:GLU:HB3	1:C:640:LEU:HG	2.03	0.41
1:C:705:LEU:HB3	1:C:755:TYR:CE2	2.55	0.41
1:D:169:TRP:CZ3	1:D:177:LEU:HB3	2.56	0.41
1:A:273:LEU:HD21	1:B:549:LEU:HD13	2.03	0.40
1:A:69:TYR:O	1:A:73:ILE:HG13	2.21	0.40
1:B:447:ARG:O	1:B:456:ILE:HD11	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:TYR:O	1:B:490:LEU:HG	2.22	0.40
1:B:814:THR:OG1	1:B:879:VAL:HG21	2.20	0.40
1:B:90:ILE:HG21	1:B:125:LYS:O	2.20	0.40
1:B:996:SER:HB3	1:B:999:PHE:HB3	2.02	0.40
1:C:1005:TRP:CZ2	1:C:1009:ILE:HD11	2.55	0.40
1:D:980:LEU:HD23	1:D:981:LEU:N	2.36	0.40
1:A:982:ILE:HD11	1:A:1024:LEU:HG	2.03	0.40
1:A:1025:MET:HA	1:A:1025:MET:CE	2.51	0.40
1:A:152:ASN:HB2	1:A:154:GLU:HG2	2.03	0.40
1:A:836:GLU:HA	1:A:839:HIS:NE2	2.36	0.40
1:A:880:LEU:HD22	1:A:907:CYS:HA	2.01	0.40
1:B:672:HIS:CE1	1:B:861:PRO:CD	3.04	0.40
1:C:661:GLU:HA	1:C:662:PRO:HD2	1.92	0.40
1:C:817:PHE:HB3	1:C:882:TRP:CE3	2.56	0.40
1:C:95:LEU:O	1:C:98:HIS:CE1	2.74	0.40
1:D:1154:LEU:CD1	1:D:1163:LEU:HD12	2.45	0.40
1:D:152:ASN:HB2	1:D:154:GLU:HG2	2.03	0.40
1:D:302:SER:CB	1:D:357:ARG:HG2	2.45	0.40
1:D:996:SER:HB3	1:D:999:PHE:HB3	2.02	0.40
1:A:671:GLN:C	1:A:671:GLN:OE1	2.60	0.40
1:A:927:GLN:O	1:A:931:GLN:HG3	2.22	0.40
1:A:930:LEU:HB3	1:A:950:ARG:HB3	2.03	0.40
1:A:982:ILE:HG21	1:A:1023:SER:HB3	2.03	0.40
1:C:177:LEU:O	1:C:180:VAL:HB	2.21	0.40
1:C:391:ASP:OD2	1:C:447:ARG:NH1	2.54	0.40
1:C:931:GLN:HG2	1:C:950:ARG:NH1	2.36	0.40
1:C:91:GLY:O	1:C:95:LEU:HG	2.21	0.40
1:D:1025:MET:HA	1:D:1025:MET:CE	2.51	0.40
1:A:217:LEU:HD22	1:A:229:VAL:CG1	2.41	0.40
1:A:817:PHE:HB3	1:A:882:TRP:CE3	2.56	0.40
1:A:996:SER:HB3	1:A:999:PHE:HB3	2.02	0.40
1:B:474:LEU:HD22	1:B:477:CYS:SG	2.62	0.40
1:B:76:VAL:HG11	1:B:90:ILE:HD11	2.04	0.40
1:B:95:LEU:HA	1:B:98:HIS:HE1	1.86	0.40
1:C:1005:TRP:CE2	1:C:1009:ILE:HD11	2.56	0.40
1:C:169:TRP:HD1	1:C:169:TRP:N	2.12	0.40
1:C:627:PHE:CE2	1:C:631:LYS:HD2	2.56	0.40
1:C:713:ILE:CG2	1:C:772:SER:HB3	2.50	0.40
1:C:36:GLN:HG3	1:C:85:VAL:HG11	2.04	0.40
1:A:1259:TYR:CE1	1:A:1263:LEU:HD11	2.56	0.40
1:A:177:LEU:O	1:A:180:VAL:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:GLN:H	1:A:565:GLN:HG2	1.53	0.40
1:A:664:ASP:OD1	1:A:664:ASP:N	2.54	0.40
1:B:763:SER:O	1:B:767:PHE:CD1	2.72	0.40
1:B:913:LYS:O	1:B:917:VAL:HG23	2.21	0.40
1:B:95:LEU:O	1:B:98:HIS:CE1	2.74	0.40
1:B:96:GLU:OE1	1:B:96:GLU:HA	2.21	0.40
1:C:1042:LEU:O	1:C:1145:PHE:HD1	2.04	0.40
1:C:814:THR:OG1	1:C:879:VAL:HG21	2.20	0.40
1:C:815:ALA:HA	1:C:819:ASP:HB3	2.04	0.40
1:D:549:LEU:HB2	1:D:567:ARG:CD	2.52	0.40
1:D:836:GLU:HA	1:D:839:HIS:NE2	2.36	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	1108/1308 (85%)	1023 (92%)	82 (7%)	3 (0%)	41	71
1	B	1045/1308 (80%)	969 (93%)	72 (7%)	4 (0%)	34	66
1	C	1108/1308 (85%)	1022 (92%)	83 (8%)	3 (0%)	41	71
1	D	1008/1308 (77%)	933 (93%)	71 (7%)	4 (0%)	34	66
All	All	4269/5232 (82%)	3947 (92%)	308 (7%)	14 (0%)	41	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	150	ASP
1	B	122	VAL
1	B	150	ASP

