



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 4B8C / pdb_00004b8c
Title : nuclease module of the yeast Ccr4-Not complex
Authors : Basquin, J.; Conti, E.
Deposited on : 2012-08-26
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

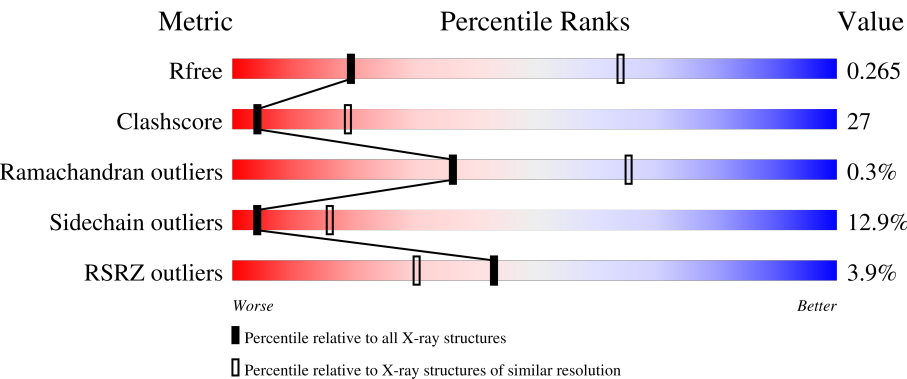
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	288	2% 57%28%6% • 7%
1	C	288	2% 56%30%6% • 7%
1	E	288	3% 59%27%6% • 7%
1	F	288	2% 60%26%6% • 7%
2	B	249	2% 61%32% • 6%

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Mol	Chain	Length	Quality of chain
2	G	249	5%59%33%6%
2	H	249	4%59%33%6%
2	I	249	4%60%31%6%
3	D	727	2%16%22%6%56%
3	J	727	2%10%13%5%71%
3	K	727	2%17%21%6%56%
3	L	727	2%10%13%6%71%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24298 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 POLY(A) RIBONUCLEASE POP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2170	1409	346	404	11			
1	C	267	Total	C	N	O	S	0	0	0
			2174	1412	347	404	11			
1	E	267	Total	C	N	O	S	0	0	0
			2174	1411	347	405	11			
1	F	267	Total	C	N	O	S	0	0	0
			2170	1409	346	404	11			

- Molecule 2 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			
2	G	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			
2	H	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			
2	I	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	752	ARG	-	expression tag	UNP P25655
B	753	SER	-	expression tag	UNP P25655
B	754	MET	-	expression tag	UNP P25655
G	752	ARG	-	expression tag	UNP P25655
G	753	SER	-	expression tag	UNP P25655
G	754	MET	-	expression tag	UNP P25655
H	752	ARG	-	expression tag	UNP P25655
H	753	SER	-	expression tag	UNP P25655

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Chain	Residue	Modelled	Actual	Comment	Reference
H	754	MET	-	expression tag	UNP P25655
I	752	ARG	-	expression tag	UNP P25655
I	753	SER	-	expression tag	UNP P25655
I	754	MET	-	expression tag	UNP P25655

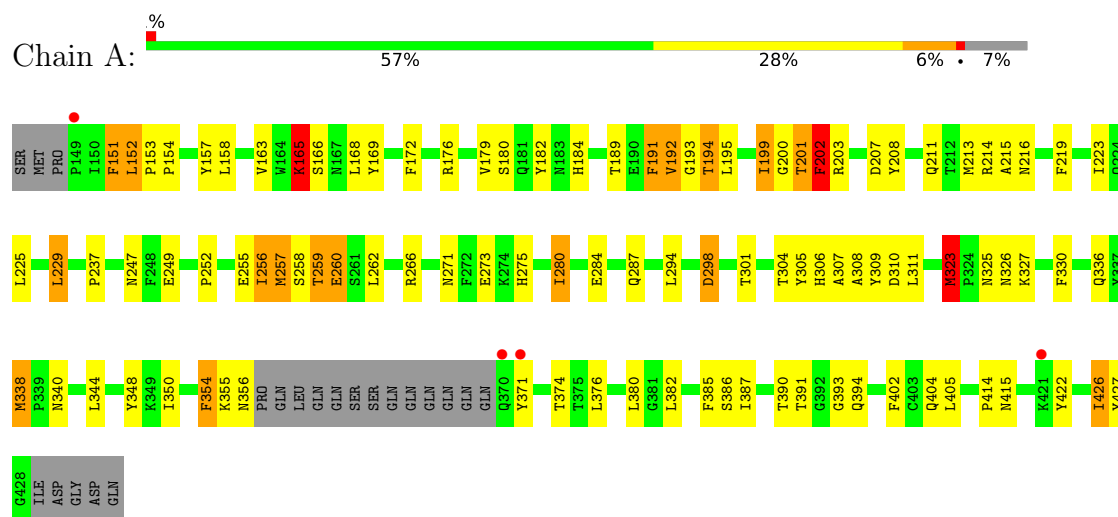
- Molecule 3 is a protein called GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	318	Total	C	N	O	S	0	0	0
			2456	1599	387	459	11			
3	J	210	Total	C	N	O	S	0	0	0
			1604	1034	266	298	6			
3	K	318	Total	C	N	O	S	0	0	0
			2470	1608	392	459	11			
3	L	210	Total	C	N	O	S	0	0	0
			1604	1034	266	298	6			

