



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:08 PM UTC

PDB ID : 4XR7 / pdb_00004xr7
Title : Structure of the *Saccharomyces cerevisiae* PAN2-PAN3 core complex
Authors : Schafer, I.B.; Rode, M.; Bonneau, F.; Schussler, S.; Conti, E.
Deposited on : 2015-01-20
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

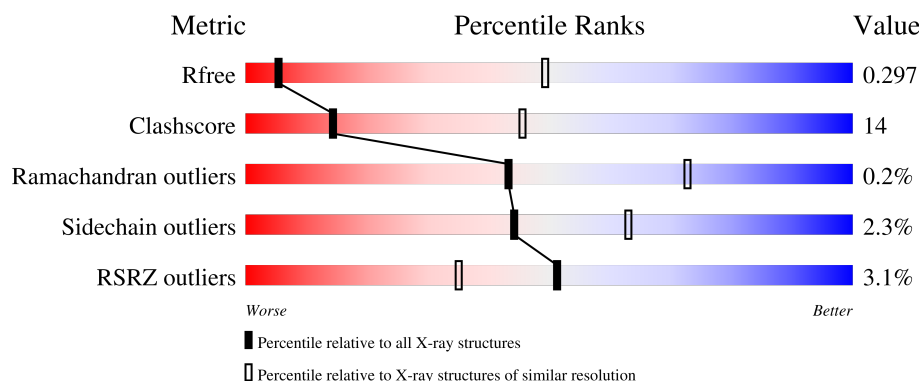
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	776	3% 66% 23% 10%
1	D	776	3% 64% 22% 12%
1	G	776	4% 63% 23% 12%
1	J	776	3% 62% 23% 12%
2	B	465	3% 59% 31% 8%

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Mol	Chain	Length	Quality of chain
2	C	465	2% 62% 32% • 5%
2	E	465	4% 60% 27% • 11%
2	F	465	2% 60% 33% • 5%
2	H	465	2% 59% 30% • 10%
2	I	465	3% 58% 34% • 6%
2	K	465	2% 65% 26% • 7%
2	L	465	% 57% 37% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46467 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 PAB-dependent poly(A)-specific ribonuclease subunit PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	683	Total	C	N	O	S	0	0	0
			4981	3160	829	972	20			
1	D	683	Total	C	N	O	S	0	0	0
			4973	3153	834	966	20			
1	J	681	Total	C	N	O	S	0	0	0
			4958	3162	810	967	19			
1	A	701	Total	C	N	O	S	0	0	0
			5217	3323	860	1012	22			

- Molecule 2 is a protein called PAB-dependent poly(A)-specific ribonuclease subunit PAN3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	441	Total	C	N	O	S	0	0	0
			3479	2243	576	646	14			
2	K	431	Total	C	N	O	S	0	0	0
			3272	2087	547	624	14			
2	E	414	Total	C	N	O	S	0	0	0
			3084	1985	509	576	14			
2	F	442	Total	C	N	O	S	0	0	0
			3381	2186	553	628	14			
2	H	420	Total	C	N	O	S	0	0	0
			3153	2020	523	596	14			
2	I	437	Total	C	N	O	S	0	0	0
			3292	2109	541	628	14			
2	C	444	Total	C	N	O	S	0	0	0
			3405	2188	561	642	14			
2	B	429	Total	C	N	O	S	0	0	0
			3272	2093	545	620	14			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	225	MET	-	initiating methionine	UNP P36102

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Chain	Residue	Modelled	Actual	Comment	Reference
L	680	HIS	-	expression tag	UNP P36102
L	681	HIS	-	expression tag	UNP P36102
L	682	HIS	-	expression tag	UNP P36102
L	683	HIS	-	expression tag	UNP P36102
L	684	HIS	-	expression tag	UNP P36102
L	685	HIS	-	expression tag	UNP P36102
L	686	HIS	-	expression tag	UNP P36102
L	687	HIS	-	expression tag	UNP P36102
L	688	HIS	-	expression tag	UNP P36102
L	689	HIS	-	expression tag	UNP P36102
K	219	MET	-	initiating methionine	UNP P36102
K	680	HIS	-	expression tag	UNP P36102
K	681	HIS	-	expression tag	UNP P36102
K	682	HIS	-	expression tag	UNP P36102
K	683	HIS	-	expression tag	UNP P36102
K	684	HIS	-	expression tag	UNP P36102
K	685	HIS	-	expression tag	UNP P36102
K	686	HIS	-	expression tag	UNP P36102
K	687	HIS	-	expression tag	UNP P36102
K	688	HIS	-	expression tag	UNP P36102
K	689	HIS	-	expression tag	UNP P36102
E	225	MET	-	initiating methionine	UNP P36102
E	680	HIS	-	expression tag	UNP P36102
E	681	HIS	-	expression tag	UNP P36102
E	682	HIS	-	expression tag	UNP P36102
E	683	HIS	-	expression tag	UNP P36102
E	684	HIS	-	expression tag	UNP P36102
E	685	HIS	-	expression tag	UNP P36102
E	686	HIS	-	expression tag	UNP P36102
E	687	HIS	-	expression tag	UNP P36102
E	688	HIS	-	expression tag	UNP P36102
E	689	HIS	-	expression tag	UNP P36102
F	225	MET	-	initiating methionine	UNP P36102
F	680	HIS	-	expression tag	UNP P36102
F	681	HIS	-	expression tag	UNP P36102
F	682	HIS	-	expression tag	UNP P36102
F	683	HIS	-	expression tag	UNP P36102
F	684	HIS	-	expression tag	UNP P36102
F	685	HIS	-	expression tag	UNP P36102
F	686	HIS	-	expression tag	UNP P36102
F	687	HIS	-	expression tag	UNP P36102
F	688	HIS	-	expression tag	UNP P36102

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Chain	Residue	Modelled	Actual	Comment	Reference
F	689	HIS	-	expression tag	UNP P36102
H	225	MET	-	initiating methionine	UNP P36102
H	680	HIS	-	expression tag	UNP P36102
H	681	HIS	-	expression tag	UNP P36102
H	682	HIS	-	expression tag	UNP P36102
H	683	HIS	-	expression tag	UNP P36102
H	684	HIS	-	expression tag	UNP P36102
H	685	HIS	-	expression tag	UNP P36102
H	686	HIS	-	expression tag	UNP P36102
H	687	HIS	-	expression tag	UNP P36102
H	688	HIS	-	expression tag	UNP P36102
H	689	HIS	-	expression tag	UNP P36102
I	225	MET	-	initiating methionine	UNP P36102
I	680	HIS	-	expression tag	UNP P36102
I	681	HIS	-	expression tag	UNP P36102
I	682	HIS	-	expression tag	UNP P36102
I	683	HIS	-	expression tag	UNP P36102
I	684	HIS	-	expression tag	UNP P36102
I	685	HIS	-	expression tag	UNP P36102
I	686	HIS	-	expression tag	UNP P36102
I	687	HIS	-	expression tag	UNP P36102
I	688	HIS	-	expression tag	UNP P36102
I	689	HIS	-	expression tag	UNP P36102
C	225	MET	-	initiating methionine	UNP P36102
C	680	HIS	-	expression tag	UNP P36102
C	681	HIS	-	expression tag	UNP P36102
C	682	HIS	-	expression tag	UNP P36102
C	683	HIS	-	expression tag	UNP P36102
C	684	HIS	-	expression tag	UNP P36102
C	685	HIS	-	expression tag	UNP P36102
C	686	HIS	-	expression tag	UNP P36102
C	687	HIS	-	expression tag	UNP P36102
C	688	HIS	-	expression tag	UNP P36102
C	689	HIS	-	expression tag	UNP P36102
B	225	MET	-	initiating methionine	UNP P36102
B	680	HIS	-	expression tag	UNP P36102
B	681	HIS	-	expression tag	UNP P36102
B	682	HIS	-	expression tag	UNP P36102
B	683	HIS	-	expression tag	UNP P36102
B	684	HIS	-	expression tag	UNP P36102
B	685	HIS	-	expression tag	UNP P36102
B	686	HIS	-	expression tag	UNP P36102

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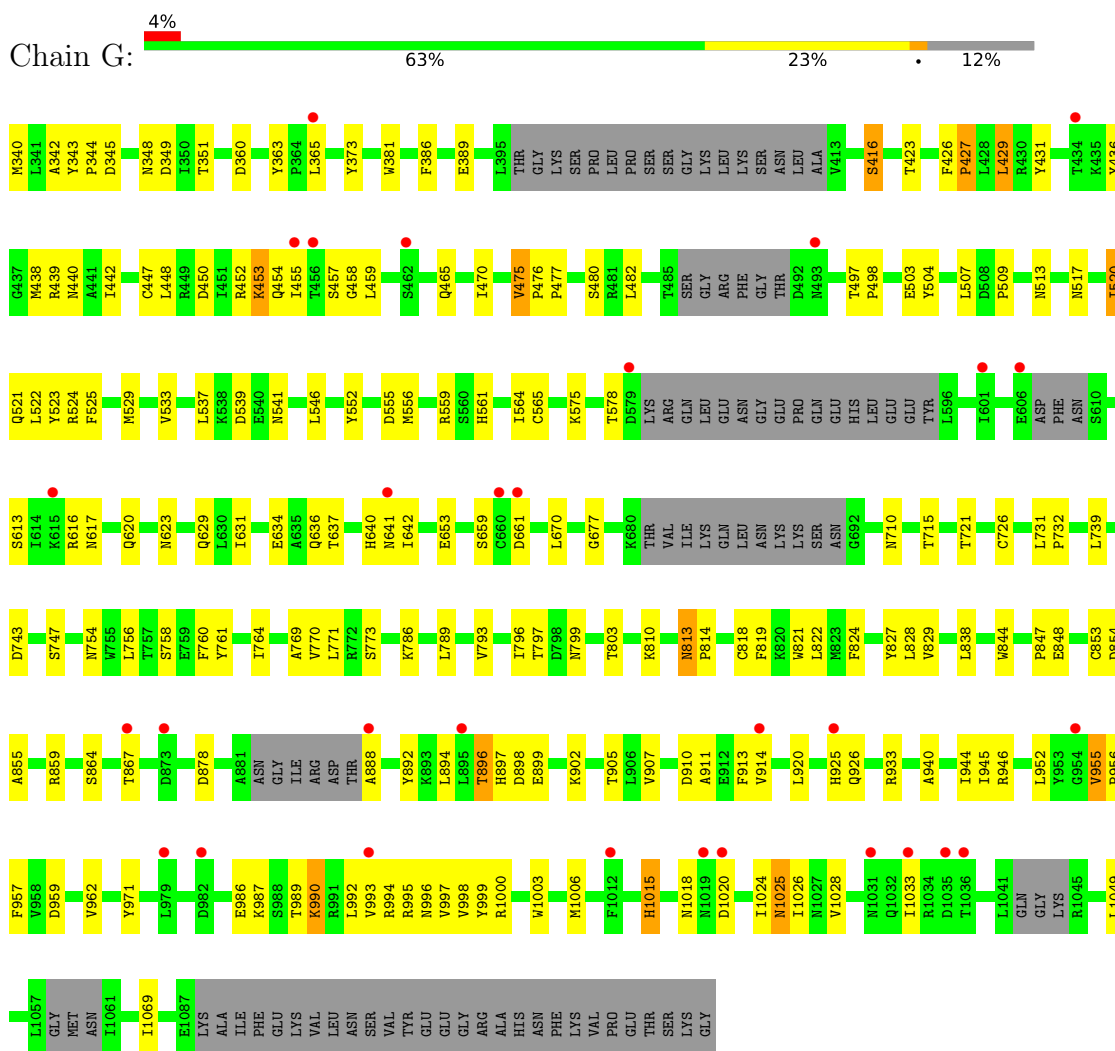
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Chain	Residue	Modelled	Actual	Comment	Reference
B	687	HIS	-	expression tag	UNP P36102
B	688	HIS	-	expression tag	UNP P36102
B	689	HIS	-	expression tag	UNP P36102

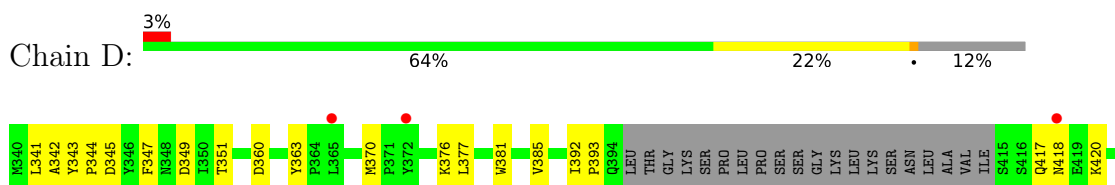
3 Residue-property plots

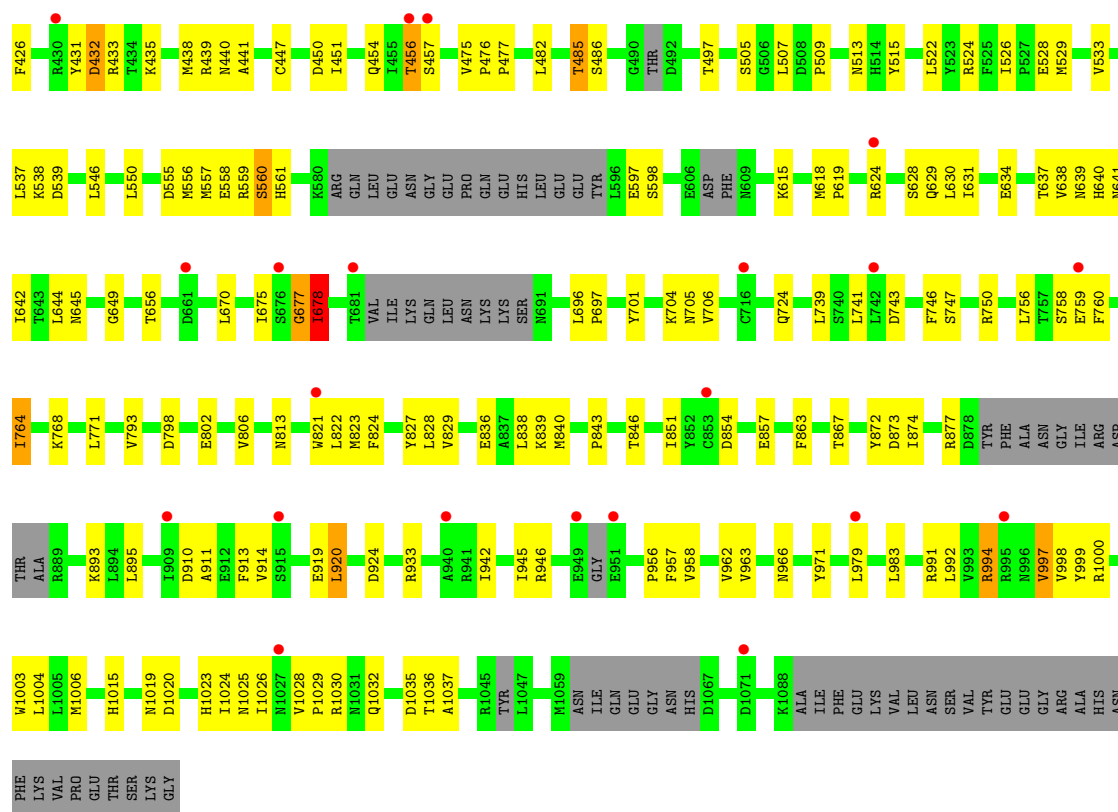
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2

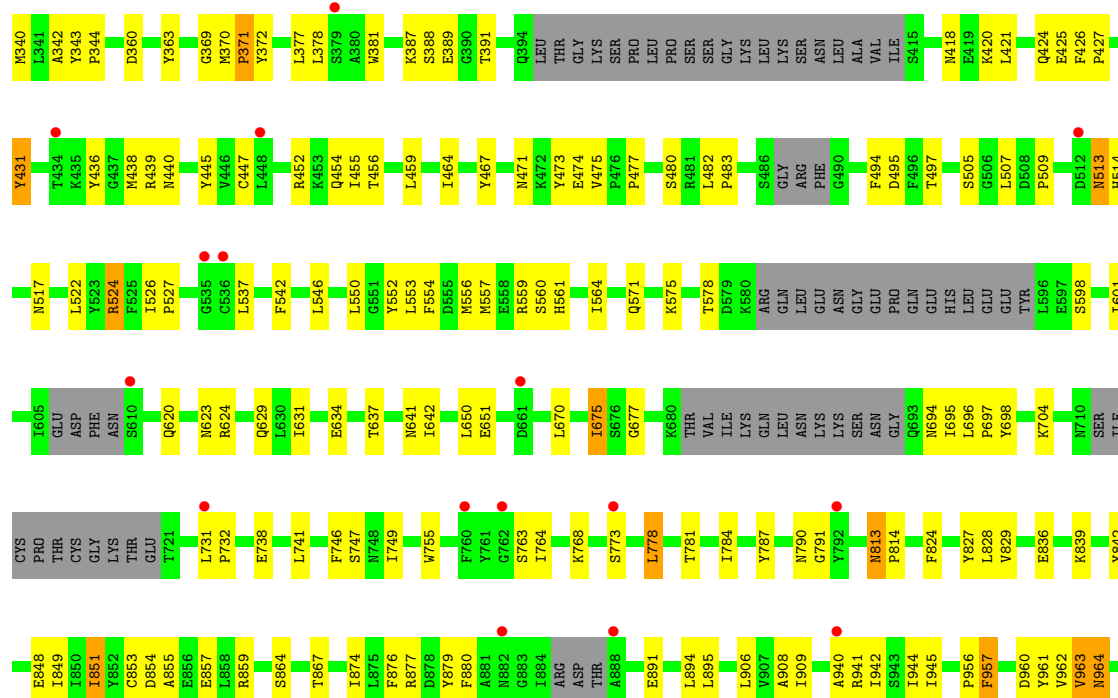


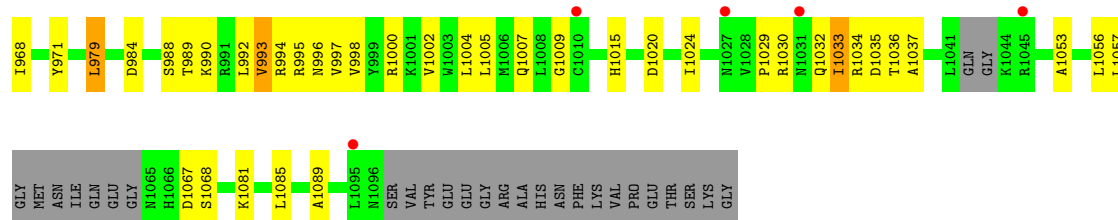
- Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2