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Mol	Chain	Res	Type
1	C	122	VAL
1	C	150	ASP
1	D	122	VAL
1	D	150	ASP
1	A	996	SER
1	B	996	SER
1	C	996	SER
1	D	452	THR
1	D	996	SER
1	B	452	THR

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	1032/1188 (87%)	917 (89%)	115 (11%)	6	23
1	B	979/1188 (82%)	867 (89%)	112 (11%)	5	22
1	C	1032/1188 (87%)	917 (89%)	115 (11%)	6	23
1	D	945/1188 (80%)	838 (89%)	107 (11%)	6	22
All	All	3988/4752 (84%)	3539 (89%)	449 (11%)	6	22

All (449) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	19	GLU
1	A	54	SER
1	A	71	CYS
1	A	81	LEU
1	A	97	VAL
1	A	99	HIS
1	A	118	GLU
1	A	119	ASP
1	A	130	LEU
1	A	169	TRP

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Mol	Chain	Res	Type
1	A	171	GLN
1	A	177	LEU
1	A	183	ASP
1	A	208	GLN
1	A	213	LEU
1	A	240	LEU
1	A	245	ARG
1	A	247	GLU
1	A	262	ASP
1	A	264	LEU
1	A	275	ILE
1	A	277	PHE
1	A	288	GLU
1	A	312	LEU
1	A	316	LEU
1	A	320	GLN
1	A	329	LEU
1	A	343	LEU
1	A	347	SER
1	A	349	PHE
1	A	359	CYS
1	A	360	VAL
1	A	376	ASP
1	A	377	HIS
1	A	378	VAL
1	A	383	ILE
1	A	397	LYS
1	A	414	THR
1	A	421	LEU
1	A	427	LEU
1	A	438	GLN
1	A	443	GLN
1	A	450	THR
1	A	451	ARG
1	A	452	THR
1	A	456	ILE
1	A	468	MET
1	A	473	ILE
1	A	477	CYS
1	A	479	LYS
1	A	488	THR
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	496	GLN
1	A	502	VAL
1	A	515	SER
1	A	519	VAL
1	A	529	LEU
1	A	530	ASP
1	A	549	LEU
1	A	552	LEU
1	A	563	VAL
1	A	565	GLN
1	A	569	ASP
1	A	579	ASN
1	A	587	ILE
1	A	597	GLN
1	A	606	ASP
1	A	612	LEU
1	A	651	LEU
1	A	659	LEU
1	A	661	GLU
1	A	663	LEU
1	A	666	LEU
1	A	699	SER
1	A	711	ARG
1	A	712	MET
1	A	743	CYS
1	A	754	GLU
1	A	759	ILE
1	A	765	SER
1	A	768	GLU
1	A	771	LEU
1	A	803	LEU
1	A	806	LEU
1	A	812	LEU
1	A	824	HIS
1	A	840	TYR
1	A	846	LEU
1	A	853	ILE
1	A	864	GLN
1	A	878	ARG
1	A	911	LEU
1	A	919	LEU
1	A	949	GLN

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Mol	Chain	Res	Type
1	A	965	LEU
1	A	980	LEU
1	A	981	LEU
1	A	982	ILE
1	A	1001	GLN
1	A	1003	LEU
1	A	1013	TYR
1	A	1024	LEU
1	A	1035	TYR
1	A	1050	HIS
1	A	1056	ILE
1	A	1071	VAL
1	A	1084	VAL
1	A	1105	SER
1	A	1142	LEU
1	A	1183	GLN
1	A	1194	THR
1	A	1200	LYS
1	A	1274	LEU
1	A	1275	MET
1	B	71	CYS
1	B	81	LEU
1	B	97	VAL
1	B	99	HIS
1	B	118	GLU
1	B	119	ASP
1	B	130	LEU
1	B	169	TRP
1	B	171	GLN
1	B	177	LEU
1	B	183	ASP
1	B	208	GLN
1	B	213	LEU
1	B	240	LEU
1	B	245	ARG
1	B	247	GLU
1	B	262	ASP
1	B	264	LEU
1	B	275	ILE
1	B	277	PHE
1	B	285	LEU
1	B	288	GLU

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Mol	Chain	Res	Type
1	B	312	LEU
1	B	316	LEU
1	B	320	GLN
1	B	329	LEU
1	B	343	LEU
1	B	347	SER
1	B	349	PHE
1	B	359	CYS
1	B	360	VAL
1	B	376	ASP
1	B	377	HIS
1	B	378	VAL
1	B	383	ILE
1	B	397	LYS
1	B	414	THR
1	B	421	LEU
1	B	427	LEU
1	B	438	GLN
1	B	443	GLN
1	B	450	THR
1	B	451	ARG
1	B	452	THR
1	B	456	ILE
1	B	468	MET
1	B	473	ILE
1	B	477	CYS
1	B	479	LYS
1	B	488	THR
1	B	493	GLN
1	B	496	GLN
1	B	502	VAL
1	B	515	SER
1	B	529	LEU
1	B	530	ASP
1	B	549	LEU
1	B	552	LEU
1	B	563	VAL
1	B	565	GLN
1	B	569	ASP
1	B	579	ASN
1	B	587	ILE
1	B	597	GLN

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Mol	Chain	Res	Type
1	B	606	ASP
1	B	612	LEU
1	B	651	LEU
1	B	659	LEU
1	B	661	GLU
1	B	663	LEU
1	B	666	LEU
1	B	699	SER
1	B	711	ARG
1	B	712	MET
1	B	743	CYS
1	B	754	GLU
1	B	759	ILE
1	B	765	SER
1	B	768	GLU
1	B	771	LEU
1	B	803	LEU
1	B	806	LEU
1	B	812	LEU
1	B	824	HIS
1	B	840	TYR
1	B	846	LEU
1	B	853	ILE
1	B	864	GLN
1	B	878	ARG
1	B	911	LEU
1	B	919	LEU
1	B	949	GLN
1	B	965	LEU
1	B	980	LEU
1	B	981	LEU
1	B	982	ILE
1	B	1001	GLN
1	B	1003	LEU
1	B	1013	TYR
1	B	1024	LEU
1	B	1035	TYR
1	B	1050	HIS
1	B	1056	ILE
1	B	1071	VAL
1	B	1084	VAL
1	B	1105	SER

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Mol	Chain	Res	Type
1	B	1142	LEU
1	B	1183	GLN
1	B	1194	THR
1	B	1200	LYS
1	B	1274	LEU
1	B	1275	MET
1	C	15	ASP
1	C	19	GLU
1	C	54	SER
1	C	71	CYS
1	C	81	LEU
1	C	97	VAL
1	C	99	HIS
1	C	118	GLU
1	C	119	ASP
1	C	130	LEU
1	C	169	TRP
1	C	171	GLN
1	C	177	LEU
1	C	183	ASP
1	C	208	GLN
1	C	213	LEU
1	C	240	LEU
1	C	245	ARG
1	C	247	GLU
1	C	262	ASP
1	C	264	LEU
1	C	275	ILE
1	C	277	PHE
1	C	285	LEU
1	C	288	GLU
1	C	312	LEU
1	C	316	LEU
1	C	329	LEU
1	C	343	LEU
1	C	347	SER
1	C	349	PHE
1	C	359	CYS
1	C	360	VAL
1	C	376	ASP
1	C	377	HIS
1	C	378	VAL