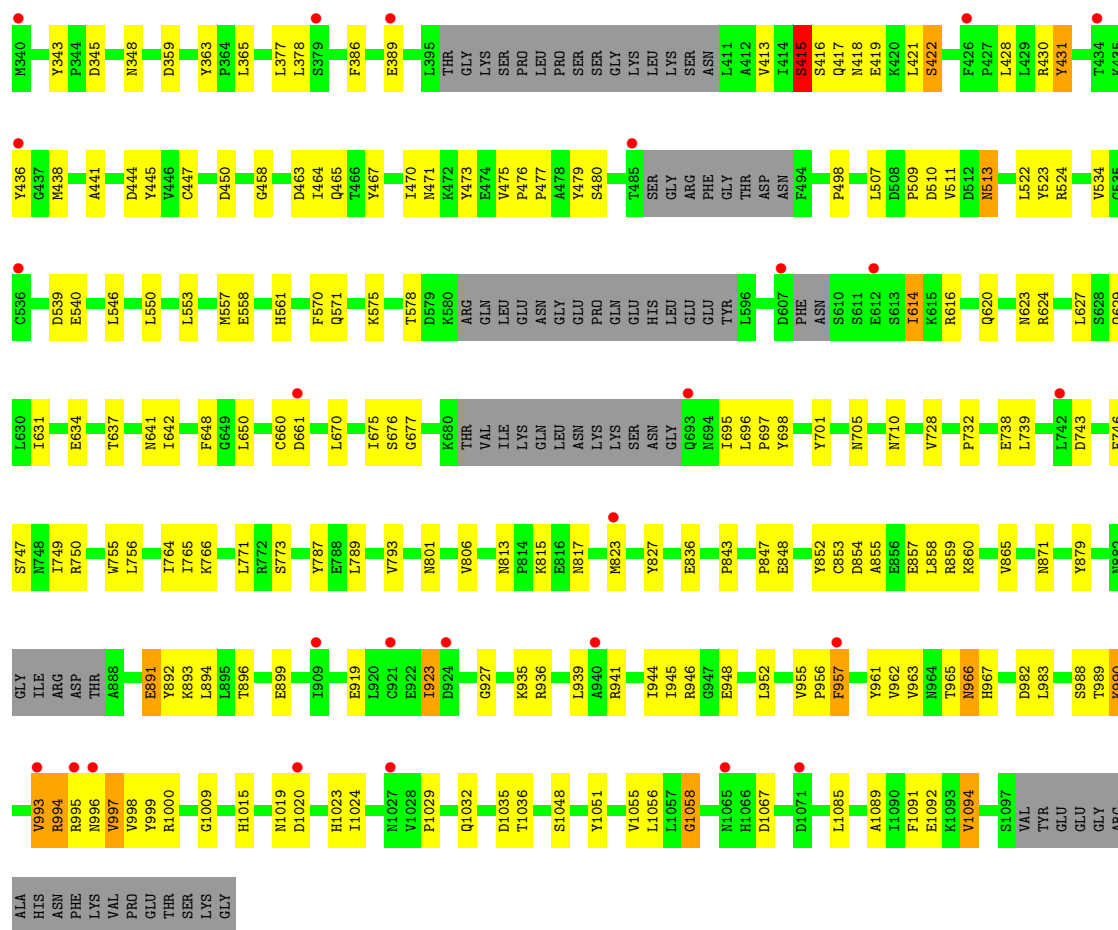


• Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2

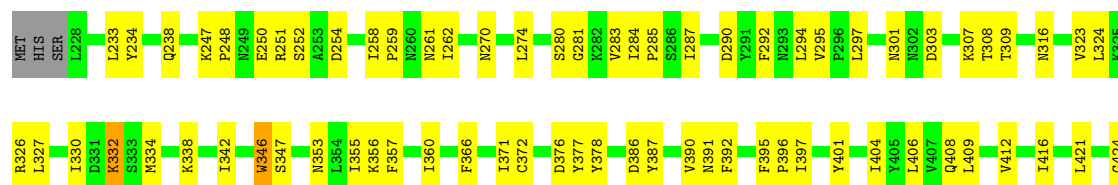


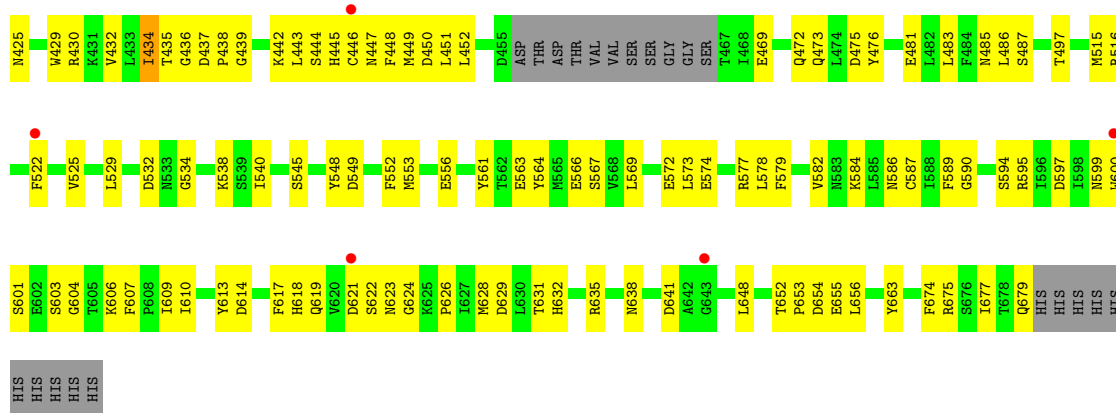


• Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2

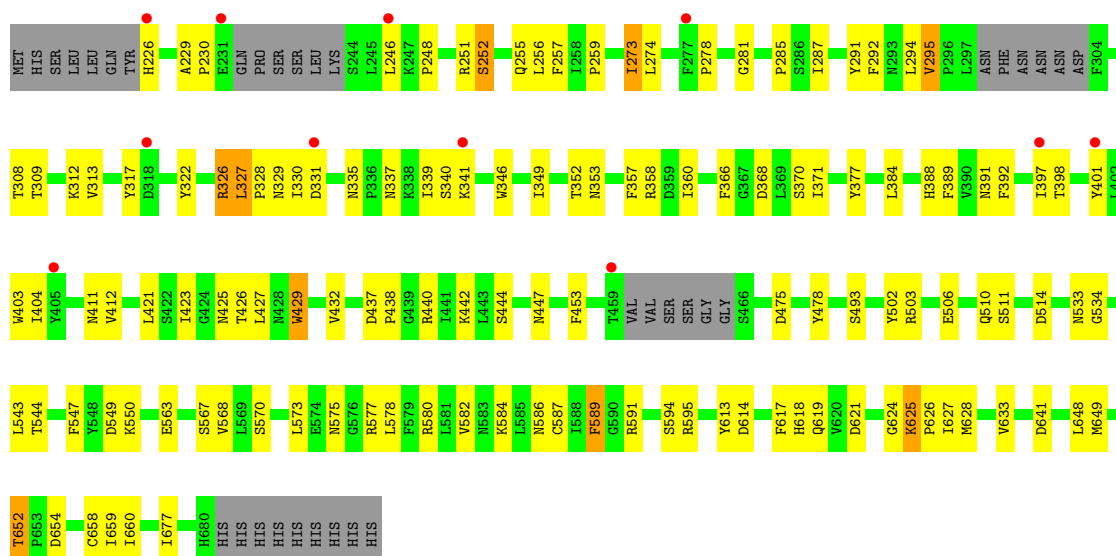


• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

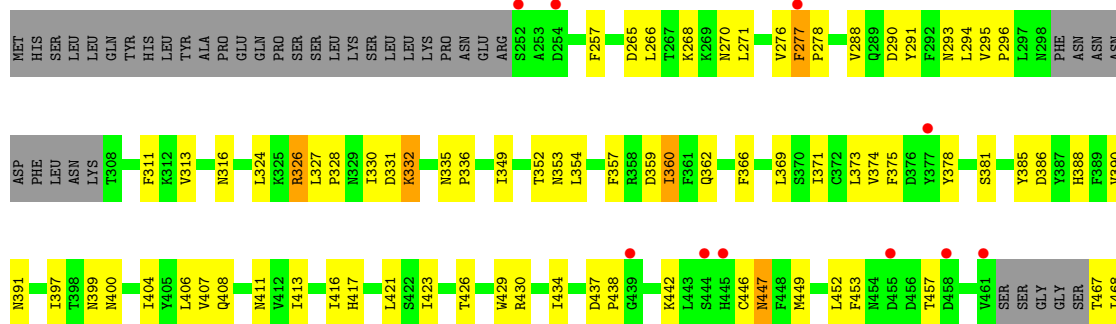


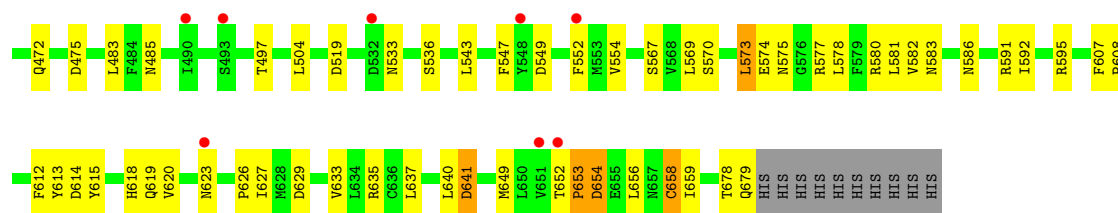


● Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

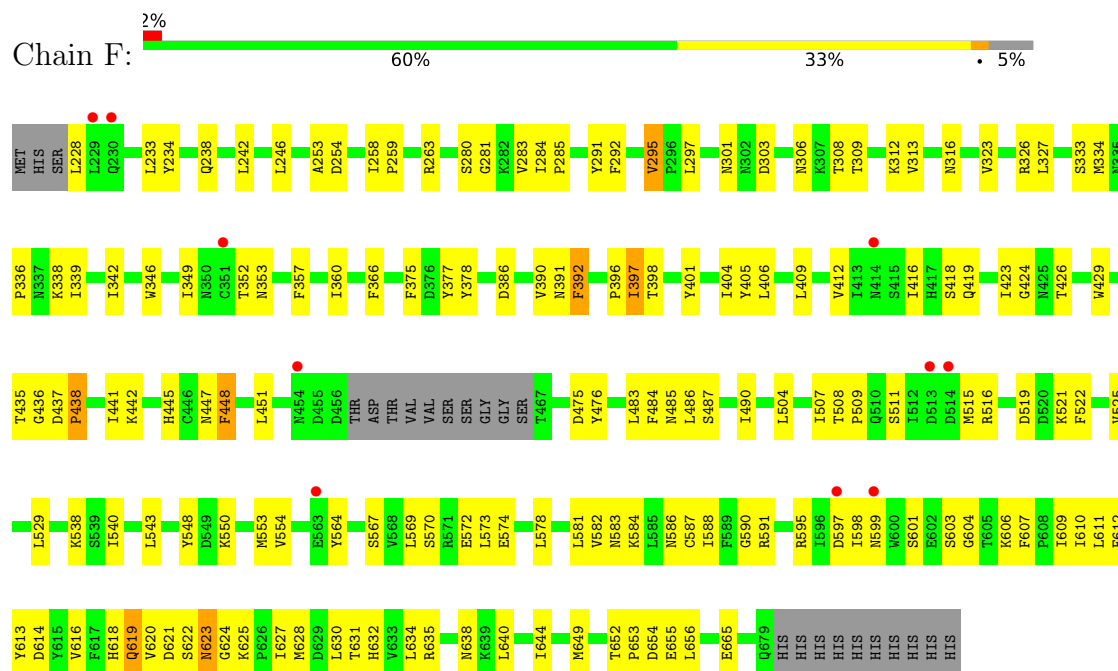


● Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

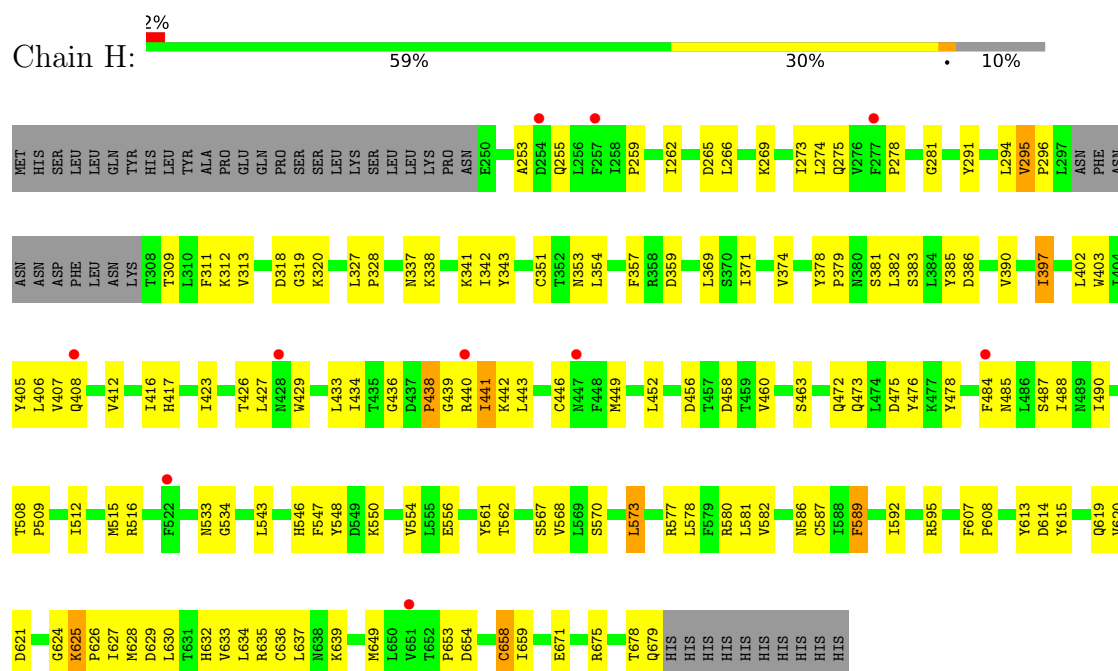




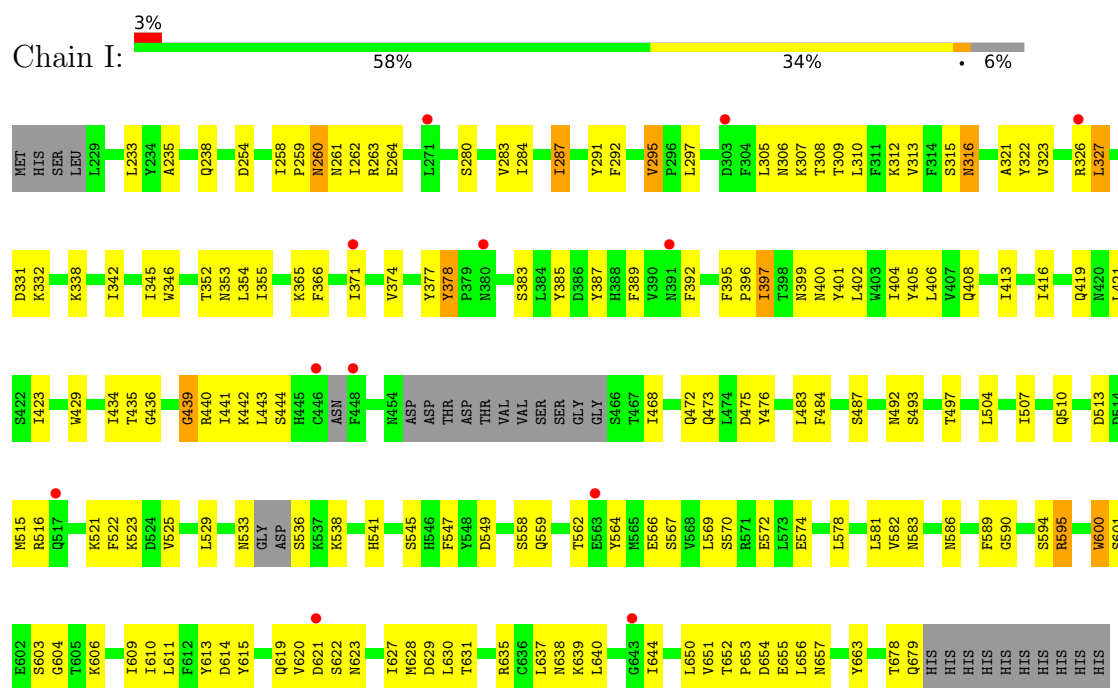
• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



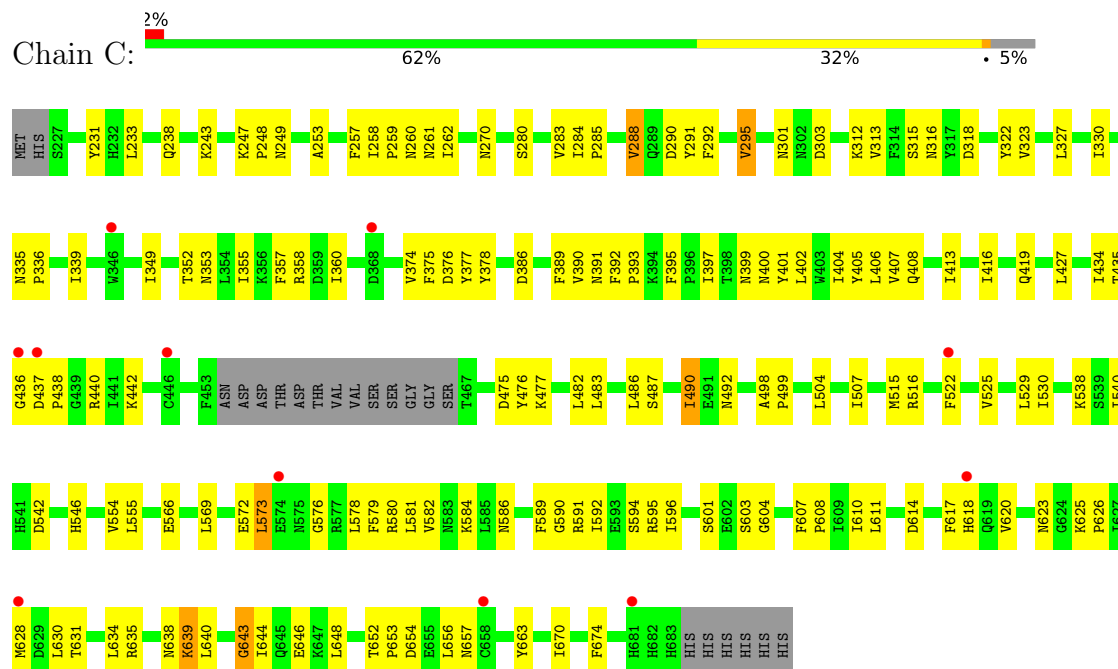
• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



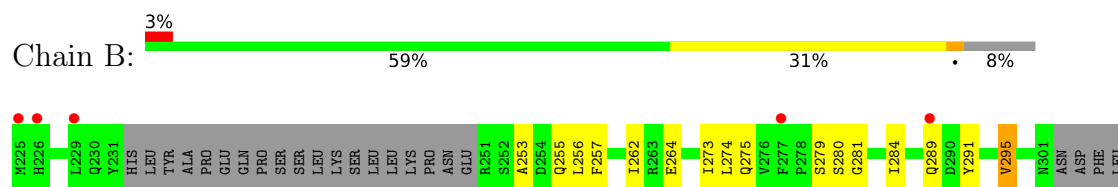
• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



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HIS	ASN	K500	T426	E501	T308	T309	L310	F311	K312	V313	D318	Y322	V323	L324	K325	R326	L327	F328	N329	I330	D331	K332	S333	M334	N335	F361	Q362	T363	T364	D368	L369	S370	I371	V374	Y378	S381	Y385	F389	F392	P393	Y401	L402	W403	I404	Y405	L406	V407	T410	I423
		E501	L504	I507	T508	F509	Q510	S511	I518	D519	D520	K521	F522	V525	L526	K527	Y528	L529	I530	K537	T544	F547	Y548	D549	F552	M553	Y554	L555	E556	Q559	S567	Y568	L569	S570	R571	E572	L573	E574	M575	M576	R577	L578	F579	Y582	M583	K584	L585	M586	C587
HIS		I588	R591	I592	R595	N599	W600	S601	E602	K606	F607	F608	I609	L610	L611	Y615	V616	F617	H618	Q619	D629	H632	V633	C636	L637	N638	K639	L640	D641	I644	T652	P653	D654	M657	C658	Y663	K667	T670	H680	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.44Å 205.30Å 234.41Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	48.83 – 3.80 48.83 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.83-3.80) 99.3 (48.83-3.80)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.285 , 0.299 0.284 , 0.297	Depositor DCC
R_{free} test set	6114 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	133.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 93.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	46467	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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	0.39	0/5327	0.94	19/7277 (0.3%)
1	D	0.37	0/5074	0.93	21/6935 (0.3%)
1	G	0.38	0/5080	0.98	31/6945 (0.4%)
1	J	0.39	0/5062	0.94	19/6924 (0.3%)
2	B	0.42	0/3341	1.06	21/4547 (0.5%)
2	C	0.38	0/3483	0.97	14/4752 (0.3%)
2	E	0.42	0/3150	0.98	16/4298 (0.4%)
2	F	0.39	0/3459	0.94	10/4723 (0.2%)
2	H	0.41	0/3221	1.02	17/4392 (0.4%)
2	I	0.39	0/3365	1.01	14/4595 (0.3%)
2	K	0.40	0/3341	1.07	23/4550 (0.5%)
2	L	0.39	0/3558	0.96	10/4837 (0.2%)
All	All	0.39	0/47461	0.98	215/64775 (0.3%)

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	4
1	D	0	2
1	G	0	1
1	J	0	2
2	C	0	1
2	F	0	1
2	H	0	1
2	L	0	1
All	All	0	13

There are no bond length outliers.