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Mol	Chain	Res	Type
1	C	383	ILE
1	C	397	LYS
1	C	414	THR
1	C	421	LEU
1	C	427	LEU
1	C	438	GLN
1	C	443	GLN
1	C	450	THR
1	C	451	ARG
1	C	452	THR
1	C	456	ILE
1	C	468	MET
1	C	473	ILE
1	C	477	CYS
1	C	479	LYS
1	C	488	THR
1	C	493	GLN
1	C	496	GLN
1	C	502	VAL
1	C	515	SER
1	C	519	VAL
1	C	529	LEU
1	C	530	ASP
1	C	549	LEU
1	C	552	LEU
1	C	563	VAL
1	C	565	GLN
1	C	569	ASP
1	C	579	ASN
1	C	587	ILE
1	C	597	GLN
1	C	606	ASP
1	C	612	LEU
1	C	651	LEU
1	C	659	LEU
1	C	661	GLU
1	C	663	LEU
1	C	666	LEU
1	C	699	SER
1	C	711	ARG
1	C	712	MET
1	C	743	CYS

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Mol	Chain	Res	Type
1	C	754	GLU
1	C	759	ILE
1	C	765	SER
1	C	768	GLU
1	C	771	LEU
1	C	803	LEU
1	C	806	LEU
1	C	812	LEU
1	C	824	HIS
1	C	840	TYR
1	C	846	LEU
1	C	853	ILE
1	C	864	GLN
1	C	878	ARG
1	C	911	LEU
1	C	919	LEU
1	C	949	GLN
1	C	965	LEU
1	C	980	LEU
1	C	981	LEU
1	C	982	ILE
1	C	1001	GLN
1	C	1003	LEU
1	C	1013	TYR
1	C	1024	LEU
1	C	1035	TYR
1	C	1050	HIS
1	C	1056	ILE
1	C	1071	VAL
1	C	1084	VAL
1	C	1105	SER
1	C	1142	LEU
1	C	1183	GLN
1	C	1194	THR
1	C	1200	LYS
1	C	1274	LEU
1	C	1275	MET
1	D	118	GLU
1	D	119	ASP
1	D	130	LEU
1	D	169	TRP
1	D	171	GLN

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Mol	Chain	Res	Type
1	D	177	LEU
1	D	183	ASP
1	D	208	GLN
1	D	213	LEU
1	D	240	LEU
1	D	245	ARG
1	D	247	GLU
1	D	262	ASP
1	D	264	LEU
1	D	275	ILE
1	D	277	PHE
1	D	285	LEU
1	D	288	GLU
1	D	312	LEU
1	D	316	LEU
1	D	329	LEU
1	D	343	LEU
1	D	347	SER
1	D	349	PHE
1	D	359	CYS
1	D	360	VAL
1	D	376	ASP
1	D	377	HIS
1	D	378	VAL
1	D	383	ILE
1	D	397	LYS
1	D	414	THR
1	D	421	LEU
1	D	427	LEU
1	D	438	GLN
1	D	443	GLN
1	D	450	THR
1	D	451	ARG
1	D	452	THR
1	D	456	ILE
1	D	468	MET
1	D	473	ILE
1	D	477	CYS
1	D	479	LYS
1	D	488	THR
1	D	493	GLN
1	D	496	GLN

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Mol	Chain	Res	Type
1	D	502	VAL
1	D	515	SER
1	D	529	LEU
1	D	530	ASP
1	D	549	LEU
1	D	552	LEU
1	D	563	VAL
1	D	565	GLN
1	D	569	ASP
1	D	579	ASN
1	D	587	ILE
1	D	597	GLN
1	D	606	ASP
1	D	612	LEU
1	D	651	LEU
1	D	659	LEU
1	D	661	GLU
1	D	663	LEU
1	D	666	LEU
1	D	699	SER
1	D	711	ARG
1	D	712	MET
1	D	743	CYS
1	D	754	GLU
1	D	759	ILE
1	D	765	SER
1	D	768	GLU
1	D	771	LEU
1	D	803	LEU
1	D	806	LEU
1	D	812	LEU
1	D	824	HIS
1	D	840	TYR
1	D	846	LEU
1	D	853	ILE
1	D	864	GLN
1	D	878	ARG
1	D	911	LEU
1	D	919	LEU
1	D	949	GLN
1	D	965	LEU
1	D	980	LEU

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Mol	Chain	Res	Type
1	D	981	LEU
1	D	982	ILE
1	D	1001	GLN
1	D	1003	LEU
1	D	1013	TYR
1	D	1024	LEU
1	D	1035	TYR
1	D	1050	HIS
1	D	1056	ILE
1	D	1071	VAL
1	D	1084	VAL
1	D	1105	SER
1	D	1142	LEU
1	D	1183	GLN
1	D	1194	THR
1	D	1200	LYS
1	D	1274	LEU
1	D	1275	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	GLN
1	A	320	GLN
1	A	377	HIS
1	A	672	HIS
1	B	320	GLN
1	B	377	HIS
1	B	433	HIS
1	B	672	HIS
1	C	377	HIS
1	C	672	HIS
1	D	377	HIS
1	D	433	HIS
1	D	672	HIS
1	D	847	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1134/1308 (86%)	0.25	85 (7%) 14 13	85, 192, 306, 410	0
1	B	1071/1308 (81%)	0.27	101 (9%) 8 9	87, 188, 306, 415	0
1	C	1134/1308 (86%)	0.25	70 (6%) 20 20	81, 191, 306, 410	0
1	D	1034/1308 (79%)	0.28	84 (8%) 12 11	84, 185, 302, 416	0
All	All	4373/5232 (83%)	0.26	340 (7%) 13 12	81, 189, 304, 416	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	ALA	12.3
1	D	250	SER	11.1
1	D	135	THR	10.9
1	D	150	ASP	8.9
1	D	299	GLY	8.7
1	D	151	LEU	7.8
1	D	165	CYS	7.6
1	D	101	PRO	7.4
1	C	258	THR	6.8
1	D	105	LEU	6.6
1	D	683	PRO	6.4
1	B	249	SER	6.4
1	D	102	GLY	6.3
1	C	400	ASP	6.3
1	A	967	SER	6.2
1	B	300	ASP	6.2
1	A	397	LYS	6.1
1	C	111	ASP	6.0
1	B	248	GLN	6.0
1	C	397	LYS	5.9
1	D	155	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	298	GLN	5.8
1	D	181	PHE	5.8
1	D	401	GLY	5.8
1	B	108	LEU	5.8
1	D	131	PRO	5.6
1	A	111	ASP	5.6
1	A	401	GLY	5.5
1	C	38	VAL	5.4
1	D	106	VAL	5.4
1	B	85	VAL	5.3
1	A	1191	ILE	5.3
1	B	156	TYR	5.3
1	A	1280	LEU	5.3
1	C	1280	LEU	5.3
1	C	398	ILE	5.2
1	A	1214	ILE	5.1
1	B	259	ALA	5.1
1	D	143	VAL	5.1
1	D	300	ASP	5.0
1	A	38	VAL	5.0
1	B	94	MET	5.0
1	A	1049	ILE	5.0
1	B	152	ASN	5.0
1	D	139	THR	4.9
1	B	102	GLY	4.9
1	D	1185	CYS	4.8
1	A	399	LEU	4.7
1	B	258	THR	4.7
1	B	399	LEU	4.7
1	B	170	PRO	4.7
1	C	399	LEU	4.6
1	D	116	VAL	4.6
1	A	400	ASP	4.6
1	C	973	PHE	4.5
1	D	169	TRP	4.5
1	D	1186	GLN	4.5
1	B	1187	SER	4.4
1	B	98	HIS	4.4
1	D	398	ILE	4.3
1	B	82	GLN	4.3
1	A	261	ALA	4.2
1	B	301	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	398	ILE	4.1
1	A	83	GLN	4.1
1	D	258	THR	4.0
1	C	259	ALA	4.0
1	B	71	CYS	4.0
1	C	1185	CYS	4.0
1	B	553	PRO	4.0
1	A	299	GLY	4.0
1	A	260	PRO	4.0
1	B	971	ASP	4.0
1	D	1190	GLY	4.0
1	B	299	GLY	4.0
1	A	1222	SER	3.9
1	A	1275	MET	3.9
1	A	258	THR	3.9
1	D	113	VAL	3.9