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	963	VAL	N-CA-C	14.41	123.97	110.42
1	D	997	VAL	N-CA-C	11.66	121.38	110.42
2	L	534	GLY	N-CA-C	-11.43	97.40	112.14
2	I	392	PHE	CA-C-N	-11.19	108.15	119.90
2	I	392	PHE	C-N-CA	-11.19	108.15	119.90
1	A	997	VAL	N-CA-C	11.15	120.89	110.74
2	H	589	PHE	N-CA-C	10.73	122.67	110.97
1	G	454	GLN	N-CA-C	10.21	122.41	111.28
2	B	335	ASN	CA-C-N	9.16	130.09	119.47
2	B	335	ASN	C-N-CA	9.16	130.09	119.47
2	E	326	ARG	N-CA-C	8.96	122.33	111.40
2	I	327	LEU	CA-C-N	8.75	129.18	120.52
2	I	327	LEU	C-N-CA	8.75	129.18	120.52
1	A	422	SER	N-CA-C	8.64	120.78	111.36
2	K	589	PHE	N-CA-C	8.58	120.56	111.03
2	E	654	ASP	N-CA-C	-8.52	96.22	109.25
2	C	335	ASN	N-CA-C	8.48	120.00	109.57
2	L	378	TYR	CA-C-N	8.47	128.50	119.78
2	L	378	TYR	C-N-CA	8.47	128.50	119.78
2	K	327	LEU	CA-C-N	8.43	128.04	118.85
2	K	327	LEU	C-N-CA	8.43	128.04	118.85
2	H	654	ASP	N-CA-C	-8.42	96.36	109.25
2	K	575	ASN	N-CA-C	8.31	120.34	111.28
1	G	561	HIS	N-CA-C	-8.16	93.63	107.99
2	C	327	LEU	CA-C-N	8.08	128.52	120.52
2	C	327	LEU	C-N-CA	8.08	128.52	120.52
1	D	432	ASP	N-CA-C	8.05	124.57	111.37
2	B	281	GLY	N-CA-C	-7.86	101.37	112.60
2	K	326	ARG	N-CA-C	7.80	121.29	111.69
2	F	392	PHE	CA-C-N	-7.78	111.89	120.14
2	F	392	PHE	C-N-CA	-7.78	111.89	120.14
2	I	378	TYR	CA-C-N	7.61	127.62	119.78
2	I	378	TYR	C-N-CA	7.61	127.62	119.78
2	K	309	THR	N-CA-C	7.56	119.60	111.36
2	C	395	PHE	CA-C-N	7.52	127.69	119.87
2	C	395	PHE	C-N-CA	7.52	127.69	119.87
2	K	335	ASN	CA-C-N	7.49	128.15	119.47
2	K	335	ASN	C-N-CA	7.49	128.15	119.47
1	J	426	PHE	N-CA-C	7.45	122.33	112.35
2	B	652	THR	CA-C-N	7.33	144.60	127.00
2	B	652	THR	C-N-CA	7.33	144.60	127.00
2	E	575	ASN	N-CA-C	7.23	120.08	111.33
1	G	898	ASP	N-CA-C	7.21	118.92	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	326	ARG	N-CA-C	7.19	120.17	111.40
1	A	616	ARG	N-CA-C	-7.14	101.08	110.43
2	K	652	THR	CA-C-N	7.12	144.08	127.00
2	K	652	THR	C-N-CA	7.12	144.08	127.00
2	B	652	THR	C-N-CD	-7.10	104.98	120.60
1	A	616	ARG	CA-C-N	-7.09	111.00	122.34
1	A	616	ARG	C-N-CA	-7.09	111.00	122.34
2	B	573	LEU	N-CA-C	7.08	120.82	111.75
2	K	328	PRO	N-CA-C	7.03	122.82	113.40
1	G	564	ILE	N-CA-C	6.99	118.11	110.21
2	H	436	GLY	N-CA-C	-6.99	104.02	112.48
1	G	426	PHE	N-CA-C	6.96	121.68	112.35
2	K	652	THR	C-N-CD	-6.95	105.30	120.60
1	G	455	ILE	N-CA-C	6.94	118.59	108.53
1	G	429	LEU	N-CA-C	6.92	121.89	113.17
1	G	677	GLY	N-CA-C	6.91	120.65	110.63
2	K	230	PRO	N-CA-CB	6.90	110.50	103.25
2	B	498	ALA	CA-C-N	6.89	127.06	120.31
2	B	498	ALA	C-N-CA	6.89	127.06	120.31
1	D	813	ASN	CA-C-N	6.89	126.69	119.05
1	D	813	ASN	C-N-CA	6.89	126.69	119.05
1	A	965	THR	N-CA-C	6.86	119.77	111.82
2	B	453	PHE	N-CA-C	6.66	118.20	111.07
2	C	643	GLY	N-CA-C	-6.60	104.50	112.48
2	B	329	ASN	N-CA-C	6.56	120.42	111.17
1	D	966	ASN	CB-CA-C	-6.49	109.07	116.54
2	L	532	ASP	N-CA-C	6.49	119.82	109.24
2	E	573	LEU	N-CA-C	6.47	119.16	111.33
2	H	253	ALA	CA-C-N	-6.33	112.21	122.34
2	H	253	ALA	C-N-CA	-6.33	112.21	122.34
1	G	613	SER	N-CA-C	6.32	118.98	111.33
1	D	497	THR	CA-C-N	-6.29	113.21	119.56
1	D	497	THR	C-N-CA	-6.29	113.21	119.56
1	G	952	LEU	CB-CA-C	-6.26	108.71	117.23
2	K	624	GLY	N-CA-C	6.25	124.30	115.30
1	A	966	ASN	N-CA-C	6.24	118.63	111.02
2	H	255	GLN	N-CA-C	-6.24	104.83	112.88
2	C	596	ILE	N-CA-C	6.23	118.15	112.29
2	B	575	ASN	N-CA-C	6.22	118.86	111.33
1	A	431	TYR	N-CA-C	6.21	120.15	108.65
1	G	431	TYR	N-CA-C	6.21	116.81	108.23
1	J	813	ASN	CA-C-N	6.17	125.39	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	813	ASN	C-N-CA	6.17	125.39	118.97
1	G	1018	ASN	N-CA-C	6.16	117.66	111.07
1	A	415	SER	N-CA-C	6.13	117.95	110.41
2	K	308	THR	N-CA-C	6.09	123.77	110.80
2	B	445	HIS	N-CA-C	6.08	117.58	111.07
2	B	588	ILE	N-CA-C	6.01	116.80	110.72
1	G	1033	ILE	N-CA-C	6.00	118.54	111.05
1	A	813	ASN	CA-C-N	6.00	125.20	118.97
1	A	813	ASN	C-N-CA	6.00	125.20	118.97
1	G	458	GLY	N-CA-C	-5.99	107.42	115.21
2	H	508	THR	CA-C-N	5.94	125.64	119.05
2	H	508	THR	C-N-CA	5.94	125.64	119.05
1	G	427	PRO	N-CA-C	5.92	120.38	111.14
2	F	378	TYR	CA-C-N	5.90	125.86	119.78
2	F	378	TYR	C-N-CA	5.90	125.86	119.78
2	B	652	THR	N-CA-C	5.88	121.69	113.57
1	G	986	GLU	N-CA-C	5.86	119.40	112.72
2	K	252	SER	N-CA-C	5.84	118.57	109.52
2	H	281	GLY	N-CA-C	5.84	118.64	111.93
2	K	281	GLY	N-CA-C	-5.83	101.48	112.10
2	I	600	TRP	N-CA-C	5.83	120.02	113.02
2	K	453	PHE	N-CA-C	5.83	119.49	112.38
1	D	426	PHE	N-CA-C	5.83	122.69	109.81
1	D	456	THR	CB-CA-C	-5.80	109.86	116.54
1	G	416	SER	CB-CA-C	-5.79	109.91	116.63
2	I	235	ALA	CA-C-N	5.79	125.98	119.90
2	I	235	ALA	C-N-CA	5.79	125.98	119.90
2	F	424	GLY	N-CA-C	5.74	122.94	112.37
2	F	625	LYS	CA-C-N	-5.74	114.02	119.76
2	F	625	LYS	C-N-CA	-5.74	114.02	119.76
2	E	574	GLU	N-CA-C	5.74	117.53	111.28
2	H	653	PRO	CA-C-N	-5.74	113.40	121.72
2	H	653	PRO	C-N-CA	-5.74	113.40	121.72
2	K	652	THR	N-CA-C	5.73	122.47	109.81
2	B	572	GLU	N-CA-C	5.70	119.95	112.89
1	G	459	LEU	N-CA-C	-5.69	104.86	113.51
2	H	439	GLY	N-CA-C	5.68	126.64	113.18
1	D	560	SER	N-CA-C	-5.66	99.30	108.41
2	K	549	ASP	N-CA-C	5.63	117.42	111.28
1	G	813	ASN	CA-C-N	5.63	124.83	118.97
1	G	813	ASN	C-N-CA	5.63	124.83	118.97
2	L	573	LEU	N-CA-C	-5.63	105.15	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	573	LEU	N-CA-C	-5.62	105.15	111.28
1	J	963	VAL	CB-CA-C	-5.62	104.62	111.87
1	A	891	GLU	CB-CA-C	-5.62	110.11	116.63
1	G	381	TRP	CA-C-N	5.60	123.75	119.66
1	G	381	TRP	C-N-CA	5.60	123.75	119.66
1	J	677	GLY	N-CA-C	5.57	118.88	110.18
2	B	275	GLN	N-CA-C	5.56	118.30	109.96
2	H	625	LYS	N-CA-C	5.55	114.52	108.14
2	K	625	LYS	CA-C-N	5.54	126.02	120.14
2	K	625	LYS	C-N-CA	5.54	126.02	120.14
1	J	438	MET	N-CA-C	5.54	119.08	111.54
2	I	439	GLY	CA-C-N	-5.52	113.77	121.99
2	I	439	GLY	C-N-CA	-5.52	113.77	121.99
2	F	623	ASN	N-CA-C	-5.51	104.13	111.02
2	B	549	ASP	N-CA-C	5.48	117.26	111.28
2	E	653	PRO	CA-C-N	-5.48	113.77	121.72
2	E	653	PRO	C-N-CA	-5.48	113.77	121.72
2	L	233	LEU	N-CA-C	-5.48	106.55	113.18
1	J	436	TYR	CB-CA-C	-5.48	110.24	116.54
1	D	385	VAL	N-CA-C	5.47	116.25	110.72
2	H	573	LEU	N-CA-C	5.47	117.94	111.33
1	J	1033	ILE	N-CA-C	5.45	115.65	110.53
2	E	497	THR	N-CA-C	5.44	117.12	108.79
2	C	378	TYR	CA-C-N	5.44	125.39	119.78
2	C	378	TYR	C-N-CA	5.44	125.39	119.78
1	A	1058	GLY	N-CA-C	5.44	123.02	112.04
2	H	328	PRO	N-CA-C	5.43	120.69	113.57
1	G	453	LYS	N-CA-C	5.42	118.36	111.69
2	E	623	ASN	N-CA-C	5.41	117.24	110.91
2	I	595	ARG	N-CA-C	5.40	119.58	113.15
2	B	262	ILE	N-CA-C	5.40	115.61	110.53
1	J	459	LEU	N-CA-C	-5.40	101.92	109.96
2	F	281	GLY	N-CA-C	-5.39	107.25	114.25
1	G	436	TYR	CB-CA-C	-5.38	109.91	117.23
1	A	999	TYR	N-CA-C	-5.38	105.41	111.28
2	L	332	LYS	N-CA-C	5.38	118.31	111.69
1	D	615	LYS	CB-CA-C	-5.37	109.93	117.23
1	J	964	ASN	N-CA-C	5.37	118.49	109.95
2	E	447	ASN	N-CA-C	5.36	118.52	111.28
1	A	661	ASP	N-CA-C	-5.34	100.60	109.46
1	G	993	VAL	N-CA-C	-5.33	102.17	109.37
2	E	457	THR	N-CA-C	5.32	117.16	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	573	LEU	N-CA-C	-5.30	105.50	111.28
1	D	638	VAL	N-CA-C	5.30	115.51	110.42
1	J	984	ASP	N-CA-C	5.30	120.82	113.45
2	H	319	GLY	N-CA-C	-5.30	108.31	115.36
1	D	381	TRP	CA-C-N	5.29	125.83	120.38
1	D	381	TRP	C-N-CA	5.29	125.83	120.38
1	J	427	PRO	N-CA-C	5.28	119.38	111.14
2	C	625	LYS	CA-C-N	-5.28	114.52	119.85
2	C	625	LYS	C-N-CA	-5.28	114.52	119.85
1	G	457	SER	N-CA-C	-5.28	106.52	113.17
1	A	614	ILE	N-CA-C	5.27	115.57	107.77
1	D	670	LEU	CA-C-N	5.25	124.57	118.85
1	D	670	LEU	C-N-CA	5.25	124.57	118.85
2	E	453	PHE	N-CA-C	5.22	119.65	113.28
2	E	332	LYS	N-CA-C	5.21	117.10	108.20
1	D	979	LEU	CA-C-N	5.20	139.48	127.00
1	D	979	LEU	C-N-CA	5.20	139.48	127.00
1	G	987	LYS	N-CA-C	5.19	117.22	108.96
1	J	731	LEU	CA-C-N	5.19	125.19	120.21
1	J	731	LEU	C-N-CA	5.19	125.19	120.21
1	G	670	LEU	CA-C-N	5.18	124.50	118.85
1	G	670	LEU	C-N-CA	5.18	124.50	118.85
1	A	436	TYR	CB-CA-C	-5.17	110.19	117.23
2	K	329	ASN	N-CA-C	5.17	117.07	108.02
2	E	277	PHE	CA-C-N	-5.17	114.59	119.76
2	E	277	PHE	C-N-CA	-5.17	114.59	119.76
1	A	413	VAL	N-CA-C	5.16	115.07	107.75
2	E	658	CYS	N-CA-C	5.15	117.01	109.24
2	C	260	ASN	N-CA-C	5.13	116.68	111.14
2	B	333	SER	N-CA-C	-5.12	102.62	110.30
1	G	955	VAL	CA-C-N	5.12	124.88	119.76
1	G	955	VAL	C-N-CA	5.12	124.88	119.76
2	I	316	ASN	N-CA-C	-5.12	105.16	111.40
2	L	534	GLY	CA-C-N	-5.10	113.34	122.32
2	L	534	GLY	C-N-CA	-5.10	113.34	122.32
2	I	260	ASN	N-CA-C	5.10	116.52	111.07
1	J	979	LEU	CA-C-N	5.09	139.22	127.00
1	J	979	LEU	C-N-CA	5.09	139.22	127.00
2	C	490	ILE	N-CA-C	5.08	115.69	110.36
1	D	768	LYS	N-CA-C	5.08	119.47	113.28
1	D	677	GLY	N-CA-C	5.07	118.93	112.13
1	J	431	TYR	N-CA-C	5.04	117.74	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	281	GLY	N-CA-C	-5.04	107.57	114.67
1	J	464	ILE	N-CA-C	-5.02	106.24	113.07
1	A	463	ASP	N-CA-C	5.02	119.28	113.20
2	H	262	ILE	N-CA-C	5.01	115.24	110.53

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1058	GLY	Peptide
1	A	422	SER	Peptide
1	A	430	ARG	Peptide
1	A	994	ARG	Peptide
2	C	288	VAL	Peptide
1	D	431	TYR	Peptide
1	D	994	ARG	Peptide
2	F	438	PRO	Peptide
1	G	453	LYS	Peptide
2	H	456	ASP	Peptide
1	J	421	LEU	Peptide
1	J	495	ASP	Peptide
2	L	366	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5217	0	4654	119	0
1	D	4973	0	4313	113	0
1	G	4981	0	4348	121	0
1	J	4958	0	4283	129	0
2	B	3272	0	2970	112	0
2	C	3405	0	3129	122	0
2	E	3084	0	2749	96	0
2	F	3381	0	3120	126	0
2	H	3153	0	2811	98	0
2	I	3292	0	2945	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	3272	0	2943	101	0
2	L	3479	0	3315	132	0
All	All	46467	0	41580	1239	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 14.