1	B	1276	GLN	3.8
1	D	994	PRO	3.8
1	A	249	SER	3.8
1	C	114	GLY	3.8
1	D	259	ALA	3.8
1	D	161	ILE	3.8
1	B	109	ALA	3.7
1	D	945	VAL	3.7
1	B	973	PHE	3.7
1	A	118	GLU	3.7
1	B	181	PHE	3.7
1	D	553	PRO	3.6
1	B	89	ILE	3.6
1	B	145	ALA	3.6
1	D	156	TYR	3.6
1	D	400	ASP	3.6
1	A	110	SER	3.6
1	A	1149	LEU	3.6
1	D	1011	LYS	3.6
1	A	973	PHE	3.6
1	B	178	THR	3.6
1	B	68	ILE	3.6
1	B	72	CYS	3.6
1	D	1187	SER	3.6
1	C	298	GLN	3.5
1	B	134	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	399	LEU	3.5
1	C	1219	ASN	3.5
1	B	302	SER	3.5
1	D	126	SER	3.5
1	A	1213	PHE	3.5
1	B	295	ALA	3.5
1	C	112	PHE	3.4
1	D	112	PHE	3.4
1	B	657	ILE	3.4
1	B	144	LEU	3.4
1	C	110	SER	3.4
1	B	148	LYS	3.4
1	C	683	PRO	3.4
1	C	698	TYR	3.4
1	B	398	ILE	3.4
1	B	697	LEU	3.3
1	B	73	ILE	3.3
1	B	1151	GLN	3.2
1	C	109	ALA	3.2
1	C	119	ASP	3.2
1	B	92	LEU	3.2
1	D	397	LYS	3.2
1	B	135	THR	3.2
1	B	692	GLU	3.2
1	B	261	ALA	3.2
1	D	249	SER	3.2
1	C	84	ASP	3.2
1	A	114	GLY	3.2
1	A	122	VAL	3.2
1	B	250	SER	3.1
1	B	1017	ASP	3.1
1	B	97	VAL	3.1
1	D	1016	GLU	3.1
1	B	1273	ASN	3.1
1	C	401	GLY	3.1
1	B	67	LYS	3.1
1	C	1190	GLY	3.1
1	D	301	PRO	3.1
1	A	1269	LYS	3.1
1	A	112	PHE	3.0
1	D	125	LYS	3.0
1	B	64	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1184	VAL	3.0
1	B	974	ASN	3.0
1	A	156	TYR	3.0
1	C	42	ALA	3.0
1	B	260	PRO	3.0
1	C	28	ASP	3.0
1	A	845	THR	3.0
1	D	168	ARG	3.0
1	A	1185	CYS	3.0
1	B	397	LYS	2.9
1	A	1218	GLN	2.9
1	A	1217	VAL	2.9
1	C	945	VAL	2.9
1	C	52	LYS	2.9
1	C	1187	SER	2.9
1	D	247	GLU	2.9
1	D	173	TYR	2.9
1	B	99	HIS	2.9
1	A	1196	GLU	2.9
1	B	157	LYS	2.9
1	B	882	TRP	2.9
1	A	972	ASP	2.9
1	A	1186	GLN	2.9
1	B	169	TRP	2.8
1	D	144	LEU	2.8
1	C	117	ARG	2.8
1	C	1154	LEU	2.8
1	A	298	GLN	2.8
1	D	152	ASN	2.8
1	D	193	LEU	2.8
1	A	1045	LEU	2.8
1	D	130	LEU	2.8
1	D	134	LEU	2.8
1	D	971	ASP	2.8
1	A	1221	SER	2.7
1	A	103	PRO	2.7
1	D	1217	VAL	2.7
1	D	127	LEU	2.7
1	D	1264	ILE	2.7
1	A	259	ALA	2.7
1	B	1280	LEU	2.7
1	B	683	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	627	PHE	2.7
1	B	694	GLU	2.7
1	C	115	ALA	2.7
1	D	1055	ASP	2.7
1	C	9	ALA	2.7
1	C	170	PRO	2.7
1	B	1277	HIS	2.7
1	D	177	LEU	2.6
1	A	151	LEU	2.6
1	C	154	GLU	2.6
1	B	150	ASP	2.6
1	A	109	ALA	2.6
1	C	118	GLU	2.6
1	B	1184	VAL	2.6
1	D	1129	LEU	2.6
1	D	639	ASP	2.6
1	B	116	VAL	2.6
1	A	962	LEU	2.6
1	A	821	ILE	2.6
1	B	90	ILE	2.6
1	C	250	SER	2.5