All (1239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:353:ASN:HA	2:I:442:LYS:HG2	1.55	0.89
2:K:256:LEU:HD13	2:K:404:ILE:HD11	1.56	0.87
2:H:586:ASN:OD1	2:I:586:ASN:ND2	2.08	0.85
2:K:577:ARG:NH1	1:J:370:MET:SD	2.49	0.85
2:B:256:LEU:HD13	2:B:404:ILE:HD11	1.60	0.83
1:J:1009:GLY:HA2	1:J:1032:GLN:HE22	1.43	0.83
2:I:611:LEU:HD22	2:I:650:LEU:HB3	1.61	0.82
2:C:644:ILE:HG22	2:C:646:GLU:H	1.45	0.82
2:I:594:SER:OG	2:I:600:TRP:O	1.98	0.82
2:L:594:SER:OG	2:L:600:TRP:O	1.95	0.82
2:F:284:ILE:HG12	2:F:285:PRO:HD2	1.61	0.81
1:G:996:ASN:O	1:G:1000:ARG:N	2.13	0.81
1:G:429:LEU:HD12	2:I:657:ASN:HB3	1.60	0.81
2:B:518:ILE:HG22	2:B:520:ASP:H	1.44	0.80
2:E:586:ASN:OD1	2:F:586:ASN:ND2	2.11	0.79
1:J:1029:PRO:HG2	1:J:1032:GLN:HG3	1.62	0.79
1:A:1085:LEU:HD21	1:A:1091:PHE:HB3	1.64	0.78
1:A:945:ILE:HA	1:A:956:PRO:HA	1.65	0.78
2:L:586:ASN:ND2	2:K:586:ASN:OD1	2.16	0.78
2:E:352:THR:O	2:E:442:LYS:NZ	2.17	0.78
1:G:747:SER:OG	2:I:623:ASN:OD1	2.02	0.78
2:H:613:TYR:OH	2:I:586:ASN:ND2	2.16	0.78
2:C:623:ASN:ND2	1:A:747:SER:OG	2.14	0.77
2:B:636:CYS:SG	1:A:348:ASN:ND2	2.58	0.77
2:F:516:ARG:NH2	1:A:773:SER:O	2.18	0.77
1:G:438:MET:HE1	1:G:743:ASP:H	1.50	0.77
2:B:295:VAL:HG22	2:B:312:LYS:HB3	1.67	0.77
2:L:346:TRP:NE1	2:L:446:CYS:SG	2.59	0.76
1:G:389:GLU:OE1	2:I:631:THR:OG1	2.02	0.76
2:L:234:TYR:HA	1:J:377:LEU:HD12	1.68	0.76
2:F:342:ILE:HD12	2:F:451:LEU:HD13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:291:TYR:HB3	2:H:313:VAL:HG21	1.68	0.76
1:J:620:GLN:NE2	1:J:848:GLU:OE1	2.18	0.76
1:G:773:SER:O	2:L:516:ARG:NH2	2.19	0.75
1:A:857:GLU:OE2	1:A:860:LYS:NZ	2.19	0.75
2:F:426:THR:HG23	2:F:447:ASN:HB2	1.68	0.75
1:G:345:ASP:OD2	2:H:615:TYR:OH	2.04	0.75
2:I:516:ARG:NH2	1:J:773:SER:O	2.20	0.75
2:C:566:GLU:OE1	2:B:440:ARG:NH2	2.20	0.75
1:G:1015:HIS:HB3	1:G:1049:LEU:HD22	1.70	0.74
2:F:285:PRO:HG3	2:F:366:PHE:HE1	1.52	0.74
2:C:397:ILE:HD11	2:C:486:LEU:HB3	1.69	0.74
1:G:465:GLN:NE2	1:G:498:PRO:O	2.19	0.74
1:J:962:VAL:HG23	1:J:994:ARG:HB3	1.70	0.74
1:A:919:GLU:HB2	1:A:935:LYS:HG3	1.69	0.74
1:G:959:ASP:OD1	1:G:990:LYS:NZ	2.20	0.73
1:J:996:ASN:O	1:J:1000:ARG:N	2.20	0.73
2:L:386:ASP:HA	2:L:390:VAL:HG22	1.69	0.73
2:E:385:TYR:HB2	2:E:429:TRP:CD1	2.24	0.73
2:H:275:GLN:HG3	2:I:644:ILE:HD13	1.70	0.73
2:L:595:ARG:NH2	2:K:614:ASP:OD2	2.21	0.73
2:C:631:THR:OG1	1:A:389:GLU:OE1	2.06	0.73
2:H:440:ARG:NH2	2:I:566:GLU:OE1	2.20	0.73
2:F:574:GLU:OE2	2:F:638:ASN:ND2	2.22	0.72
2:I:331:ASP:OD1	2:I:332:LYS:N	2.20	0.72
1:A:620:GLN:NE2	1:A:848:GLU:OE1	2.22	0.72
1:D:439:ARG:NH1	1:D:440:ASN:OD1	2.22	0.72
2:E:266:LEU:HD21	2:F:570:SER:HA	1.71	0.72
1:D:597:GLU:OE1	1:D:629:GLN:NE2	2.23	0.71
1:A:941:ARG:NH1	1:A:1067:ASP:OD2	2.23	0.71
2:K:291:TYR:HB3	2:K:313:VAL:HG21	1.72	0.71
2:L:284:ILE:HG12	2:L:285:PRO:HD2	1.70	0.71
2:C:482:LEU:HD22	2:C:483:LEU:HD12	1.71	0.71
1:G:348:ASN:ND2	2:H:636:CYS:SG	2.64	0.71
2:E:614:ASP:OD2	2:F:595:ARG:NH2	2.22	0.71
1:J:763:SER:HB2	1:J:784:ILE:HA	1.72	0.71
2:K:584:LYS:NZ	1:J:378:LEU:O	2.24	0.71
1:J:439:ARG:NH1	1:J:440:ASN:OD1	2.24	0.71
2:H:385:TYR:HB2	2:H:429:TRP:CD1	2.26	0.70
1:J:874:ILE:HG21	1:J:1000:ARG:HG2	1.72	0.70
2:E:331:ASP:OD1	2:E:332:LYS:N	2.24	0.70
2:L:301:ASN:HD22	2:L:308:THR:HA	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:TYR:HB2	2:B:429:TRP:CD1	2.27	0.70
2:C:291:TYR:HB3	2:C:313:VAL:HG21	1.72	0.70
2:L:574:GLU:OE2	2:L:638:ASN:ND2	2.25	0.69
2:L:481:GLU:O	2:L:485:ASN:ND2	2.25	0.69
2:B:485:ASN:HD21	2:B:501:GLU:HA	1.57	0.69
2:E:378:TYR:O	2:E:381:SER:OG	2.11	0.69
2:B:619:GLN:HE21	1:A:343:TYR:HB2	1.57	0.69
1:J:513:ASN:OD1	1:J:571:GLN:NE2	2.26	0.69
2:I:280:SER:HB2	2:I:283:VAL:HG12	1.75	0.69
2:I:287:ILE:HD12	2:I:292:PHE:HB3	1.74	0.69
1:A:1092:GLU:HG3	1:A:1094:VAL:H	1.57	0.68
1:G:994:ARG:O	1:G:997:VAL:N	2.23	0.68
2:K:357:PHE:HZ	2:K:360:ILE:HB	1.56	0.68
1:D:806:VAL:HG21	1:D:823:MET:HE3	1.73	0.68
1:D:914:VAL:HG23	1:D:971:TYR:HA	1.75	0.68
2:I:434:ILE:HD11	2:I:439:GLY:HA2	1.74	0.68
2:L:529:LEU:O	2:L:538:LYS:NZ	2.27	0.68
2:E:295:VAL:O	2:E:311:PHE:HB2	1.94	0.68
1:D:963:VAL:HG23	1:D:983:LEU:HA	1.75	0.68
2:E:426:THR:HG21	2:E:446:CYS:H	1.59	0.68
2:H:615:TYR:O	2:H:619:GLN:NE2	2.27	0.68
1:J:854:ASP:HB3	1:J:857:GLU:HB2	1.74	0.68
2:L:613:TYR:CE2	2:L:618:HIS:HE1	2.12	0.67
2:E:406:LEU:HD13	2:E:483:LEU:HD11	1.76	0.67
2:F:632:HIS:HA	2:F:635:ARG:HE	1.60	0.67
1:D:874:ILE:HG21	1:D:1000:ARG:HG2	1.76	0.67
2:I:389:PHE:HE1	2:I:493:SER:HB2	1.60	0.67
2:L:285:PRO:HG2	2:L:294:LEU:HD21	1.75	0.67
1:D:675:ILE:HD13	1:D:739:LEU:HD23	1.77	0.67
1:D:920:LEU:HD23	1:D:933:ARG:HD3	1.76	0.67
2:B:489:ASN:ND2	2:B:500:LYS:O	2.27	0.67
2:F:613:TYR:HE1	2:F:618:HIS:HE1	1.41	0.67
2:B:652:THR:OG1	2:B:654:ASP:O	2.13	0.67
2:B:667:LYS:HG3	1:A:378:LEU:HD12	1.77	0.67
2:C:601:SER:OG	2:C:603:SER:O	2.13	0.66
2:E:573:LEU:HD22	2:F:263:ARG:HG3	1.77	0.66
1:D:559:ARG:HH22	1:D:1003:TRP:HE1	1.44	0.66
2:F:623:ASN:OD1	1:D:747:SER:OG	2.11	0.66
2:B:291:TYR:HB3	2:B:313:VAL:HG21	1.78	0.66
2:H:658:CYS:SG	2:H:659:ILE:N	2.67	0.66
2:L:425:ASN:OD1	2:L:447:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:291:TYR:HB3	2:E:313:VAL:HG21	1.78	0.66
2:F:285:PRO:HG3	2:F:366:PHE:CE1	2.29	0.66
2:E:678:THR:HG22	2:E:679:GLN:H	1.60	0.66
1:D:750:ARG:NH1	1:D:843:PRO:O	2.29	0.66
1:J:704:LYS:HD3	1:J:768:LYS:HA	1.77	0.65
2:C:504:LEU:HD23	2:C:507:ILE:HD12	1.78	0.65
1:A:990:LYS:HE2	1:A:990:LYS:H	1.62	0.65
2:L:654:ASP:OD1	2:L:656:LEU:N	2.27	0.65
1:G:439:ARG:HH12	2:I:614:ASP:HB3	1.62	0.65
2:F:654:ASP:OD1	2:F:656:LEU:N	2.30	0.65
2:H:440:ARG:HH21	2:H:561:TYR:HE2	1.45	0.65
2:B:449:MET:O	2:B:452:LEU:HG	1.96	0.65
1:G:442:ILE:HD11	2:I:619:GLN:HB3	1.79	0.65
1:A:417:GLN:N	1:A:419:GLU:OE1	2.28	0.65
1:G:507:LEU:HD11	1:G:520:ILE:HD11	1.79	0.65
2:E:278:PRO:HG3	2:E:296:PRO:HD2	1.78	0.65
1:D:743:ASP:HA	1:D:746:PHE:HD2	1.61	0.65
1:J:945:ILE:HA	1:J:956:PRO:HA	1.79	0.65
1:G:429:LEU:HB3	2:I:657:ASN:HD22	1.62	0.65
2:E:658:CYS:SG	2:E:659:ILE:N	2.69	0.65
2:C:249:ASN:ND2	1:A:389:GLU:O	2.27	0.65
2:E:276:VAL:HG23	2:E:293:ASN:OD1	1.97	0.64
2:I:258:ILE:N	2:I:572:GLU:OE2	2.30	0.64
2:C:657:ASN:ND2	1:A:418:ASN:OD1	2.30	0.64
1:D:597:GLU:OE2	1:D:628:SER:OG	2.12	0.64
2:E:533:ASN:HB3	2:E:536:SER:HA	1.78	0.64
2:H:337:ASN:ND2	1:J:494:PHE:O	2.30	0.64
2:H:327:LEU:HB3	2:H:371:ILE:O	1.98	0.64
2:K:613:TYR:HE1	2:K:617:PHE:CD2	2.16	0.64
2:B:326:ARG:NH2	2:B:368:ASP:OD1	2.30	0.64
2:F:258:ILE:N	2:F:572:GLU:OE2	2.31	0.63
2:C:357:PHE:HD2	2:C:375:PHE:HE1	1.44	0.63
1:A:1029:PRO:HG2	1:A:1032:GLN:HG3	1.79	0.63
2:F:448:PHE:O	2:F:451:LEU:HG	1.98	0.63
2:C:270:ASN:OD1	2:B:570:SER:OG	2.15	0.63
2:K:295:VAL:HG13	2:K:312:LYS:HB3	1.80	0.63
1:G:797:THR:HG22	1:G:803:THR:HG22	1.79	0.63
2:K:652:THR:OG1	2:K:654:ASP:O	2.15	0.63
1:D:758:SER:HB2	1:D:838:LEU:HD21	1.81	0.63
2:B:331:ASP:OD1	2:B:332:LYS:N	2.32	0.63
2:L:258:ILE:N	2:L:572:GLU:OE2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:991:ARG:O	1:D:991:ARG:NH1	2.31	0.63
2:C:349:ILE:HG22	2:C:419:GLN:HG3	1.81	0.63
1:A:923:ILE:HD11	1:A:927:GLY:HA2	1.81	0.63
1:G:945:ILE:HA	1:G:956:PRO:HA	1.81	0.63
1:G:1006:MET:HE2	1:G:1028:VAL:HG23	1.81	0.63
2:F:397:ILE:HD11	2:F:486:LEU:HB3	1.81	0.63
2:C:408:GLN:NE2	2:B:559:GLN:OE1	2.32	0.63
1:A:1009:GLY:HA2	1:A:1032:GLN:HE22	1.63	0.62
1:D:505:SER:OG	1:D:560:SER:O	2.17	0.62
2:L:487:SER:OG	2:L:515:MET:SD	2.51	0.62
1:J:732:PRO:O	1:J:787:TYR:OH	2.14	0.62
2:I:309:THR:HA	2:I:326:ARG:HG2	1.81	0.62
1:J:1085:LEU:O	1:J:1089:ALA:N	2.32	0.62
2:L:601:SER:HB3	2:L:607:PHE:HD1	1.63	0.62
2:K:533:ASN:OD1	2:K:534:GLY:N	2.31	0.62
2:H:582:VAL:O	2:H:586:ASN:ND2	2.29	0.62
2:I:529:LEU:O	2:I:538:LYS:NZ	2.33	0.62
1:G:710:ASN:HA	1:G:721:THR:HA	1.80	0.62
2:K:570:SER:HA	2:K:573:LEU:HD23	1.82	0.62
2:K:352:THR:O	2:K:442:LYS:NZ	2.29	0.61
1:D:417:GLN:HA	1:D:420:LYS:HB2	1.82	0.61
2:B:606:LYS:O	2:B:609:ILE:HG22	2.00	0.61
1:A:963:VAL:HG23	1:A:983:LEU:HA	1.82	0.61
2:H:412:VAL:HG11	2:H:443:LEU:HD21	1.82	0.61
2:H:397:ILE:HD11	2:H:490:ILE:HB	1.82	0.61
2:F:238:GLN:NE2	2:F:253:ALA:HB3	2.16	0.61
2:H:378:TYR:O	2:H:381:SER:OG	2.13	0.61
2:F:613:TYR:CE1	2:F:618:HIS:HE1	2.18	0.61
2:I:406:LEU:HG	2:I:483:LEU:HD21	1.81	0.61
1:J:790:ASN:HB3	1:J:851:ILE:HD12	1.81	0.61
1:J:855:ALA:HB1	1:J:859:ARG:HH12	1.65	0.61
1:A:465:GLN:NE2	1:A:498:PRO:O	2.33	0.61
2:L:238:GLN:HE21	2:L:252:SER:HB2	1.65	0.61
2:K:226:HIS:HB2	1:J:369:GLY:HA2	1.82	0.61
1:J:941:ARG:NH1	1:J:961:TYR:OH	2.34	0.61
2:L:406:LEU:HD21	2:L:525:VAL:HG11	1.83	0.61
1:J:522:LEU:HD21	1:J:851:ILE:HG12	1.83	0.61
1:D:438:MET:HE1	1:D:743:ASP:H	1.65	0.61
2:H:512:ILE:HA	2:H:515:MET:HG3	1.81	0.61
1:J:360:ASP:OD1	1:J:363:TYR:N	2.33	0.61
1:G:497:THR:HG21	2:K:337:ASN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:559:GLN:O	2:I:562:THR:OG1	2.13	0.61
1:G:892:TYR:HA	1:G:956:PRO:HD2	1.83	0.60
2:F:238:GLN:HE22	2:F:253:ALA:HB3	1.66	0.60
2:B:378:TYR:O	2:B:381:SER:OG	2.14	0.60
1:G:477:PRO:O	1:G:480:SER:OG	2.18	0.60
2:C:284:ILE:HG13	2:C:285:PRO:HD2	1.83	0.60
1:A:891:GLU:OE2	1:A:990:LYS:NZ	2.34	0.60
2:K:330:ILE:HG13	2:K:371:ILE:HG23	1.84	0.60
2:H:295:VAL:HG13	2:H:312:LYS:HB3	1.83	0.60
2:C:648:LEU:HG	2:C:663:TYR:HE1	1.65	0.60
2:K:341:LYS:HA	2:K:341:LYS:HE2	1.83	0.60
2:C:258:ILE:N	2:C:572:GLU:OE2	2.35	0.60
1:G:497:THR:HB	2:K:341:LYS:HE3	1.83	0.60
2:L:473:GLN:OE1	2:L:538:LYS:N	2.34	0.60
2:E:388:HIS:HB3	2:E:397:ILE:HD11	1.84	0.60
1:D:1035:ASP:OD1	1:D:1037:ALA:N	2.34	0.60
2:C:292:PHE:HE2	2:C:316:ASN:HA	1.67	0.60
2:L:631:THR:OG1	1:J:389:GLU:OE1	2.20	0.59
2:I:305:LEU:HD12	2:I:306:ASN:HB2	1.84	0.59
2:C:402:LEU:HA	2:C:405:TYR:HD2	1.67	0.59
2:F:418:SER:OG	2:F:419:GLN:OE1	2.17	0.59
2:C:614:ASP:OD2	2:B:595:ARG:NH2	2.35	0.59
2:I:323:VAL:HG23	2:I:377:TYR:HA	1.84	0.59
1:J:391:THR:HG22	1:J:445:TYR:HD1	1.67	0.59
2:C:529:LEU:O	2:C:538:LYS:NZ	2.34	0.59
2:C:580:ARG:NH2	1:A:363:TYR:O	2.35	0.59
2:K:567:SER:O	2:K:570:SER:OG	2.14	0.59
2:H:449:MET:HA	2:H:452:LEU:HG	1.84	0.59
2:C:628:MET:HE3	2:B:587:CYS:HB2	1.83	0.59
2:F:301:ASN:HD22	2:F:308:THR:HA	1.68	0.59
2:C:492:ASN:ND2	2:C:498:ALA:O	2.31	0.59
2:L:584:LYS:HG3	2:L:674:PHE:CD2	2.37	0.59
2:K:389:PHE:HE2	2:K:429:TRP:HZ3	1.50	0.59
2:K:423:ILE:N	2:K:475:ASP:OD2	2.35	0.59
2:H:678:THR:HG22	2:H:679:GLN:H	1.66	0.59
1:J:477:PRO:O	1:J:480:SER:OG	2.20	0.58
1:J:623:ASN:HD22	1:J:849:ILE:HD13	1.67	0.58
2:F:346:TRP:HZ2	2:F:448:PHE:HB3	1.67	0.58
2:I:355:ILE:HD12	2:I:378:TYR:HD2	1.68	0.58
1:G:1025:ASN:ND2	1:G:1025:ASN:O	2.34	0.58
1:J:994:ARG:O	1:J:997:VAL:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:436:GLY:HA3	2:I:440:ARG:CZ	2.33	0.58
2:C:643:GLY:O	2:C:644:ILE:HG13	2.02	0.58
1:A:854:ASP:HB3	1:A:857:GLU:HB3	1.85	0.58
2:E:399:ASN:ND2	2:E:519:ASP:OD2	2.36	0.58
2:C:323:VAL:HG23	2:C:377:TYR:HA	1.86	0.58
2:L:652:THR:HG22	2:L:653:PRO:HD2	1.84	0.58
1:J:909:ILE:HD11	1:J:942:ILE:HD11	1.85	0.58
2:L:654:ASP:OD2	1:J:420:LYS:HG3	2.04	0.58
2:E:467:THR:OG1	2:E:468:ILE:N	2.35	0.58
2:F:619:GLN:HB2	2:F:627:ILE:O	2.04	0.58
2:L:290:ASP:O	2:L:316:ASN:N	2.37	0.58
2:E:429:TRP:HZ3	2:E:485:ASN:HB3	1.69	0.58
2:F:487:SER:OG	2:F:515:MET:SD	2.57	0.58
2:F:529:LEU:O	2:F:538:LYS:NZ	2.37	0.58
1:D:522:LEU:HD22	1:D:793:VAL:HG23	1.85	0.58
1:G:914:VAL:HG23	1:G:971:TYR:HA	1.86	0.57
1:D:750:ARG:NH2	1:D:846:THR:OG1	2.37	0.57
1:J:909:ILE:HD12	1:J:944:ILE:HD12	1.87	0.57
2:C:584:LYS:HE3	1:A:359:ASP:HB2	1.86	0.57
2:L:623:ASN:OD1	1:J:747:SER:HB2	2.04	0.57
2:F:336:PRO:O	2:F:339:ILE:HG13	2.04	0.57
1:A:438:MET:HB3	1:A:441:ALA:HB2	1.86	0.57
1:J:675:ILE:HD11	1:J:741:LEU:HD21	1.87	0.57
1:G:439:ARG:NH1	2:I:614:ASP:HB3	2.18	0.57
2:I:402:LEU:HA	2:I:405:TYR:HD2	1.69	0.57
1:A:558:GLU:O	1:A:561:HIS:ND1	2.37	0.57
2:L:601:SER:OG	2:L:603:SER:O	2.22	0.57
2:K:257:PHE:HA	2:K:438:PRO:HB2	1.87	0.57
2:E:296:PRO:HA	2:E:311:PHE:HB3	1.87	0.57
2:F:297:LEU:O	2:F:308:THR:HG21	2.05	0.57
2:L:437:ASP:HB2	2:L:438:PRO:HA	1.86	0.57
2:E:649:MET:H	1:D:347:PHE:HE2	1.53	0.57
1:D:618:MET:N	1:D:619:PRO:HD2	2.20	0.57
2:B:544:THR:HA	2:B:547:PHE:HD2	1.69	0.57
1:G:1025:ASN:C	1:G:1025:ASN:HD22	2.13	0.57
1:D:447:CYS:HB3	1:D:450:ASP:HB2	1.87	0.57
2:I:487:SER:OG	2:I:515:MET:SD	2.58	0.57
1:G:416:SER:HA	1:G:429:LEU:HD23	1.86	0.56
2:I:292:PHE:HE2	2:I:316:ASN:HA	1.70	0.56
2:K:658:CYS:SG	2:K:659:ILE:N	2.78	0.56
2:H:556:GLU:HG3	2:I:352:THR:OG1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:567:SER:O	2:H:570:SER:OG	2.18	0.56
2:C:437:ASP:HB2	2:C:438:PRO:HA	1.86	0.56
1:G:342:ALA:HB1	2:H:620:VAL:O	2.06	0.56
1:D:942:ILE:HG13	1:D:998:VAL:HG11	1.87	0.56
2:B:257:PHE:HA	2:B:438:PRO:HB2	1.87	0.56
2:I:654:ASP:OD1	2:I:656:LEU:N	2.39	0.56
2:C:336:PRO:O	2:C:339:ILE:HG13	2.05	0.56
2:C:406:LEU:HG	2:C:483:LEU:HD21	1.87	0.56
1:A:522:LEU:HD22	1:A:793:VAL:HG23	1.87	0.56
2:L:424:GLY:HA3	2:L:447:ASN:HB3	1.86	0.56
2:L:635:ARG:NH1	1:J:389:GLU:OE1	2.35	0.56
2:F:652:THR:OG1	2:F:654:ASP:OD1	2.23	0.56
1:D:546:LEU:HD12	1:D:629:GLN:HG2	1.88	0.56
2:B:403:TRP:CH2	2:B:522:PHE:HB3	2.41	0.56
2:L:297:LEU:O	2:L:308:THR:HG21	2.05	0.56
2:E:423:ILE:N	2:E:475:ASP:OD2	2.38	0.56
2:F:258:ILE:HG13	2:F:259:PRO:HD2	1.87	0.56
2:I:291:TYR:HB3	2:I:313:VAL:HG11	1.88	0.56
1:A:477:PRO:O	1:A:480:SER:OG	2.19	0.56
1:G:1015:HIS:H	1:G:1015:HIS:CD2	2.22	0.56
2:L:357:PHE:HZ	2:L:360:ILE:HB	1.71	0.56
2:B:423:ILE:N	2:B:475:ASP:OD2	2.35	0.56
1:A:513:ASN:OD1	1:A:571:GLN:NE2	2.38	0.56
2:E:276:VAL:HG12	2:F:644:ILE:HG12	1.86	0.56
2:H:417:HIS:CE1	2:H:472:GLN:HG3	2.41	0.56
2:H:427:LEU:HB2	2:H:478:TYR:HB3	1.88	0.56
2:B:466:SER:OG	2:B:467:THR:N	2.38	0.56
1:A:746:PHE:O	1:A:749:ILE:HG13	2.06	0.56
1:G:482:LEU:HD21	1:G:828:LEU:HB2	1.87	0.56
1:A:631:ILE:O	1:A:634:GLU:HG2	2.06	0.56
2:H:533:ASN:OD1	2:H:534:GLY:N	2.39	0.55
2:B:615:TYR:OH	1:A:345:ASP:OD2	2.13	0.55
1:G:522:LEU:HD22	1:G:793:VAL:HG23	1.87	0.55
2:L:429:TRP:HZ2	2:L:485:ASN:HB3	1.71	0.55
2:K:621:ASP:N	2:K:625:LYS:O	2.36	0.55
2:K:617:PHE:HE1	2:K:633:VAL:HG13	1.71	0.55
1:A:892:TYR:HA	1:A:956:PRO:HG2	1.89	0.55
2:F:301:ASN:OD1	2:F:303:ASP:N	2.40	0.55
2:I:423:ILE:HG21	2:I:475:ASP:HB3	1.87	0.55
2:B:429:TRP:HA	2:B:432:VAL:HG12	1.89	0.55
2:E:353:ASN:ND2	2:E:411:ASN:HD22	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:LEU:HD21	1:D:557:MET:SD	2.47	0.55
1:A:546:LEU:HD12	1:A:629:GLN:HG2	1.89	0.55
1:J:968:ILE:HG13	1:J:971:TYR:CZ	2.41	0.55
2:F:437:ASP:HA	2:F:438:PRO:C	2.31	0.55
2:B:582:VAL:O	2:B:586:ASN:ND2	2.34	0.55
2:B:619:GLN:NE2	1:A:343:TYR:HB2	2.22	0.55
2:I:574:GLU:OE2	2:I:638:ASN:ND2	2.39	0.55
1:A:523:TYR:OH	1:A:623:ASN:OD1	2.23	0.55
2:L:617:PHE:O	2:L:628:MET:HE1	2.06	0.54
2:I:291:TYR:HB3	2:I:313:VAL:CG1	2.37	0.54
2:C:358:ARG:O	2:C:374:VAL:HB	2.07	0.54
2:B:601:SER:OG	2:B:602:GLU:N	2.37	0.54
1:A:1035:ASP:OD1	1:A:1036:THR:N	2.41	0.54
2:L:274:LEU:HD11	2:K:229:ALA:HA	1.89	0.54
2:K:577:ARG:HA	2:K:580:ARG:HE	1.71	0.54
2:H:403:TRP:CE3	2:H:550:LYS:HG3	2.41	0.54
2:B:567:SER:O	2:B:570:SER:HB3	2.08	0.54
1:G:760:PHE:CE1	1:G:771:LEU:HD23	2.42	0.54
2:F:357:PHE:HD1	2:F:375:PHE:HE1	1.53	0.54
2:E:257:PHE:HA	2:E:438:PRO:HB2	1.88	0.54
1:D:1032:GLN:OE1	1:D:1032:GLN:N	2.40	0.54
2:B:327:LEU:HB2	2:B:371:ILE:O	2.06	0.54
2:F:508:THR:O	2:F:511:SER:OG	2.17	0.54
2:H:619:GLN:O	2:H:626:PRO:HA	2.07	0.54
2:I:492:ASN:O	2:I:497:THR:N	2.37	0.54
2:L:429:TRP:HE1	2:L:485:ASN:HB2	1.73	0.54
2:L:391:ASN:OD1	2:L:392:PHE:N	2.39	0.54
2:C:542:ASP:O	2:C:546:HIS:ND1	2.33	0.54
2:B:644:ILE:O	2:B:663:TYR:HB2	2.08	0.54
2:L:586:ASN:ND2	2:K:613:TYR:OH	2.41	0.54
1:J:944:ILE:HG12	1:J:957:PHE:CZ	2.43	0.54
1:A:806:VAL:HG21	1:A:823:MET:HE3	1.88	0.54
2:L:621:ASP:OD1	2:L:622:SER:N	2.41	0.54
2:K:511:SER:HA	2:K:514:ASP:HB2	1.89	0.54
2:H:385:TYR:HB2	2:H:429:TRP:HD1	1.73	0.54
2:I:327:LEU:HB2	2:I:371:ILE:O	2.08	0.54
2:C:280:SER:HB3	2:C:283:VAL:HG22	1.90	0.54
2:B:289:GLN:HG2	2:B:361:PHE:CG	2.43	0.54
2:E:417:HIS:CE1	2:E:472:GLN:HG3	2.42	0.53
2:F:653:PRO:HA	1:D:439:ARG:HE	1.74	0.53
1:D:992:LEU:HD23	1:D:997:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:LEU:HG	2:B:547:PHE:CZ	2.43	0.53
2:B:407:VAL:O	2:B:410:THR:OG1	2.23	0.53
2:E:615:TYR:HD1	1:D:341:LEU:HD13	1.73	0.53
1:G:940:ALA:O	1:G:962:VAL:HG12	2.08	0.53
2:H:614:ASP:OD2	2:I:595:ARG:NH2	2.38	0.53
2:I:652:THR:OG1	2:I:654:ASP:OD1	2.24	0.53
1:J:1030:ARG:O	1:J:1033:ILE:HG12	2.07	0.53
1:A:962:VAL:HG21	1:A:994:ARG:HB2	1.89	0.53
2:L:353:ASN:O	2:L:442:LYS:HA	2.09	0.53
2:L:449:MET:HA	2:L:452:LEU:HD12	1.91	0.53
2:H:296:PRO:HA	2:H:311:PHE:HD1	1.73	0.53
2:C:290:ASP:O	2:C:316:ASN:N	2.38	0.53
2:K:425:ASN:O	2:K:425:ASN:ND2	2.42	0.53
2:L:628:MET:HE3	2:K:587:CYS:HB2	1.89	0.53
2:K:259:PRO:HB3	2:K:438:PRO:HD3	1.91	0.53
2:I:385:TYR:HB2	2:I:429:TRP:HB3	1.90	0.53
1:J:1067:ASP:OD1	1:J:1068:SER:N	2.41	0.53
2:B:508:THR:OG1	2:B:511:SER:HB3	2.09	0.53
2:E:357:PHE:CE1	2:E:360:ILE:HG13	2.43	0.53
1:A:511:VAL:O	1:A:936:ARG:NH2	2.42	0.53
2:L:258:ILE:HG13	2:L:259:PRO:HD2	1.91	0.53
2:K:287:ILE:HG22	2:K:292:PHE:HB3	1.91	0.53
1:A:966:ASN:OD1	1:A:967:HIS:N	2.38	0.53
1:G:855:ALA:HB1	1:G:859:ARG:HH12	1.74	0.53
2:L:248:PRO:HG3	2:K:317:TYR:CZ	2.44	0.53
2:E:591:ARG:HA	2:F:618:HIS:HD2	1.73	0.53
2:E:591:ARG:HA	2:F:618:HIS:CD2	2.44	0.53
2:F:295:VAL:HG13	2:F:312:LYS:HB3	1.90	0.53
2:I:383:SER:O	2:I:387:TYR:N	2.40	0.53
1:J:454:GLN:C	1:J:456:THR:H	2.17	0.53
2:K:429:TRP:H	2:K:429:TRP:CD1	2.27	0.53
2:E:437:ASP:N	2:E:438:PRO:HD2	2.23	0.53
2:F:338:LYS:O	2:F:342:ILE:HG12	2.09	0.53
2:I:578:LEU:HD22	2:I:637:LEU:HB3	1.91	0.53
1:J:514:HIS:O	1:J:517:ASN:ND2	2.29	0.53
1:J:988:SER:O	1:J:989:THR:OG1	2.26	0.53
2:B:572:GLU:OE2	2:B:575:ASN:ND2	2.41	0.52
2:L:545:SER:HA	2:L:548:TYR:CE2	2.43	0.52
2:E:349:ILE:HD11	2:E:421:LEU:HD12	1.91	0.52
2:E:404:ILE:HG22	2:E:408:GLN:HE21	1.75	0.52
2:K:426:THR:HG21	2:K:444:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:ILE:O	1:D:634:GLU:HG2	2.09	0.52
1:D:836:GLU:HA	1:D:839:LYS:HE3	1.92	0.52
2:F:607:PHE:O	2:F:610:ILE:HG13	2.09	0.52
2:B:325:LYS:HD3	2:B:445:HIS:HE1	1.74	0.52
2:L:435:THR:HG22	2:L:436:GLY:H	1.73	0.52
2:L:569:LEU:HD11	2:K:568:VAL:HG13	1.91	0.52
1:D:957:PHE:HD1	1:D:958:VAL:HG22	1.74	0.52
2:H:426:THR:HG21	2:H:446:CYS:HA	1.91	0.52
2:I:238:GLN:OE1	2:I:238:GLN:N	2.37	0.52
2:I:601:SER:OG	2:I:603:SER:O	2.27	0.52
1:A:996:ASN:O	1:A:1000:ARG:HB2	2.09	0.52
1:G:878:ASP:HB2	1:G:894:LEU:HD21	1.91	0.52
2:K:510:GLN:NE2	2:K:514:ASP:OD1	2.42	0.52
2:F:606:LYS:O	2:F:609:ILE:HG12	2.09	0.52
2:H:405:TYR:HA	2:H:441:ILE:HD13	1.92	0.52
1:J:698:TYR:HE2	1:J:755:TRP:HE1	1.56	0.52
2:C:435:THR:HG22	2:C:436:GLY:H	1.74	0.52