1	B	1185	CYS	2.5
1	D	133	ILE	2.5
1	B	1012	GLU	2.5
1	A	971	ASP	2.5
1	C	260	PRO	2.5
1	A	1190	GLY	2.5
1	B	400	ASP	2.5
1	B	88	GLU	2.5
1	C	47	LEU	2.5
1	D	1014	SER	2.5
1	A	60	ASP	2.5
1	C	1279	LYS	2.5
1	C	299	GLY	2.5
1	B	106	VAL	2.5
1	C	261	ALA	2.5
1	A	13	THR	2.5
1	C	168	ARG	2.5
1	D	178	THR	2.5
1	C	563	VAL	2.4
1	D	947	VAL	2.4
1	A	36	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	142	GLU	2.4
1	C	105	LEU	2.4
1	B	77	GLU	2.4
1	A	1183	GLN	2.4
1	D	1276	GLN	2.4
1	B	69	TYR	2.4
1	C	15	ASP	2.4
1	A	1056	ILE	2.4
1	A	41	ARG	2.4
1	B	1193	ASN	2.4
1	A	823	SER	2.4
1	C	764	LYS	2.4
1	B	991	LEU	2.4
1	A	963	LEU	2.4
1	B	927	GLN	2.3
1	A	1042	LEU	2.3
1	B	80	ASP	2.3
1	B	125	LYS	2.3
1	C	1186	GLN	2.3
1	A	822	GLN	2.3
1	D	172	ARG	2.3
1	A	799	VAL	2.3
1	A	1017	ASP	2.3
1	C	1210	CYS	2.3
1	A	117	ARG	2.3
1	D	297	GLN	2.3
1	D	298	GLN	2.3
1	D	1280	LEU	2.3
1	A	113	VAL	2.3
1	A	1	MET	2.3
1	B	926	VAL	2.3
1	C	131	PRO	2.3
1	C	169	TRP	2.3
1	D	1015	GLN	2.3
1	A	300	ASP	2.3
1	D	142	GLU	2.3
1	B	1014	SER	2.3
1	A	3	LEU	2.3
1	B	1186	GLN	2.3
1	A	698	TYR	2.3
1	D	184	VAL	2.3
1	B	1221	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	991	LEU	2.3
1	C	967	SER	2.3
1	A	1159	CYS	2.3
1	A	977	GLU	2.3
1	B	1190	GLY	2.3
1	B	915	PHE	2.3
1	B	1188	SER	2.3
1	B	146	CYS	2.2
1	A	1171	TYR	2.2
1	C	113	VAL	2.2
1	D	697	LEU	2.2
1	B	1274	LEU	2.2
1	B	1220	LYS	2.2
1	C	165	CYS	2.2
1	C	297	GLN	2.2
1	C	1183	GLN	2.2
1	D	110	SER	2.2
1	C	48	ARG	2.2
1	B	820	SER	2.2
1	C	141	LYS	2.2
1	A	72	CYS	2.2
1	A	248	GLN	2.2
1	D	170	PRO	2.2
1	D	681	VAL	2.2
1	B	105	LEU	2.2
1	C	859	SER	2.2
1	A	119	ASP	2.2
1	B	1010	CYS	2.2
1	D	108	LEU	2.1
1	B	141	LYS	2.1
1	C	4	LYS	2.1
1	A	452	THR	2.1
1	C	66	TYR	2.1
1	C	958	PHE	2.1
1	A	2	ASP	2.1
1	A	123	ASN	2.1
1	B	999	PHE	2.1
1	C	106	VAL	2.1
1	C	72	CYS	2.1
1	D	302	SER	2.1
1	A	116	VAL	2.1
1	A	1211	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	692	GLU	2.1
1	A	1157	GLY	2.1
1	D	693	GLU	2.1
1	C	116	VAL	2.1
1	A	115	ALA	2.1
1	A	165	CYS	2.1
1	D	1213	PHE	2.1
1	A	148	LYS	2.1
1	A	105	LEU	2.1
1	A	4	LYS	2.0
1	A	694	GLU	2.0
1	A	1279	LYS	2.0
1	B	357	ARG	2.0
1	C	70	SER	2.0
1	B	817	PHE	2.0
1	B	155	GLU	2.0
1	B	1191	ILE	2.0
1	C	102	GLY	2.0
1	D	642	PRO	2.0
1	B	139	THR	2.0
1	B	297	GLN	2.0
1	C	284	GLU	2.0
1	B	839	HIS	2.0
1	B	1183	GLN	2.0
1	C	51	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.