2:C:578:LEU:O	2:C:582:VAL:HG23	2.10	0.52
2:K:391:ASN:OD1	2:K:392:PHE:N	2.43	0.52
2:K:425:ASN:HB3	2:K:478:TYR:CZ	2.44	0.52
2:F:409:LEU:HD11	2:F:441:ILE:HG21	1.92	0.52
2:H:484:PHE:CE1	2:H:488:ILE:HG13	2.45	0.52
2:I:473:GLN:HE22	2:I:533:ASN:CG	2.18	0.52
2:C:291:TYR:HB3	2:C:313:VAL:CG2	2.40	0.52
2:H:429:TRP:HZ3	2:H:485:ASN:ND2	2.07	0.52
2:H:595:ARG:HD3	2:I:600:TRP:CD1	2.44	0.52
2:C:573:LEU:HD23	2:B:572:GLU:HG2	1.91	0.52
2:B:392:PHE:CD1	2:B:393:PRO:HA	2.44	0.52
2:L:280:SER:HB2	2:L:283:VAL:HG22	1.91	0.52
2:L:444:SER:HG	2:L:445:HIS:CE1	2.28	0.52
2:K:437:ASP:N	2:K:438:PRO:HD2	2.25	0.52
2:E:583:ASN:ND2	2:F:628:MET:SD	2.82	0.52
2:C:386:ASP:HA	2:C:390:VAL:HB	1.92	0.52
2:B:401:TYR:HD1	2:B:404:ILE:HD12	1.75	0.52
2:F:435:THR:HG22	2:F:436:GLY:H	1.74	0.52
2:F:590:GLY:O	2:F:595:ARG:NH1	2.43	0.52
1:D:418:ASN:C	1:D:420:LYS:H	2.18	0.52
2:I:297:LEU:O	2:I:308:THR:HG21	2.10	0.52
2:C:591:ARG:O	2:C:594:SER:OG	2.22	0.52
1:G:899:GLU:CD	1:G:899:GLU:H	2.18	0.51
2:E:620:VAL:O	1:D:342:ALA:HB1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:910:ASP:OD1	1:D:911:ALA:N	2.42	0.51
2:H:386:ASP:HA	2:H:390:VAL:HG12	1.92	0.51
2:H:581:LEU:HD23	2:H:637:LEU:HB3	1.92	0.51
2:E:386:ASP:HA	2:E:390:VAL:HB	1.91	0.51
2:L:334:MET:HB2	2:L:338:LYS:HE3	1.91	0.51
2:K:278:PRO:HD3	2:K:295:VAL:HB	1.92	0.51
2:I:258:ILE:HG13	2:I:259:PRO:HD2	1.92	0.51
2:C:540:ILE:HG23	2:B:548:TYR:OH	2.10	0.51
2:F:631:THR:O	2:F:635:ARG:HG3	2.11	0.51
2:H:408:GLN:CD	2:H:441:ILE:HD12	2.35	0.51
2:H:592:ILE:HD12	2:I:653:PRO:HB3	1.91	0.51
2:I:413:ILE:O	2:I:416:ILE:HG13	2.11	0.51
2:L:301:ASN:ND2	2:L:308:THR:HA	2.25	0.51
2:L:429:TRP:CZ2	2:L:485:ASN:HB3	2.45	0.51
2:E:386:ASP:HB3	2:E:391:ASN:OD1	2.10	0.51
2:H:548:TYR:OH	2:I:545:SER:OG	2.25	0.51
2:I:263:ARG:NH1	2:I:264:GLU:HG3	2.25	0.51
2:I:619:GLN:HB2	2:I:627:ILE:O	2.11	0.51
2:E:449:MET:HA	2:E:452:LEU:HD12	1.91	0.51
1:D:854:ASP:HB3	1:D:857:GLU:HB3	1.92	0.51
1:J:1015:HIS:HD1	1:J:1036:THR:HG1	1.55	0.51
2:C:399:ASN:OD1	2:C:400:ASN:N	2.43	0.51
2:L:287:ILE:HG13	2:L:292:PHE:HB3	1.93	0.51
2:H:407:VAL:HG11	2:H:554:VAL:HG11	1.93	0.51
2:H:607:PHE:N	2:H:608:PRO:HD2	2.26	0.51
2:I:321:ALA:O	2:I:322:TYR:CG	2.64	0.51
2:C:569:LEU:HD11	2:B:568:VAL:HG13	1.93	0.51
1:G:1003:TRP:O	1:G:1006:MET:HG3	2.11	0.51
1:D:677:GLY:O	1:D:678:ILE:HG13	2.11	0.51
1:D:893:LYS:O	1:D:946:ARG:NH2	2.38	0.51
1:J:482:LEU:HD21	1:J:828:LEU:HB2	1.92	0.51
2:C:247:LYS:HB3	2:C:248:PRO:HD2	1.92	0.51
1:G:758:SER:HB2	1:G:838:LEU:HD21	1.93	0.50
2:K:627:ILE:HD11	1:J:343:TYR:CG	2.45	0.50
2:H:274:LEU:HD21	2:I:639:LYS:HA	1.93	0.50
2:H:543:LEU:O	2:H:546:HIS:HB2	2.10	0.50
2:C:584:LYS:HG2	2:C:674:PHE:CE2	2.47	0.50
2:C:657:ASN:HD21	1:A:415:SER:HB2	1.76	0.50
2:B:525:VAL:O	2:B:528:TYR:HB3	2.11	0.50
2:L:540:ILE:HD12	2:L:540:ILE:H	1.77	0.50
2:H:343:TYR:HA	2:H:357:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:487:SER:HB2	2:H:515:MET:HE1	1.93	0.50
1:J:524:ARG:HD2	1:J:557:MET:HE3	1.93	0.50
2:C:352:THR:OG1	2:B:556:GLU:HG2	2.12	0.50
2:B:575:ASN:HB3	1:A:365:LEU:HD12	1.92	0.50
2:L:437:ASP:OD1	2:L:437:ASP:N	2.42	0.50
2:E:429:TRP:CD1	2:E:430:ARG:N	2.79	0.50
2:F:309:THR:O	2:F:326:ARG:HB3	2.11	0.50
2:B:518:ILE:HG22	2:B:520:ASP:N	2.21	0.50
2:E:613:TYR:OH	2:F:586:ASN:ND2	2.43	0.50
1:A:952:LEU:O	1:A:955:VAL:HG12	2.11	0.50
2:K:389:PHE:HE1	2:K:493:SER:HB3	1.76	0.50
2:H:318:ASP:HB3	2:H:320:LYS:HB2	1.94	0.50
2:H:341:LYS:HA	1:J:497:THR:HG21	1.92	0.50
1:J:853:CYS:SG	1:J:854:ASP:N	2.84	0.50
2:C:586:ASN:ND2	2:B:586:ASN:OD1	2.45	0.50
2:E:357:PHE:HE1	2:E:360:ILE:HG13	1.76	0.50
2:H:402:LEU:HD11	2:H:487:SER:HB3	1.94	0.50
2:L:574:GLU:HG2	2:L:578:LEU:HD13	1.92	0.50
1:D:528:GLU:HG3	1:D:857:GLU:OE2	2.11	0.50
1:D:945:ILE:HG23	1:D:956:PRO:HA	1.93	0.50
2:E:592:ILE:HD12	2:F:653:PRO:HB3	1.94	0.50
2:I:397:ILE:HD11	2:I:402:LEU:HD21	1.93	0.50
2:C:603:SER:OG	2:C:604:GLY:N	2.44	0.50
1:A:997:VAL:HG23	1:A:998:VAL:N	2.26	0.50
2:F:649:MET:HG2	1:D:435:LYS:HE2	1.94	0.50
1:J:507:LEU:HD21	1:J:557:MET:SD	2.52	0.50
2:B:389:PHE:CD2	2:B:499:PRO:HG3	2.46	0.50
2:L:238:GLN:HE22	2:L:254:ASP:H	1.60	0.49
2:F:280:SER:HB2	2:F:283:VAL:HG22	1.94	0.49
2:H:265:ASP:O	2:H:269:LYS:HG3	2.12	0.49
1:J:467:TYR:HD2	1:J:836:GLU:HG2	1.76	0.49
1:J:505:SER:OG	1:J:561:HIS:O	2.18	0.49
1:J:1000:ARG:HE	1:J:1004:LEU:HD11	1.77	0.49
2:C:238:GLN:NE2	2:C:253:ALA:HB3	2.27	0.49
2:B:331:ASP:OD1	2:B:332:LYS:HG2	2.12	0.49
2:B:667:LYS:HG3	1:A:378:LEU:HB2	1.94	0.49
1:A:701:TYR:O	1:A:705:ASN:HB3	2.12	0.49
1:G:764:ILE:HG22	1:G:769:ALA:HA	1.94	0.49
2:L:387:TYR:CE2	2:L:434:ILE:HD12	2.48	0.49
2:E:607:PHE:N	2:E:608:PRO:HD2	2.27	0.49
2:I:306:ASN:OD1	2:I:307:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:579:PHE:HE1	2:B:582:VAL:HG21	1.77	0.49
1:G:373:TYR:HE1	2:I:233:LEU:HB2	1.77	0.49
2:F:397:ILE:HG23	2:F:490:ILE:HG13	1.93	0.49
1:G:546:LEU:HD12	1:G:629:GLN:HG2	1.95	0.49
1:G:761:TYR:CE1	1:G:786:LYS:HG3	2.48	0.49
2:L:677:ILE:O	2:K:626:PRO:HG2	2.13	0.49
2:F:349:ILE:HG22	2:F:419:GLN:HE21	1.77	0.49
2:H:273:ILE:HD11	2:H:379:PRO:HG3	1.94	0.49
2:I:558:SER:O	2:I:562:THR:HG23	2.13	0.49
1:G:925:HIS:O	1:G:926:GLN:HG2	2.12	0.49
2:L:675:ARG:O	2:L:679:GLN:HG2	2.12	0.49
1:J:1033:ILE:HG13	1:J:1034:ARG:N	2.28	0.49
1:A:695:ILE:O	1:A:698:TYR:HB2	2.13	0.49
1:G:796:ILE:HG23	1:G:844:TRP:HD1	1.77	0.49
2:K:577:ARG:HH21	2:K:578:LEU:HD11	1.77	0.49
2:F:292:PHE:CE2	2:F:316:ASN:HA	2.48	0.49
2:H:509:PRO:O	2:H:512:ILE:HG13	2.13	0.49
1:J:942:ILE:HG21	1:J:998:VAL:CG1	2.42	0.49
2:C:555:LEU:HD11	2:B:554:VAL:HG13	1.93	0.49
2:B:362:GLN:HB3	1:A:923:ILE:HG23	1.94	0.49
1:A:467:TYR:CD2	1:A:836:GLU:HG2	2.48	0.49
1:A:855:ALA:HB1	1:A:859:ARG:HH12	1.77	0.49
2:I:295:VAL:HG13	2:I:312:LYS:HB3	1.94	0.49
2:I:533:ASN:ND2	2:I:536:SER:O	2.46	0.49
1:G:620:GLN:NE2	1:G:848:GLU:OE1	2.46	0.49
1:G:796:ILE:HG23	1:G:844:TRP:CD1	2.47	0.49
2:L:483:LEU:HD23	2:L:522:PHE:CE1	2.48	0.49
2:F:564:TYR:O	2:F:567:SER:OG	2.29	0.49
1:J:418:ASN:C	1:J:420:LYS:H	2.20	0.49
2:C:318:ASP:OD2	2:C:322:TYR:OH	2.24	0.49
1:A:962:VAL:CG2	1:A:994:ARG:HB2	2.42	0.49
1:A:1019:ASN:O	1:A:1023:HIS:ND1	2.46	0.49
2:H:405:TYR:HD1	2:H:441:ILE:HD11	1.78	0.49
2:C:238:GLN:OE1	2:C:243:LYS:NZ	2.46	0.49
2:C:295:VAL:HG13	2:C:312:LYS:HB3	1.95	0.49
1:A:641:ASN:O	1:A:642:ILE:HG13	2.13	0.49
1:G:340:MET:HE1	2:H:649:MET:SD	2.53	0.49
1:G:756:LEU:HD21	1:G:789:LEU:HD22	1.94	0.49
2:L:587:CYS:HB2	2:K:628:MET:SD	2.52	0.49
2:L:629:ASP:OD1	2:L:631:THR:HG22	2.12	0.49
2:K:252:SER:HB2	2:K:255:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:577:ARG:HA	2:E:580:ARG:HE	1.79	0.48
2:F:312:LYS:HG3	2:F:377:TYR:HE2	1.78	0.48
1:D:1015:HIS:HD1	1:D:1036:THR:HG1	1.55	0.48
2:H:458:ASP:CB	1:J:1030:ARG:H	2.26	0.48
2:I:549:ASP:OD1	2:I:549:ASP:N	2.46	0.48
2:C:437:ASP:OD1	2:C:437:ASP:N	2.44	0.48
2:L:301:ASN:OD1	2:L:303:ASP:N	2.46	0.48
2:L:579:PHE:CE1	2:K:578:LEU:HB3	2.48	0.48
2:K:349:ILE:HD11	2:K:421:LEU:HD12	1.94	0.48
2:F:601:SER:OG	2:F:603:SER:O	2.29	0.48
1:J:559:ARG:O	1:J:561:HIS:ND1	2.45	0.48
2:C:582:VAL:O	2:C:586:ASN:HB2	2.12	0.48
2:C:631:THR:O	2:C:635:ARG:HG3	2.13	0.48
2:B:325:LYS:HD3	2:B:445:HIS:CE1	2.48	0.48
2:B:437:ASP:N	2:B:438:PRO:HD2	2.28	0.48
1:A:853:CYS:SG	1:A:854:ASP:N	2.86	0.48
2:F:397:ILE:HG21	2:F:490:ILE:HA	1.96	0.48
1:J:631:ILE:O	1:J:634:GLU:HG2	2.13	0.48
2:B:507:ILE:O	2:B:509:PRO:HD3	2.13	0.48
1:G:799:ASN:N	1:G:799:ASN:OD1	2.44	0.48
2:E:429:TRP:CZ3	2:E:485:ASN:HB3	2.47	0.48
1:D:432:ASP:OD1	1:D:433:ARG:N	2.47	0.48
2:C:353:ASN:H	2:C:442:LYS:NZ	2.12	0.48
2:C:576:GLY:O	2:C:579:PHE:HB3	2.14	0.48
2:L:590:GLY:O	2:L:595:ARG:NH1	2.46	0.48
2:E:612:PHE:HE2	2:E:640:LEU:HD22	1.79	0.48
2:F:429:TRP:CZ2	2:F:485:ASN:HB3	2.49	0.48
1:D:537:LEU:O	1:D:1000:ARG:NH1	2.44	0.48
2:H:359:ASP:H	2:H:374:VAL:HG12	1.79	0.48
2:B:264:GLU:OE2	2:B:264:GLU:N	2.45	0.48
1:G:653:GLU:O	1:G:726:CYS:HA	2.13	0.48
1:G:824:PHE:CE1	1:G:829:VAL:HG13	2.49	0.48
1:G:910:ASP:OD1	1:G:911:ALA:N	2.45	0.48
2:L:355:ILE:HG23	2:L:376:ASP:HB2	1.94	0.48
2:I:513:ASP:HA	2:I:523:LYS:HD3	1.96	0.48
2:I:631:THR:O	2:I:635:ARG:HG3	2.13	0.48
2:C:638:ASN:CG	2:B:274:LEU:HD11	2.38	0.48
1:A:676:SER:OG	1:A:677:GLY:N	2.46	0.48
1:G:348:ASN:OD1	2:H:639:LYS:NZ	2.31	0.48
2:E:567:SER:O	2:E:570:SER:OG	2.24	0.48
2:F:597:ASP:HB3	2:F:599:ASN:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:CYS:O	1:D:451:ILE:N	2.47	0.48
1:J:537:LEU:HD21	1:J:552:TYR:HE1	1.78	0.48
2:B:616:VAL:HA	2:B:632:HIS:HE1	1.79	0.48
1:A:765:ILE:HD12	1:A:766:LYS:HG3	1.94	0.48
1:G:853:CYS:SG	1:G:854:ASP:N	2.87	0.48
2:L:323:VAL:HG23	2:L:377:TYR:HA	1.95	0.48
2:K:248:PRO:HD2	2:K:251:ARG:HE	1.79	0.48
2:F:581:LEU:HD21	2:F:640:LEU:HD22	1.96	0.48
1:D:895:LEU:HD21	1:D:957:PHE:CE2	2.48	0.48
2:I:406:LEU:HD12	2:I:522:PHE:CE1	2.48	0.48
2:C:477:LYS:O	2:C:504:LEU:HD21	2.12	0.48
2:L:270:ASN:HD21	2:K:570:SER:HB2	1.78	0.48
2:L:553:MET:O	2:L:556:GLU:HB2	2.13	0.48
2:L:603:SER:OG	2:L:604:GLY:N	2.47	0.48
2:E:277:PHE:CD2	2:E:278:PRO:HD3	2.48	0.48
2:F:540:ILE:HD12	2:F:540:ILE:H	1.78	0.48
1:J:624:ARG:NH1	1:J:738:GLU:OE1	2.47	0.48
2:L:409:LEU:HA	2:L:412:VAL:HG22	1.95	0.48
2:K:353:ASN:HB2	2:K:412:VAL:HG13	1.96	0.48
2:H:568:VAL:HG13	2:I:569:LEU:HD11	1.96	0.48
2:H:619:GLN:HB2	2:H:627:ILE:O	2.14	0.48
2:C:620:VAL:O	1:A:441:ALA:HA	2.14	0.48
2:B:599:ASN:OD1	2:B:599:ASN:N	2.40	0.48
1:G:999:TYR:CE1	1:G:1026:ILE:HB	2.49	0.47
2:L:606:LYS:O	2:L:609:ILE:HG13	2.13	0.47
2:K:285:PRO:HG3	2:K:366:PHE:HE1	1.79	0.47
2:F:416:ILE:HG13	2:F:423:ILE:HD13	1.95	0.47
1:J:696:LEU:HB2	1:J:697:PRO:HD3	1.96	0.47
2:B:607:PHE:CE2	2:B:611:LEU:HD11	2.48	0.47
1:A:993:VAL:HG22	1:A:995:ARG:H	1.79	0.47
1:G:789:LEU:HD23	1:G:821:TRP:HH2	1.80	0.47
2:L:432:VAL:HG22	2:L:443:LEU:HD13	1.96	0.47
2:I:475:ASP:OD1	2:I:476:TYR:N	2.47	0.47
2:I:581:LEU:HD21	2:I:640:LEU:HD22	1.96	0.47
1:J:467:TYR:CD2	1:J:836:GLU:HG2	2.48	0.47
2:B:495:ASN:OD1	2:B:496:ASN:N	2.45	0.47
1:A:696:LEU:HB2	1:A:697:PRO:HD3	1.96	0.47
1:G:631:ILE:O	1:G:634:GLU:HG2	2.13	0.47
1:G:888:ALA:HA	1:G:989:THR:HA	1.96	0.47
1:G:1020:ASP:O	1:G:1024:ILE:HG13	2.13	0.47
1:G:1069:ILE:HD12	1:G:1069:ILE:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:566:GLU:OE2	2:K:440:ARG:NH2	2.46	0.47
2:K:326:ARG:NH2	2:K:368:ASP:OD2	2.46	0.47
1:D:456:THR:OG1	1:D:457:SER:N	2.47	0.47
2:H:587:CYS:HB2	2:I:628:MET:SD	2.55	0.47
1:A:1048:SER:HB2	1:A:1051:TYR:HB2	1.96	0.47
1:G:659:SER:C	1:G:661:ASP:H	2.22	0.47
2:F:578:LEU:O	2:F:582:VAL:HG23	2.14	0.47
2:H:562:THR:OG1	2:I:562:THR:HG22	2.15	0.47
1:J:483:PRO:O	1:J:827:TYR:OH	2.32	0.47
2:B:291:TYR:HB3	2:B:313:VAL:CG2	2.43	0.47
1:G:641:ASN:C	1:G:642:ILE:HG13	2.39	0.47
2:L:475:ASP:OD1	2:L:476:TYR:N	2.47	0.47
2:K:312:LYS:HD2	2:K:377:TYR:CE2	2.50	0.47
2:E:641:ASP:HB3	1:D:370:MET:HE1	1.95	0.47
2:F:654:ASP:OD1	2:F:655:GLU:N	2.47	0.47
2:C:353:ASN:H	2:C:442:LYS:HZ3	1.62	0.47
2:B:410:THR:HG21	2:B:547:PHE:CE2	2.49	0.47
2:B:423:ILE:HG23	2:B:446:CYS:SG	2.54	0.47
1:G:503:GLU:HG2	1:G:504:TYR:CD1	2.50	0.47
2:L:401:TYR:HA	2:L:404:ILE:HD12	1.96	0.47
2:K:246:LEU:O	2:K:248:PRO:HD3	2.13	0.47
2:K:584:LYS:HG3	1:J:381:TRP:CZ3	2.50	0.47
2:E:618:HIS:CD2	2:F:591:ARG:HD2	2.50	0.47
2:C:589:PHE:O	2:B:618:HIS:NE2	2.48	0.47
2:B:253:ALA:C	2:B:255:GLN:H	2.23	0.47
1:G:955:VAL:HA	1:G:956:PRO:HD3	1.77	0.47
2:L:234:TYR:CZ	2:K:577:ARG:HD3	2.49	0.47
2:K:589:PHE:CG	2:K:613:TYR:HD2	2.33	0.47
2:F:291:TYR:HB3	2:F:313:VAL:CG1	2.45	0.47
1:D:485:THR:HG22	1:D:486:SER:H	1.78	0.47
2:H:463:SER:HB3	1:J:1007:GLN:O	2.14	0.47
2:I:338:LYS:O	2:I:342:ILE:HG13	2.15	0.47
2:I:355:ILE:HG12	2:I:444:SER:HA	1.97	0.47
2:I:611:LEU:HD21	2:I:651:VAL:O	2.15	0.47
2:C:391:ASN:CG	2:C:392:PHE:H	2.23	0.47
2:C:578:LEU:HD21	2:C:638:ASN:HA	1.97	0.47
2:C:579:PHE:CE1	2:B:582:VAL:HG21	2.49	0.47
2:C:652:THR:HG22	2:C:653:PRO:HD2	1.96	0.47
2:B:280:SER:OG	2:B:284:ILE:O	2.24	0.47
2:B:318:ASP:OD2	2:B:322:TYR:OH	2.25	0.47
2:B:323:VAL:O	2:B:374:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:652:THR:HG21	2:B:657:ASN:HB2	1.96	0.47
1:G:365:LEU:HD23	2:H:578:LEU:HD22	1.97	0.47
1:D:641:ASN:C	1:D:642:ILE:HG13	2.40	0.47
2:H:383:SER:HA	2:H:433:LEU:HA	1.96	0.47
2:H:628:MET:SD	2:I:583:ASN:ND2	2.88	0.47
1:J:424:GLN:HG3	1:J:425:GLU:H	1.78	0.47
2:C:406:LEU:HD11	2:C:525:VAL:HG11	1.96	0.47
1:A:698:TYR:HE2	1:A:755:TRP:HE1	1.61	0.47
2:L:549:ASP:OD1	2:L:549:ASP:N	2.48	0.47
2:L:631:THR:OG1	2:L:635:ARG:NH1	2.48	0.47
2:E:406:LEU:CD1	2:E:483:LEU:HD11	2.44	0.47
2:F:603:SER:OG	2:F:604:GLY:N	2.47	0.47
2:C:483:LEU:HD23	2:C:522:PHE:CE1	2.49	0.47
2:C:623:ASN:HA	1:A:743:ASP:HB3	1.96	0.47
2:B:401:TYR:HA	2:B:404:ILE:HD12	1.97	0.47
2:H:259:PRO:HB3	2:H:438:PRO:HD3	1.96	0.47
1:J:940:ALA:O	1:J:962:VAL:HG12	2.14	0.47
1:A:507:LEU:HD21	1:A:557:MET:SD	2.55	0.47
1:A:624:ARG:NH1	1:A:738:GLU:OE1	2.48	0.47
2:L:631:THR:O	2:L:635:ARG:HG3	2.15	0.46
2:B:469:GLU:O	2:B:473:GLN:HG2	2.15	0.46
1:A:988:SER:O	1:A:989:THR:OG1	2.29	0.46
1:G:440:ASN:CG	2:I:615:TYR:HA	2.40	0.46
1:G:525:PHE:CE1	1:G:824:PHE:HE2	2.33	0.46
2:L:247:LYS:HB2	2:L:248:PRO:HD2	1.98	0.46
2:I:261:ASN:OD1	2:I:262:ILE:N	2.49	0.46
2:C:301:ASN:ND2	2:C:303:ASP:O	2.48	0.46
1:A:467:TYR:HD2	1:A:836:GLU:HG2	1.79	0.46
1:G:896:THR:HG22	1:G:897:HIS:H	1.80	0.46
2:K:322:TYR:CE1	2:K:358:ARG:HD2	2.50	0.46
2:F:353:ASN:O	2:F:442:LYS:HA	2.15	0.46
2:H:570:SER:HA	2:H:573:LEU:HD23	1.97	0.46
2:I:326:ARG:HB2	2:I:366:PHE:HE2	1.79	0.46
2:I:640:LEU:HA	2:I:663:TYR:HD2	1.79	0.46
1:J:908:ALA:O	1:J:944:ILE:HG13	2.15	0.46
2:C:427:LEU:O	2:C:482:LEU:HD12	2.15	0.46
2:L:556:GLU:OE2	2:K:411:ASN:ND2	2.24	0.46
2:K:619:GLN:O	2:K:626:PRO:HA	2.16	0.46
2:F:406:LEU:HG	2:F:483:LEU:HD11	1.96	0.46
1:D:1020:ASP:O	1:D:1024:ILE:HG13	2.15	0.46
2:C:475:ASP:OD1	2:C:476:TYR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:607:PHE:HB3	2:C:608:PRO:HD3	1.97	0.46
2:B:401:TYR:O	2:B:405:TYR:HD1	1.98	0.46
2:E:413:ILE:HD13	2:E:423:ILE:HD12	1.98	0.46
2:F:429:TRP:HZ2	2:F:485:ASN:HB3	1.80	0.46
2:I:355:ILE:HD12	2:I:378:TYR:CD2	2.49	0.46
2:C:617:PHE:O	2:C:628:MET:HE1	2.15	0.46
2:C:639:LYS:NZ	2:C:663:TYR:OH	2.48	0.46
2:L:408:GLN:NE2	2:L:439:GLY:O	2.39	0.46
2:L:561:TYR:HD1	2:L:564:TYR:HB3	1.81	0.46
2:E:569:LEU:HB2	2:F:569:LEU:HD13	1.96	0.46
2:I:254:ASP:OD1	2:I:254:ASP:N	2.49	0.46
2:I:473:GLN:NE2	2:I:533:ASN:OD1	2.38	0.46
1:A:939:LEU:HG	1:A:962:VAL:HG11	1.98	0.46
2:E:543:LEU:HG	2:E:547:PHE:CE2	2.51	0.46
2:E:591:ARG:HG2	2:F:618:HIS:CD2	2.51	0.46
2:F:409:LEU:HA	2:F:412:VAL:HG12	1.98	0.46
1:D:701:TYR:O	1:D:705:ASN:HB3	2.15	0.46
2:I:603:SER:OG	2:I:604:GLY:N	2.48	0.46
1:J:526:ILE:HG12	1:J:790:ASN:ND2	2.31	0.46
2:C:258:ILE:HG13	2:C:259:PRO:HD2	1.97	0.46
2:B:450:ASP:OD1	2:B:454:ASN:ND2	2.48	0.46
1:D:634:GLU:O	1:D:637:THR:HG22	2.16	0.46
2:I:401:TYR:HD1	2:I:404:ILE:HD12	1.81	0.46
2:C:413:ILE:O	2:C:416:ILE:HG13	2.16	0.46
1:G:556:MET:HE2	1:G:565:CYS:HB3	1.96	0.46
2:K:330:ILE:HG22	2:K:331:ASP:O	2.16	0.46
2:K:384:LEU:HD13	2:K:432:VAL:HG13	1.96	0.46
2:K:429:TRP:CD1	2:K:429:TRP:N	2.82	0.46
2:C:654:ASP:C	2:C:656:LEU:H	2.23	0.46
2:B:334:MET:HE1	2:B:452:LEU:HB2	1.97	0.46
1:G:920:LEU:HD13	1:G:933:ARG:HD3	1.98	0.46
2:E:359:ASP:O	2:E:374:VAL:HG12	2.15	0.46
2:F:233:LEU:HD12	1:D:376:LYS:HA	1.97	0.46
2:F:621:ASP:OD1	2:F:622:SER:N	2.48	0.46
1:D:913:PHE:CZ	1:D:1020:ASP:HA	2.50	0.46
2:B:406:LEU:HD13	2:B:483:LEU:HD13	1.97	0.46
1:A:634:GLU:O	1:A:637:THR:HG22	2.16	0.46
1:A:1085:LEU:O	1:A:1089:ALA:N	2.49	0.46
1:G:386:PHE:HD2	2:I:631:THR:HG22	1.81	0.45
2:L:442:LYS:NZ	2:K:563:GLU:OE2	2.39	0.45
2:L:614:ASP:OD2	2:K:595:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:635:ARG:HH22	1:J:388:SER:HB3	1.81	0.45
2:E:429:TRP:HD1	2:E:430:ARG:N	2.14	0.45
1:D:630:LEU:HD23	1:D:630:LEU:HA	1.73	0.45
2:H:278:PRO:HG2	2:H:296:PRO:HD3	1.98	0.45
2:I:644:ILE:O	2:I:663:TYR:HB2	2.16	0.45
1:J:1053:ALA:O	1:J:1057:LEU:N	2.49	0.45
2:B:592:ILE:HA	2:B:595:ARG:HG3	1.98	0.45
1:G:634:GLU:CD	1:G:642:ILE:HA	2.41	0.45
2:K:278:PRO:HG3	2:K:294:LEU:O	2.16	0.45
2:E:290:ASP:OD1	2:E:316:ASN:HB3	2.16	0.45
1:D:558:GLU:O	1:D:561:HIS:ND1	2.49	0.45
1:J:1020:ASP:O	1:J:1024:ILE:HG13	2.17	0.45
2:C:389:PHE:CE1	2:C:499:PRO:HB3	2.51	0.45
2:C:492:ASN:HD21	2:C:498:ALA:C	2.23	0.45
2:B:570:SER:HA	2:B:573:LEU:HD23	1.97	0.45
1:A:575:LYS:O	1:A:578:THR:HG22	2.17	0.45
2:L:561:TYR:HE1	2:L:564:TYR:HD2	1.65	0.45
2:L:621:ASP:O	2:L:624:GLY:HA2	2.17	0.45
2:K:649:MET:SD	1:J:340:MET:HE1	2.57	0.45
1:D:873:ASP:O	1:D:877:ARG:HG2	2.16	0.45
2:H:266:LEU:HD23	2:I:570:SER:HB3	1.97	0.45
2:H:543:LEU:HG	2:H:547:PHE:CE2	2.51	0.45
2:I:504:LEU:HA	2:I:507:ILE:HG12	1.98	0.45
2:I:606:LYS:O	2:I:609:ILE:HG13	2.16	0.45
1:J:575:LYS:O	1:J:578:THR:HG22	2.17	0.45
1:J:641:ASN:C	1:J:642:ILE:HG13	2.41	0.45
2:E:581:LEU:HD23	2:E:637:LEU:HB3	1.98	0.45
2:F:357:PHE:HZ	2:F:360:ILE:HB	1.81	0.45
2:F:574:GLU:HG2	2:F:578:LEU:HD13	1.97	0.45
2:I:578:LEU:O	2:I:582:VAL:HG23	2.17	0.45
1:G:555:ASP:OD1	1:G:559:ARG:NH1	2.50	0.45
1:G:641:ASN:O	1:G:642:ILE:HG13	2.16	0.45
2:L:347:SER:O	2:L:356:LYS:NZ	2.48	0.45
2:F:292:PHE:HE2	2:F:316:ASN:HA	1.81	0.45
1:D:656:THR:HG22	1:D:724:GLN:HG2	1.98	0.45
2:I:352:THR:C	2:I:354:LEU:H	2.24	0.45
1:J:537:LEU:HD21	1:J:552:TYR:CE1	2.51	0.45
2:L:261:ASN:OD1	2:L:262:ILE:N	2.49	0.45
2:F:654:ASP:OD2	1:D:420:LYS:HG3	2.17	0.45
1:D:641:ASN:O	1:D:642:ILE:HG13	2.16	0.45
1:D:696:LEU:HB2	1:D:697:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:539:ASP:HB2	1:G:541:ASN:HD21	1.81	0.45
1:G:552:TYR:OH	1:G:1000:ARG:HD2	2.16	0.45
1:G:620:GLN:HE22	1:G:848:GLU:C	2.23	0.45
1:G:946:ARG:HD2	1:G:955:VAL:HG23	1.98	0.45
2:L:654:ASP:OD1	2:L:655:GLU:N	2.50	0.45
1:D:509:PRO:HD3	1:D:827:TYR:HD2	1.82	0.45
1:D:538:LYS:HG3	1:D:539:ASP:OD1	2.17	0.45
1:D:555:ASP:OD1	1:D:559:ARG:NH1	2.50	0.45
2:H:354:LEU:HD13	2:H:416:ILE:HD11	1.98	0.45
1:J:445:TYR:OH	1:J:447:CYS:HB3	2.17	0.45
2:B:640:LEU:HD21	1:A:378:LEU:HD13	1.98	0.45
1:A:641:ASN:C	1:A:642:ILE:HG13	2.42	0.45
2:K:403:TRP:CE3	2:K:550:LYS:HG3	2.51	0.45
2:K:578:LEU:O	2:K:582:VAL:HG22	2.17	0.45
2:H:338:LYS:O	2:H:342:ILE:HG12	2.17	0.45
2:C:357:PHE:CZ	2:C:360:ILE:HB	2.52	0.45
1:A:476:PRO:HB2	1:A:479:TYR:HD1	1.80	0.45
1:G:360:ASP:OD1	1:G:363:TYR:N	2.50	0.45
2:F:346:TRP:CZ2	2:F:448:PHE:HB3	2.51	0.45
1:J:452:ARG:O	1:J:454:GLN:HG3	2.17	0.45
1:J:960:ASP:HB3	1:J:992:LEU:HD11	1.99	0.45
2:C:618:HIS:CG	2:B:591:ARG:HD2	2.52	0.45
2:C:630:LEU:HB2	1:A:386:PHE:CE2	2.52	0.45
2:B:389:PHE:CG	2:B:499:PRO:HG3	2.51	0.45
2:L:356:LYS:HB3	2:L:376:ASP:OD1	2.17	0.45
2:K:371:ILE:HG13	2:K:371:ILE:O	2.15	0.45
2:K:401:TYR:HD1	2:K:404:ILE:HD12	1.81	0.45
2:E:619:GLN:O	2:E:626:PRO:HA	2.17	0.45
1:D:550:LEU:HD13	1:D:630:LEU:HD11	1.99	0.45
1:G:429:LEU:HB3	2:I:657:ASN:ND2	2.29	0.44
2:L:327:LEU:O	2:L:330:ILE:HD11	2.17	0.44
2:C:330:ILE:HG13	2:C:330:ILE:O	2.17	0.44
2:B:639:LYS:HB3	2:B:663:TYR:CD2	2.51	0.44
2:K:327:LEU:HB2	2:K:371:ILE:O	2.16	0.44
2:K:398:THR:HG23	2:K:401:TYR:H	1.80	0.44
2:F:398:THR:HG23	2:F:401:TYR:H	1.81	0.44
2:F:621:ASP:O	2:F:624:GLY:HA2	2.17	0.44
1:D:392:ILE:HA	1:D:393:PRO:HD3	1.85	0.44
2:I:621:ASP:OD1	2:I:622:SER:N	2.49	0.44
2:C:507:ILE:HG21	2:C:530:ILE:HG21	1.99	0.44
1:G:447:CYS:SG	1:G:450:ASP:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:309:THR:OG1	2:L:326:ARG:O	2.30	0.44
2:F:323:VAL:HG23	2:F:377:TYR:HA	1.99	0.44
2:F:333:SER:OG	2:F:334:MET:N	2.49	0.44
1:J:526:ILE:HG12	1:J:790:ASN:HD22	1.82	0.44
2:B:273:ILE:O	2:B:312:LYS:NZ	2.51	0.44
1:A:510:ASP:OD1	1:A:936:ARG:NH1	2.51	0.44
1:A:896:THR:HG22	1:A:899:GLU:HG2	1.99	0.44
1:A:1055:VAL:HG12	1:A:1056:LEU:HD12	2.00	0.44
2:E:294:LEU:HB3	2:E:311:PHE:CE1	2.52	0.44
2:E:635:ARG:NH1	1:D:351:THR:OG1	2.48	0.44
1:D:756:LEU:HD23	1:D:840:MET:HE2	1.99	0.44
1:D:1015:HIS:ND1	1:D:1036:THR:OG1	2.29	0.44
2:H:351:CYS:HB3	2:H:354:LEU:HB3	2.00	0.44
2:H:621:ASP:N	2:H:625:LYS:O	2.32	0.44
2:I:295:VAL:HG11	2:I:312:LYS:HE3	1.98	0.44
1:J:546:LEU:HD12	1:J:629:GLN:HG2	1.99	0.44
1:J:891:GLU:OE1	1:J:990:LYS:NZ	2.41	0.44
1:J:963:VAL:HG13	1:J:964:ASN:N	2.32	0.44
2:C:355:ILE:HD11	2:C:376:ASP:O	2.18	0.44
2:C:401:TYR:HA	2:C:404:ILE:HD12	1.99	0.44
1:G:761:TYR:HE1	1:G:786:LYS:HG3	1.82	0.44
2:L:450:ASP:OD1	2:L:451:LEU:N	2.50	0.44
1:D:919:GLU:HA	1:D:933:ARG:O	2.17	0.44
1:D:1006:MET:HE2	1:D:1028:VAL:HG23	2.00	0.44
2:H:548:TYR:OH	2:I:541:HIS:O	2.34	0.44
2:I:395:PHE:HA	2:I:396:PRO:HD3	1.73	0.44
1:A:650:LEU:HG	1:A:670:LEU:O	2.17	0.44
1:G:423:THR:HB	1:G:427:PRO:HG3	1.98	0.44
1:G:537:LEU:O	1:G:1000:ARG:NH2	2.50	0.44
1:G:864:SER:O	1:G:867:THR:HG22	2.17	0.44
2:E:615:TYR:OH	1:D:345:ASP:OD2	2.34	0.44
2:H:460:VAL:O	1:J:1029:PRO:HB3	2.18	0.44
2:C:610:ILE:HG13	2:C:611:LEU:N	2.33	0.44
2:B:527:LYS:HA	2:B:530:ILE:HG22	1.99	0.44
1:G:351:THR:HG21	2:H:635:ARG:CZ	2.47	0.44
1:G:634:GLU:O	1:G:637:THR:HG22	2.18	0.44
2:L:552:PHE:O	2:L:556:GLU:HG2	2.18	0.44
2:F:612:PHE:O	2:F:616:VAL:HG12	2.18	0.44
2:F:620:VAL:O	1:D:441:ALA:HA	2.17	0.44
1:D:347:PHE:CD1	1:D:347:PHE:N	2.84	0.44
1:D:597:GLU:HG3	1:D:598:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:287:ILE:O	2:I:365:LYS:HE3	2.18	0.44
1:J:340:MET:C	1:J:342:ALA:H	2.26	0.44
1:J:1056:LEU:HD23	1:J:1081:LYS:HG3	1.99	0.44
2:C:630:LEU:O	2:C:634:LEU:HD12	2.18	0.44
2:C:657:ASN:ND2	1:A:415:SER:HB2	2.33	0.44
2:E:362:GLN:HG3	2:E:371:ILE:HG22	1.99	0.44
2:F:426:THR:HG21	2:F:445:HIS:ND1	2.32	0.44
1:D:913:PHE:HZ	1:D:1020:ASP:HA	1.83	0.44
1:J:371:PRO:HG2	1:J:372:TYR:H	1.82	0.44
1:J:550:LEU:HD21	1:J:554:PHE:CE2	2.52	0.44
1:J:877:ARG:HH12	1:J:879:TYR:HD2	1.66	0.44
2:C:652:THR:OG1	2:C:657:ASN:HB2	2.18	0.44
2:B:427:LEU:O	2:B:482:LEU:HD22	2.18	0.44
2:B:641:ASP:OD1	1:A:378:LEU:N	2.51	0.44
1:G:349:ASP:CG	2:H:632:HIS:HD1	2.25	0.44
2:L:626:PRO:HG2	2:K:677:ILE:O	2.18	0.44
2:K:248:PRO:HD2	2:K:251:ARG:HG3	2.00	0.44
1:D:1030:ARG:CB	2:B:457:THR:H	2.30	0.44
2:H:353:ASN:O	2:H:442:LYS:HA	2.18	0.44
2:H:621:ASP:O	2:H:624:GLY:N	2.49	0.44
1:J:650:LEU:HG	1:J:670:LEU:O	2.18	0.44
1:J:880:PHE:CE1	1:J:990:LYS:HB3	2.52	0.44
2:C:626:PRO:HB3	2:B:591:ARG:HH22	1.83	0.44
2:B:577:ARG:NH2	2:B:638:ASN:OD1	2.45	0.44
1:A:540:GLU:OE2	1:A:871:ASN:ND2	2.51	0.44
1:A:966:ASN:O	1:A:967:HIS:HB2	2.17	0.44
1:G:509:PRO:HD3	1:G:827:TYR:HD1	1.83	0.43
1:G:754:ASN:ND2	1:G:754:ASN:O	2.51	0.43
2:L:589:PHE:O	2:K:618:HIS:NE2	2.49	0.43
2:L:618:HIS:HD2	2:K:591:ARG:HA	1.83	0.43
2:K:337:ASN:O	2:K:340:SER:OG	2.22	0.43
2:K:353:ASN:O	2:K:442:LYS:HA	2.18	0.43
2:C:261:ASN:OD1	2:C:262:ILE:N	2.51	0.43
2:C:487:SER:O	2:C:490:ILE:HG22	2.18	0.43
1:A:627:LEU:HD22	1:A:648:PHE:HD2	1.83	0.43
2:K:388:HIS:ND1	2:K:397:ILE:HG13	2.33	0.43
2:E:627:ILE:HD11	1:D:343:TYR:CD2	2.52	0.43
2:F:409:LEU:CD1	2:F:441:ILE:HG21	2.48	0.43
1:D:482:LEU:HD21	1:D:828:LEU:HB2	2.00	0.43
1:D:1029:PRO:HG2	1:D:1032:GLN:OE1	2.19	0.43
2:I:423:ILE:CG2	2:I:475:ASP:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:542:PHE:CE2	1:J:997:VAL:HG12	2.53	0.43
2:B:385:TYR:HB2	2:B:429:TRP:HD1	1.80	0.43
1:A:893:LYS:O	1:A:957:PHE:HA	2.18	0.43
1:A:1015:HIS:HD1	1:A:1036:THR:HG1	1.63	0.43
1:G:994:ARG:O	1:G:996:ASN:N	2.52	0.43
2:E:595:ARG:NH2	2:F:614:ASP:OD2	2.51	0.43
1:D:872:TYR:HA	1:D:1004:LEU:HD13	1.99	0.43
1:A:789:LEU:HA	1:A:852:TYR:CD1	2.53	0.43
2:E:326:ARG:CZ	2:E:328:PRO:HB3	2.48	0.43
2:F:611:LEU:HD12	2:F:611:LEU:HA	1.87	0.43
1:D:759:GLU:OE1	2:C:516:ARG:NH1	2.52	0.43
1:D:760:PHE:CE1	1:D:771:LEU:HD23	2.53	0.43
2:I:308:THR:HG22	2:I:310:LEU:H	1.84	0.43
2:I:399:ASN:OD1	2:I:400:ASN:N	2.52	0.43
1:J:598:SER:HA	1:J:601:ILE:HG22	2.00	0.43
1:A:416:SER:HB2	1:A:710:ASN:CB	2.48	0.43
2:L:483:LEU:HD23	2:L:522:PHE:HE1	1.83	0.43
2:F:301:ASN:ND2	2:F:308:THR:HA	2.34	0.43
2:F:352:THR:OG1	2:F:353:ASN:N	2.51	0.43
2:F:405:TYR:CD1	2:F:441:ILE:HD11	2.53	0.43
1:D:360:ASP:OD1	1:D:363:TYR:N	2.47	0.43
1:D:513:ASN:HB3	1:D:515:TYR:CE2	2.54	0.43
2:C:291:TYR:HD1	2:C:315:SER:HA	1.83	0.43
2:C:407:VAL:HG21	2:C:554:VAL:HG21	2.01	0.43
1:A:523:TYR:CE2	1:A:627:LEU:HD21	2.52	0.43
2:F:254:ASP:OD1	2:F:254:ASP:N	2.51	0.43
1:D:999:TYR:OH	1:D:1026:ILE:HD13	2.19	0.43
2:I:406:LEU:HD11	2:I:525:VAL:HG11	2.01	0.43
2:I:423:ILE:HG21	2:I:475:ASP:CB	2.48	0.43
2:C:401:TYR:HD1	2:C:404:ILE:HD12	1.84	0.43
2:C:427:LEU:O	2:C:427:LEU:HD23	2.18	0.43
1:A:447:CYS:SG	1:A:450:ASP:HB2	2.59	0.43
2:L:397:ILE:HD11	2:L:486:LEU:HB3	2.01	0.43
2:E:357:PHE:HD1	2:E:375:PHE:HE1	1.66	0.43
2:E:408:GLN:O	2:E:411:ASN:HB3	2.19	0.43
2:F:349:ILE:HG22	2:F:419:GLN:NE2	2.34	0.43
2:H:577:ARG:HA	2:H:580:ARG:HE	1.83	0.43
2:I:468:ILE:O	2:I:472:GLN:HG3	2.19	0.43
1:J:694:ASN:O	1:J:697:PRO:HD2	2.19	0.43
2:C:353:ASN:HA	2:C:442:LYS:HG2	2.01	0.43
2:C:652:THR:CG2	2:C:653:PRO:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:LYS:HD3	1:A:815:LYS:HA	1.83	0.43
1:G:529:MET:O	1:G:533:VAL:HG23	2.19	0.43
1:G:818:CYS:SG	1:G:819:PHE:N	2.92	0.43
1:G:994:ARG:O	1:G:995:ARG:C	2.62	0.43
2:E:330:ILE:HG22	2:E:369:LEU:HB3	1.99	0.43
2:I:567:SER:O	2:I:570:SER:OG	2.33	0.43
2:B:405:TYR:HA	2:B:441:ILE:HD13	1.99	0.43
1:G:523:TYR:OH	1:G:623:ASN:OD1	2.29	0.43
1:G:770:VAL:C	1:G:771:LEU:HD12	2.44	0.43
2:L:648:LEU:HG	2:L:663:TYR:HE1	1.84	0.43
2:K:427:LEU:HD23	2:K:427:LEU:HA	1.83	0.43
2:E:294:LEU:HD23	2:E:311:PHE:CE1	2.54	0.43
2:E:327:LEU:HB2	2:E:371:ILE:O	2.18	0.43
2:E:591:ARG:HG2	2:F:618:HIS:HD2	1.83	0.43
2:E:612:PHE:CE2	2:E:640:LEU:HD22	2.53	0.43
2:F:419:GLN:OE1	2:F:419:GLN:N	2.52	0.43
1:D:345:ASP:O	1:D:349:ASP:HB2	2.19	0.43
1:J:695:ILE:O	1:J:698:TYR:HB2	2.19	0.43
2:C:288:VAL:O	2:C:291:TYR:N	2.32	0.43
1:A:445:TYR:OH	1:A:447:CYS:HB3	2.19	0.43
2:L:250:GLU:OE2	1:J:387:LYS:NZ	2.49	0.43
2:E:296:PRO:HA	2:E:311:PHE:CB	2.48	0.43
2:E:324:LEU:HD22	2:E:373:LEU:O	2.19	0.43
2:E:354:LEU:HD13	2:E:416:ILE:HD11	2.01	0.43
2:E:652:THR:HB	2:E:654:ASP:H	1.84	0.43
1:D:526:ILE:HD11	1:D:851:ILE:HG21	2.01	0.43
2:H:382:LEU:O	2:H:434:ILE:HG22	2.19	0.43
2:I:260:ASN:O	2:I:263:ARG:NH1	2.52	0.43
2:I:355:ILE:HG12	2:I:443:LEU:O	2.19	0.43
1:A:853:CYS:HB3	1:A:858:LEU:HD12	2.01	0.43
2:L:564:TYR:O	2:L:567:SER:OG	2.27	0.42
2:K:346:TRP:CZ2	2:K:421:LEU:HD13	2.54	0.42
2:E:654:ASP:O	2:E:656:LEU:N	2.51	0.42
2:F:504:LEU:HA	2:F:507:ILE:HG12	2.01	0.42
2:F:588:ILE:HG21	2:F:609:ILE:HD11	2.01	0.42
2:H:635:ARG:HG2	2:H:639:LYS:HE2	2.00	0.42
2:I:435:THR:O	2:I:440:ARG:HB2	2.19	0.42
1:J:675:ILE:O	1:J:675:ILE:HG13	2.18	0.42
1:A:961:TYR:CD2	1:A:989:THR:HG21	2.54	0.42
1:A:1020:ASP:O	1:A:1024:ILE:HG13	2.19	0.42
2:L:338:LYS:O	2:L:342:ILE:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:421:LEU:HB3	2:L:448:PHE:HZ	1.84	0.42
1:D:529:MET:O	1:D:533:VAL:HG23	2.19	0.42
2:H:671:GLU:OE2	2:H:675:ARG:NH2	2.50	0.42
2:I:408:GLN:NE2	2:I:441:ILE:H	2.16	0.42
1:A:539:ASP:O	1:A:1000:ARG:NH1	2.53	0.42
1:A:946:ARG:NH1	1:A:955:VAL:HG13	2.34	0.42
1:G:343:TYR:HA	1:G:344:PRO:HA	1.85	0.42
1:G:992:LEU:O	1:G:992:LEU:HD12	2.18	0.42
2:K:389:PHE:CE2	2:K:429:TRP:HZ3	2.34	0.42
2:E:270:ASN:OD1	2:E:271:LEU:N	2.52	0.42
2:E:629:ASP:O	2:E:633:VAL:HG23	2.19	0.42
2:C:581:LEU:HD21	2:C:640:LEU:HD22	2.01	0.42
2:C:584:LYS:HE2	2:C:674:PHE:CE2	2.55	0.42
2:C:643:GLY:C	2:C:644:ILE:HG13	2.44	0.42
2:B:640:LEU:HD11	2:B:670:ILE:HD12	2.01	0.42
1:G:944:ILE:O	1:G:957:PHE:N	2.52	0.42
2:L:476:TYR:O	2:L:529:LEU:HD23	2.20	0.42
2:L:619:GLN:HE22	2:L:632:HIS:HB3	1.84	0.42
2:K:426:THR:OG1	2:K:447:ASN:N	2.52	0.42
2:E:265:ASP:O	2:E:268:LYS:HB3	2.20	0.42
2:E:549:ASP:O	2:E:552:PHE:HB2	2.20	0.42
2:F:401:TYR:HA	2:F:404:ILE:HD12	2.01	0.42
1:D:798:ASP:OD1	1:D:802:GLU:N	2.52	0.42
1:D:1019:ASN:O	1:D:1023:HIS:ND1	2.53	0.42
2:I:620:VAL:HG12	2:I:621:ASP:O	2.20	0.42
1:J:471:ASN:OD1	1:J:473:TYR:N	2.50	0.42
2:C:257:PHE:CZ	2:B:579:PHE:HD2	2.37	0.42
2:C:590:GLY:O	2:C:595:ARG:NH1	2.52	0.42
2:C:592:ILE:CD1	2:B:653:PRO:HG3	2.49	0.42
2:B:591:ARG:O	2:B:595:ARG:HG3	2.19	0.42
1:G:470:ILE:HD12	1:G:470:ILE:H	1.84	0.42
2:L:601:SER:HB2	2:L:610:ILE:HD12	2.02	0.42
2:I:280:SER:HB2	2:I:283:VAL:CG1	2.46	0.42
1:J:537:LEU:HD23	1:J:537:LEU:O	2.20	0.42
1:J:791:GLY:O	1:J:851:ILE:HG13	2.19	0.42
1:J:992:LEU:HD12	1:J:992:LEU:O	2.20	0.42
1:J:997:VAL:HG23	1:J:998:VAL:N	2.35	0.42
1:A:464:ILE:HA	1:A:477:PRO:HB2	2.02	0.42
1:G:902:LYS:H	1:G:905:THR:HG1	1.61	0.42
2:L:578:LEU:O	2:L:582:VAL:HG23	2.20	0.42
2:L:652:THR:CG2	2:L:653:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:556:MET:HE3	1:J:556:MET:HB2	1.83	0.42
1:J:746:PHE:O	1:J:749:ILE:HG13	2.20	0.42
1:G:959:ASP:OD2	1:G:1069:ILE:HD11	2.20	0.42
2:L:250:GLU:O	2:L:251:ARG:HD3	2.19	0.42
2:K:577:ARG:HH12	1:J:370:MET:CG	2.28	0.42
2:K:591:ARG:HB2	2:K:594:SER:CB	2.50	0.42
2:E:426:THR:OG1	2:E:447:ASN:HB2	2.19	0.42
2:E:633:VAL:HG11	2:F:583:ASN:HD21	1.85	0.42
2:F:242:LEU:O	2:F:246:LEU:HG	2.20	0.42
2:F:386:ASP:O	2:F:390:VAL:HB	2.20	0.42
2:F:484:PHE:CD2	2:F:507:ILE:HD12	2.55	0.42
2:F:487:SER:O	2:F:490:ILE:HG22	2.19	0.42
1:D:524:ARG:HG3	1:D:557:MET:HE3	2.01	0.42
1:D:962:VAL:HG21	1:D:994:ARG:HB3	2.01	0.42
2:H:586:ASN:OD1	2:I:613:TYR:OH	2.10	0.42
2:B:484:PHE:CD1	2:B:488:ILE:HD13	2.55	0.42
1:A:534:VAL:HG12	1:A:865:VAL:HB	2.00	0.42
1:G:475:VAL:HA	1:G:476:PRO:HD3	1.89	0.42
2:L:577:ARG:NE	2:L:641:ASP:OD2	2.45	0.42
2:K:589:PHE:CG	2:K:613:TYR:CD2	3.08	0.42
2:F:521:LYS:O	2:F:525:VAL:HG23	2.19	0.42
1:D:645:ASN:O	1:D:649:GLY:HA3	2.20	0.42
2:I:589:PHE:CD1	2:I:610:ILE:HG23	2.55	0.42
1:J:634:GLU:O	1:J:637:THR:HG22	2.20	0.42
2:L:327:LEU:HB2	2:L:371:ILE:HG23	2.01	0.42
2:E:294:LEU:HD12	2:E:294:LEU:H	1.84	0.42
2:F:610:ILE:O	2:F:613:TYR:HB3	2.20	0.42
2:I:629:ASP:OD1	2:I:630:LEU:N	2.53	0.42
1:A:750:ARG:NH1	1:A:843:PRO:O	2.53	0.42
2:L:652:THR:HB	2:L:654:ASP:OD1	2.19	0.42
2:K:502:TYR:CD1	2:K:506:GLU:OE1	2.73	0.42
2:E:578:LEU:O	2:E:582:VAL:HG22	2.20	0.42
2:F:404:ILE:HG12	2:F:554:VAL:HG22	2.02	0.42
1:D:556:MET:HE3	1:D:556:MET:HB2	1.77	0.42
1:D:639:ASN:HB3	1:D:641:ASN:ND2	2.35	0.42
1:J:509:PRO:HD3	1:J:827:TYR:HD1	1.84	0.42
1:J:813:ASN:HA	1:J:814:PRO:HD3	1.86	0.42
2:B:426:THR:OG1	2:B:447:ASN:N	2.52	0.42
1:A:471:ASN:OD1	1:A:473:TYR:N	2.49	0.42
1:G:448:LEU:O	1:G:452:ARG:HG2	2.20	0.41
1:G:637:THR:HG23	1:G:640:HIS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:261:ASN:OD1	2:L:262:ILE:HG12	2.20	0.41
2:K:401:TYR:HA	2:K:404:ILE:HD12	2.02	0.41
2:E:407:VAL:HG11	2:E:554:VAL:HG11	2.02	0.41
2:I:263:ARG:NH1	2:I:263:ARG:HB3	2.35	0.41
2:B:324:LEU:HD11	2:B:361:PHE:HZ	1.84	0.41
1:A:756:LEU:HD21	1:A:789:LEU:HD22	2.02	0.41
2:K:273:ILE:HG13	2:K:274:LEU:N	2.34	0.41
2:F:597:ASP:OD1	2:F:598:ILE:N	2.52	0.41
1:D:924:ASP:OD1	1:D:924:ASP:N	2.50	0.41
2:H:629:ASP:O	2:H:633:VAL:HG23	2.20	0.41
1:J:864:SER:O	1:J:867:THR:HG22	2.21	0.41
1:J:876:PHE:CD1	1:J:895:LEU:HB2	2.56	0.41
1:A:509:PRO:HD3	1:A:827:TYR:HD2	1.84	0.41
1:A:994:ARG:O	1:A:995:ARG:C	2.64	0.41
1:G:821:TRP:C	1:G:822:LEU:HD12	2.46	0.41
2:L:324:LEU:HD21	2:L:372:CYS:HB3	2.02	0.41
2:L:430:ARG:C	2:L:432:VAL:H	2.28	0.41
2:F:429:TRP:HE1	2:F:485:ASN:HB2	1.85	0.41
1:D:920:LEU:HD13	1:D:920:LEU:HA	1.92	0.41
2:I:564:TYR:O	2:I:567:SER:OG	2.33	0.41
1:J:634:GLU:CD	1:J:642:ILE:HA	2.45	0.41
2:L:563:GLU:OE2	2:K:442:LYS:NZ	2.34	0.41
2:L:586:ASN:HB3	2:K:617:PHE:CD2	2.56	0.41
2:L:597:ASP:HB3	2:L:599:ASN:O	2.20	0.41
2:K:368:ASP:OD1	2:K:370:SER:OG	2.38	0.41
2:K:543:LEU:HG	2:K:547:PHE:CE2	2.55	0.41
2:F:475:ASP:OD1	2:F:476:TYR:N	2.54	0.41
2:F:519:ASP:O	2:F:522:PHE:N	2.54	0.41
2:I:291:TYR:HD1	2:I:315:SER:HA	1.84	0.41
2:I:484:PHE:CD2	2:I:507:ILE:HD12	2.56	0.41
1:J:553:LEU:O	1:J:557:MET:HG3	2.19	0.41
1:J:994:ARG:HG3	1:J:995:ARG:N	2.35	0.41
2:C:392:PHE:HB3	2:C:393:PRO:HD3	2.01	0.41
1:G:810:LYS:HE3	1:G:821:TRP:CZ2	2.55	0.41
2:L:330:ILE:HG22	2:L:332:LYS:H	1.85	0.41
2:F:619:GLN:OE1	2:F:632:HIS:ND1	2.53	0.41
2:F:630:LEU:O	2:F:634:LEU:HD12	2.21	0.41
1:D:677:GLY:C	1:D:678:ILE:HG13	2.45	0.41
2:H:294:LEU:HD23	2:H:311:PHE:CD2	2.55	0.41
2:H:406:LEU:HG	2:H:547:PHE:CZ	2.56	0.41
2:C:291:TYR:CE2	2:C:374:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:416:ILE:HG22	2:L:421:LEU:O	2.21	0.41
2:L:469:GLU:O	2:L:473:GLN:HG2	2.21	0.41
1:D:454:GLN:HE22	1:A:458:GLY:HA3	1.86	0.41
1:D:476:PRO:HA	1:D:477:PRO:HD3	1.94	0.41
1:D:556:MET:HE1	1:D:1025:ASN:O	2.20	0.41
1:D:764:ILE:H	1:D:764:ILE:HG13	1.73	0.41
2:H:460:VAL:HG22	1:J:560:SER:HA	2.02	0.41
2:H:473:GLN:O	2:H:476:TYR:HB2	2.21	0.41
2:H:589:PHE:CD1	2:H:613:TYR:HD2	2.39	0.41
1:J:564:ILE:HD12	1:J:564:ILE:H	1.85	0.41
1:A:739:LEU:HD12	1:A:847:PRO:HB2	2.01	0.41
2:E:652:THR:N	2:E:653:PRO:HA	2.36	0.41
2:F:550:LYS:O	2:F:553:MET:HB3	2.20	0.41
2:H:578:LEU:O	2:H:582:VAL:HG22	2.20	0.41
2:H:630:LEU:O	2:H:634:LEU:HD12	2.20	0.41
2:I:521:LYS:HD3	2:I:547:PHE:HB3	2.03	0.41
2:B:403:TRP:O	2:B:407:VAL:HG23	2.21	0.41
2:B:436:GLY:C	2:B:438:PRO:HD2	2.46	0.41
1:A:553:LEU:O	1:A:557:MET:HG3	2.20	0.41
1:G:509:PRO:HD3	1:G:827:TYR:CD1	2.55	0.41
1:G:517:ASN:O	1:G:520:ILE:HG13	2.21	0.41
1:G:894:LEU:H	1:G:894:LEU:HD12	1.86	0.41
2:I:345:ILE:HG13	2:I:346:TRP:N	2.34	0.41
1:J:1035:ASP:OD1	1:J:1037:ALA:N	2.53	0.41
2:C:352:THR:O	2:C:353:ASN:HB2	2.21	0.41
2:B:468:ILE:O	2:B:472:GLN:HG3	2.21	0.41
1:A:444:ASP:HB3	1:A:801:ASN:ND2	2.36	0.41
1:A:650:LEU:HD13	1:A:728:VAL:HG11	2.01	0.41
1:G:813:ASN:HA	1:G:814:PRO:HD3	1.92	0.41
2:L:395:PHE:HA	2:L:396:PRO:HD3	1.75	0.41
2:L:552:PHE:HE1	2:K:544:THR:HG21	1.84	0.41
2:E:288:VAL:HG11	2:E:366:PHE:CE1	2.56	0.41
2:F:397:ILE:HG23	2:F:397:ILE:O	2.21	0.41
2:H:423:ILE:N	2:H:475:ASP:OD2	2.46	0.41
2:I:654:ASP:OD1	2:I:655:GLU:N	2.53	0.41
2:C:406:LEU:HD12	2:C:522:PHE:CE1	2.56	0.41
2:B:450:ASP:CG	2:B:454:ASN:HD21	2.28	0.41
2:B:549:ASP:O	2:B:552:PHE:HB2	2.21	0.41
2:B:629:ASP:O	2:B:633:VAL:HG23	2.21	0.41
1:A:550:LEU:HB2	1:A:570:PHE:HE2	1.85	0.41
1:A:946:ARG:HG3	1:A:957:PHE:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:994:ARG:O	1:G:997:VAL:HG22	2.20	0.41
2:E:416:ILE:HG22	2:E:421:LEU:O	2.20	0.41
2:F:391:ASN:CG	2:F:392:PHE:H	2.29	0.41
1:D:741:LEU:HB2	1:D:746:PHE:CE2	2.55	0.41
1:D:863:PHE:HD1	1:D:867:THR:HG21	1.86	0.41
2:I:589:PHE:CG	2:I:590:GLY:N	2.89	0.41
1:J:471:ASN:HB3	1:J:474:GLU:HB3	2.03	0.41
1:J:963:VAL:CG1	1:J:993:VAL:HA	2.50	0.41
2:C:640:LEU:HD11	2:C:670:ILE:HD12	2.03	0.41
2:B:652:THR:OG1	2:B:654:ASP:N	2.54	0.41
1:G:913:PHE:HZ	1:G:1020:ASP:HA	1.86	0.40
2:K:291:TYR:HB3	2:K:313:VAL:CG2	2.46	0.40
2:F:508:THR:HA	2:F:509:PRO:HD3	1.96	0.40
2:F:584:LYS:O	2:F:587:CYS:HB3	2.21	0.40
1:J:979:LEU:HD12	1:J:979:LEU:H	1.86	0.40
1:G:575:LYS:O	1:G:578:THR:HG22	2.21	0.40
1:G:739:LEU:HD12	1:G:847:PRO:HB2	2.02	0.40
1:G:913:PHE:CZ	1:G:1020:ASP:HA	2.56	0.40
2:L:589:PHE:CD1	2:L:610:ILE:HG23	2.57	0.40
2:F:548:TYR:HD1	2:F:548:TYR:HA	1.71	0.40
2:H:405:TYR:HD1	2:H:441:ILE:CD1	2.34	0.40
1:J:641:ASN:O	1:J:642:ILE:HG13	2.20	0.40
2:K:339:ILE:HG23	2:K:360:ILE:HD13	2.02	0.40
2:E:353:ASN:O	2:E:442:LYS:HA	2.21	0.40
2:F:291:TYR:HB3	2:F:313:VAL:HG13	2.03	0.40
1:D:539:ASP:O	1:D:1000:ARG:NH1	2.52	0.40
2:I:291:TYR:CE2	2:I:374:VAL:HG21	2.56	0.40
2:I:678:THR:O	2:I:679:GLN:HB2	2.22	0.40
1:J:526:ILE:HA	1:J:527:PRO:HD3	1.95	0.40
1:J:778:LEU:HD22	1:J:784:ILE:HD11	2.04	0.40
1:J:839:LYS:HD3	1:J:842:TYR:CE2	2.56	0.40
1:J:961:TYR:CE2	1:J:989:THR:HG21	2.55	0.40
2:C:434:ILE:HG13	2:C:440:ARG:O	2.22	0.40
2:C:487:SER:OG	2:C:515:MET:SD	2.71	0.40
1:A:732:PRO:O	1:A:787:TYR:OH	2.18	0.40
1:G:507:LEU:HD12	1:G:517:ASN:HB3	2.03	0.40
1:G:739:LEU:CD1	1:G:847:PRO:HB2	2.52	0.40
2:L:429:TRP:HE1	2:L:485:ASN:CB	2.34	0.40
2:E:335:ASN:HA	2:E:336:PRO:HD2	1.90	0.40
2:F:396:PRO:O	2:F:397:ILE:C	2.64	0.40
1:D:634:GLU:OE2	1:D:644:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:821:TRP:C	1:D:822:LEU:HD12	2.46	0.40
2:I:352:THR:O	2:I:353:ASN:HB2	2.21	0.40
2:I:387:TYR:CE2	2:I:434:ILE:HD13	2.57	0.40
1:J:824:PHE:CD2	1:J:829:VAL:HG22	2.56	0.40
1:J:1002:VAL:HA	1:J:1005:LEU:HD12	2.04	0.40
2:C:231:TYR:O	2:C:233:LEU:HG	2.22	0.40
2:B:584:LYS:HD2	1:A:378:LEU:HD21	2.02	0.40
1:A:815:LYS:C	1:A:817:ASN:H	2.28	0.40
1:G:731:LEU:HA	1:G:732:PRO:HD3	1.84	0.40
2:E:400:ASN:O	2:E:404:ILE:HG12	2.21	0.40
2:F:234:TYR:HA	1:D:377:LEU:HD12	2.03	0.40
1:D:824:PHE:CD2	1:D:829:VAL:HG22	2.56	0.40
2:H:416:ILE:HG21	2:H:423:ILE:HG12	2.03	0.40
2:I:399:ASN:O	2:I:402:LEU:HB2	2.22	0.40
2:I:419:GLN:C	2:I:421:LEU:H	2.30	0.40
1:J:343:TYR:HA	1:J:344:PRO:HA	1.82	0.40
2:C:233:LEU:O	1:A:377:LEU:HD13	2.22	0.40
2:C:653:PRO:HB3	2:B:592:ILE:HD12	2.04	0.40
1:A:899:GLU:CD	1:A:946:ARG:HE	2.29	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	687/776 (88%)	652 (95%)	34 (5%)	1 (0%)	48	79
1	D	663/776 (85%)	622 (94%)	39 (6%)	2 (0%)	36	67
1	G	665/776 (86%)	631 (95%)	32 (5%)	2 (0%)	36	67
1	J	661/776 (85%)	624 (94%)	35 (5%)	2 (0%)	36	67
2	B	421/465 (90%)	397 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	440/465 (95%)	417 (95%)	23 (5%)	0	100	100
2	E	408/465 (88%)	384 (94%)	24 (6%)	0	100	100
2	F	438/465 (94%)	415 (95%)	22 (5%)	1 (0%)	43	73
2	H	416/465 (90%)	394 (95%)	21 (5%)	1 (0%)	43	73
2	I	429/465 (92%)	404 (94%)	24 (6%)	1 (0%)	43	73
2	K	423/465 (91%)	408 (96%)	15 (4%)	0	100	100
2	L	437/465 (94%)	416 (95%)	21 (5%)	0	100	100
All	All	6088/6824 (89%)	5764 (95%)	314 (5%)	10 (0%)	43	73

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	455	ILE
1	G	616	ARG
2	F	397	ILE
1	A	660	CYS
1	G	715	THR
2	H	438	PRO
1	J	371	PRO
2	I	397	ILE
1	D	678	ILE
1	D	344	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/712 (72%)	487 (96%)	22 (4%)	26	50
1	D	465/712 (65%)	456 (98%)	9 (2%)	50	66
1	G	469/712 (66%)	456 (97%)	13 (3%)	38	58
1	J	462/712 (65%)	448 (97%)	14 (3%)	36	57
2	B	332/444 (75%)	323 (97%)	9 (3%)	39	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	352/444 (79%)	350 (99%)	2 (1%)	78	79
2	E	297/444 (67%)	293 (99%)	4 (1%)	61	71
2	F	348/444 (78%)	340 (98%)	8 (2%)	44	63
2	H	307/444 (69%)	300 (98%)	7 (2%)	44	63
2	I	331/444 (74%)	327 (99%)	4 (1%)	63	72
2	K	328/444 (74%)	321 (98%)	7 (2%)	47	64
2	L	375/444 (84%)	369 (98%)	6 (2%)	55	68
All	All	4575/6400 (72%)	4470 (98%)	105 (2%)	44	63

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	475	VAL
1	G	513	ASN
1	G	520	ILE
1	G	521	GLN
1	G	524	ARG
1	G	617	ASN
1	G	636	GLN
1	G	896	THR
1	G	907	VAL
1	G	990	LYS
1	G	998	VAL
1	G	1015	HIS
1	G	1025	ASN
2	L	295	VAL
2	L	307	LYS
2	L	346	TRP
2	L	434	ILE
2	L	472	GLN
2	L	497	THR
2	K	273	ILE
2	K	295	VAL
2	K	429	TRP
2	K	503	ARG
2	K	641	ASP
2	K	648	LEU
2	K	660	ILE
2	E	360	ILE
2	E	434	ILE

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Mol	Chain	Res	Type
2	E	504	LEU
2	E	641	ASP
2	F	228	LEU
2	F	295	VAL
2	F	306	ASN
2	F	327	LEU
2	F	448	PHE
2	F	543	LEU
2	F	619	GLN
2	F	665	GLU
1	D	475	VAL
1	D	485	THR
1	D	624	ARG
1	D	640	HIS
1	D	678	ILE
1	D	704	LYS
1	D	706	VAL
1	D	764	ILE
1	D	920	LEU
2	H	295	VAL
2	H	309	THR
2	H	369	LEU
2	H	397	ILE
2	H	441	ILE
2	H	516	ARG
2	H	658	CYS
2	I	284	ILE
2	I	287	ILE
2	I	295	VAL
2	I	510	GLN
1	J	431	TYR
1	J	475	VAL
1	J	513	ASN
1	J	524	ARG
1	J	651	GLU
1	J	675	ILE
1	J	764	ILE
1	J	778	LEU
1	J	781	THR
1	J	851	ILE
1	J	894	LEU
1	J	906	LEU

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Mol	Chain	Res	Type
1	J	957	PHE
1	J	993	VAL
2	C	295	VAL
2	C	639	LYS
2	B	279	SER
2	B	295	VAL
2	B	309	THR
2	B	369	LEU
2	B	434	ILE
2	B	504	LEU
2	B	537	LYS
2	B	619	GLN
2	B	658	CYS
1	A	415	SER
1	A	421	LEU
1	A	428	LEU
1	A	431	TYR
1	A	470	ILE
1	A	475	VAL
1	A	513	ASN
1	A	524	ARG
1	A	614	ILE
1	A	675	ILE
1	A	764	ILE
1	A	771	LEU
1	A	879	TYR
1	A	894	LEU
1	A	923	ILE
1	A	944	ILE
1	A	948	GLU
1	A	957	PHE
1	A	982	ASP
1	A	990	LYS
1	A	993	VAL
1	A	1094	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	394	GLN
1	G	521	GLN
1	G	1007	GLN

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Mol	Chain	Res	Type
2	L	238	GLN
2	L	472	GLN
2	L	618	HIS
2	K	425	ASN
2	K	494	ASN
2	E	411	ASN
2	E	473	GLN
2	E	485	ASN
2	E	583	ASN
2	E	632	HIS
2	F	353	ASN
2	F	411	ASN
2	F	583	ASN
2	F	618	HIS
2	F	619	GLN
1	D	629	GLN
1	D	640	HIS
1	D	801	ASN
2	H	353	ASN
2	H	417	HIS
2	H	472	GLN
2	H	485	ASN
2	I	249	ASN
2	I	353	ASN
2	I	411	ASN
1	J	521	GLN
1	J	623	ASN
1	J	754	ASN
1	J	1032	GLN
2	C	623	ASN
2	C	657	ASN
2	B	270	ASN
2	B	289	GLN
2	B	420	ASN
2	B	445	HIS
2	B	485	ASN
2	B	489	ASN
2	B	632	HIS
1	A	348	ASN
1	A	418	ASN
1	A	800	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	701/776 (90%)	0.52	26 (3%)	45	31	86, 110, 163, 211	0
1	D	683/776 (88%)	0.53	24 (3%)	47	33	89, 128, 188, 213	0
1	G	683/776 (88%)	0.55	30 (4%)	39	28	81, 108, 195, 233	0
1	J	681/776 (87%)	0.56	21 (3%)	51	35	91, 118, 146, 174	0
2	B	429/465 (92%)	0.51	12 (2%)	55	38	66, 111, 155, 177	0
2	C	444/465 (95%)	0.47	11 (2%)	58	40	72, 114, 151, 172	0
2	E	414/465 (89%)	0.45	18 (4%)	40	28	67, 109, 139, 161	0
2	F	442/465 (95%)	0.52	10 (2%)	61	42	86, 104, 125, 136	0
2	H	420/465 (90%)	0.46	10 (2%)	59	41	73, 103, 141, 160	0
2	I	437/465 (93%)	0.46	12 (2%)	56	38	80, 112, 146, 161	0
2	K	431/465 (92%)	0.50	11 (2%)	57	39	80, 116, 151, 168	0
2	L	441/465 (94%)	0.41	5 (1%)	78	56	80, 99, 127, 156	0
All	All	6206/6824 (90%)	0.50	190 (3%)	51	35	66, 112, 160, 233	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	HIS	5.8
1	J	661	ASP	4.9
1	A	1027	ASN	4.5
1	G	434	THR	4.1
1	J	536	CYS	4.1
1	A	995	ARG	4.0
1	J	1027	ASN	3.9
2	I	446	CYS	3.8
1	A	661	ASP	3.6
1	G	1036	THR	3.6
2	C	346	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	940	ALA	3.4
2	K	277	PHE	3.4
2	H	428	ASN	3.4
2	F	351	CYS	3.3
1	D	1027	ASN	3.3
2	F	414	ASN	3.3
1	A	957	PHE	3.2
2	B	225	MET	3.2
2	F	513	ASP	3.2
2	E	254	ASP	3.2
2	I	621	ASP	3.1
2	F	599	ASN	3.1
1	G	365	LEU	3.1
2	C	574	GLU	3.0
2	E	461	VAL	3.0
1	G	982	ASP	3.0
2	E	490	ILE	3.0
2	E	458	ASP	3.0
1	D	821	TRP	2.9
2	B	311	PHE	2.9
1	D	457	SER	2.9
2	B	487	SER	2.9
1	G	615	LYS	2.9
2	F	597	ASP	2.9
2	F	230	GLN	2.9
2	I	448	PHE	2.9
2	C	658	CYS	2.9
1	G	661	ASP	2.8
1	A	436	TYR	2.8
1	G	456	THR	2.8
1	A	993	VAL	2.8
2	B	229	LEU	2.8
1	D	456	THR	2.8
2	H	651	VAL	2.8
2	L	621	ASP	2.8
1	D	940	ALA	2.8
2	E	377	TYR	2.7
2	H	277	PHE	2.7
1	A	996	ASN	2.7
1	D	372	TYR	2.7
1	G	455	ILE	2.7
1	J	434	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	1019	ASN	2.7
1	G	1035	ASP	2.7
2	F	454	ASN	2.7
1	J	448	LEU	2.7
1	G	1033	ILE	2.7
1	J	1031	ASN	2.7
1	G	979	LEU	2.7
1	G	1031	ASN	2.6
1	J	882	ASN	2.6
1	J	762	GLY	2.6
2	E	439	GLY	2.6
2	C	628	MET	2.6
1	D	853	CYS	2.6
2	H	484	PHE	2.6
2	E	493	SER	2.6
1	A	921	CYS	2.5
2	B	405	TYR	2.5
1	J	1045	ARG	2.5
2	H	447	ASN	2.5
2	I	391	ASN	2.5
2	E	252	SER	2.5
2	I	563	GLU	2.5
1	D	1071	ASP	2.5
1	G	1020	ASP	2.5
2	F	563	GLU	2.4
2	L	600	TRP	2.4
2	I	643	GLY	2.4
1	A	1020	ASP	2.4
1	G	660	CYS	2.4
2	L	446	CYS	2.4
1	G	993	VAL	2.4
1	A	426	PHE	2.4
1	G	606	GLU	2.4
1	J	888	ALA	2.4
2	L	643	GLY	2.4
2	E	548	TYR	2.4
1	D	915	SER	2.4
2	K	459	THR	2.4
1	J	1095	LEU	2.4
1	D	716	CYS	2.4
2	C	446	CYS	2.4
2	I	380	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	485	THR	2.4
1	J	512	ASP	2.4
2	K	405	TYR	2.4
1	D	624	ARG	2.4
1	A	940	ALA	2.4
1	D	676	SER	2.4
1	D	681	THR	2.4
2	F	514	ASP	2.4
2	H	440	ARG	2.4
1	G	954	GLY	2.3
2	B	446	CYS	2.3
1	A	340	MET	2.3
1	D	759	GLU	2.3
1	A	924	ASP	2.3
2	E	532	ASP	2.3
1	J	760	PHE	2.3
1	J	535	GLY	2.3
2	L	522	PHE	2.3
2	I	303	ASP	2.3
2	E	651	VAL	2.3
2	B	460	VAL	2.3
1	G	493	ASN	2.3
1	G	867	THR	2.3
2	E	652	THR	2.3
2	C	618	HIS	2.3
1	J	1010	CYS	2.3
1	A	536	CYS	2.3
1	G	462	SER	2.3
2	E	623	ASN	2.2
2	K	231	GLU	2.2
1	D	995	ARG	2.2
1	G	873	ASP	2.2
1	D	979	LEU	2.2
2	K	318	ASP	2.2
1	G	925	HIS	2.2
1	D	418	ASN	2.2
2	I	371	ILE	2.2
1	G	888	ALA	2.2
1	A	693	GLN	2.2
1	D	951	GLU	2.2
2	E	552	PHE	2.2
1	A	742	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	326	ARG	2.2
2	B	364	THR	2.2
1	A	607	ASP	2.2
1	D	365	LEU	2.2
1	A	379	SER	2.2
2	H	408	GLN	2.2
2	I	517	GLN	2.2
1	G	895	LEU	2.2
1	D	661	ASP	2.1
1	J	379	SER	2.1
2	E	455	ASP	2.1
2	K	397	ILE	2.1
1	G	1012	PHE	2.1
1	A	389	GLU	2.1
1	A	434	THR	2.1
1	G	641	ASN	2.1
1	J	773	SER	2.1
1	D	909	ILE	2.1
1	A	1071	ASP	2.1
2	H	522	PHE	2.1
1	G	914	VAL	2.1
2	H	257	PHE	2.1
2	C	368	ASP	2.1
2	K	401	TYR	2.1
2	C	436	GLY	2.1
2	C	522	PHE	2.1
2	K	246	LEU	2.1
2	K	331	ASP	2.1
1	G	601	ILE	2.1
1	A	909	ILE	2.1
1	A	1065	ASN	2.1
2	E	277	PHE	2.1
2	I	271	LEU	2.1
2	C	681	HIS	2.1
1	J	792	TYR	2.1
1	G	579	ASP	2.1
1	A	612	GLU	2.1
2	K	341	LYS	2.1
1	J	610	SER	2.1
2	B	484	PHE	2.1
2	K	226	HIS	2.0
2	E	445	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	430	ARG	2.0
2	H	254	ASP	2.0
2	B	277	PHE	2.0
2	F	229	LEU	2.0
1	A	823	MET	2.0
1	D	949	GLU	2.0
2	C	437	ASP	2.0
1	D	742	LEU	2.0
2	E	444	SER	2.0
2	B	289	GLN	2.0
1	J	731	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.