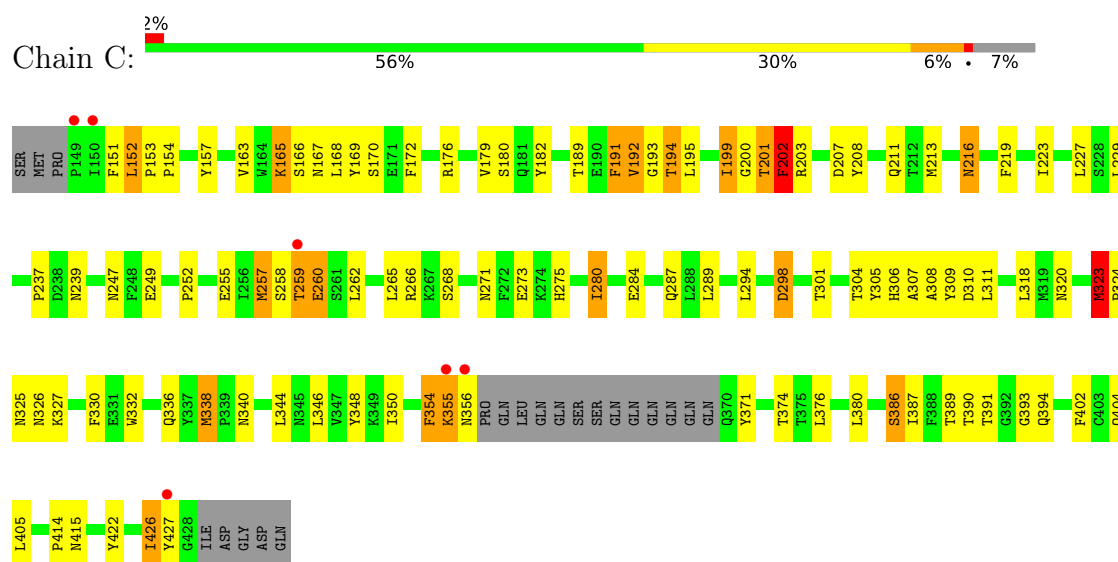
3 Residue-property plots

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: POLY(A) RIBONUCLEASE POP2

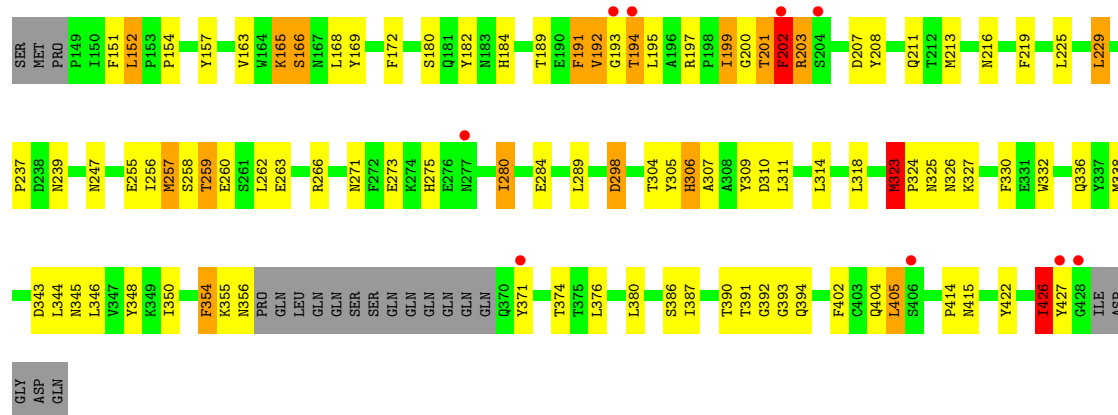


• Molecule 1: POLY(A) RIBONUCLEASE POP2

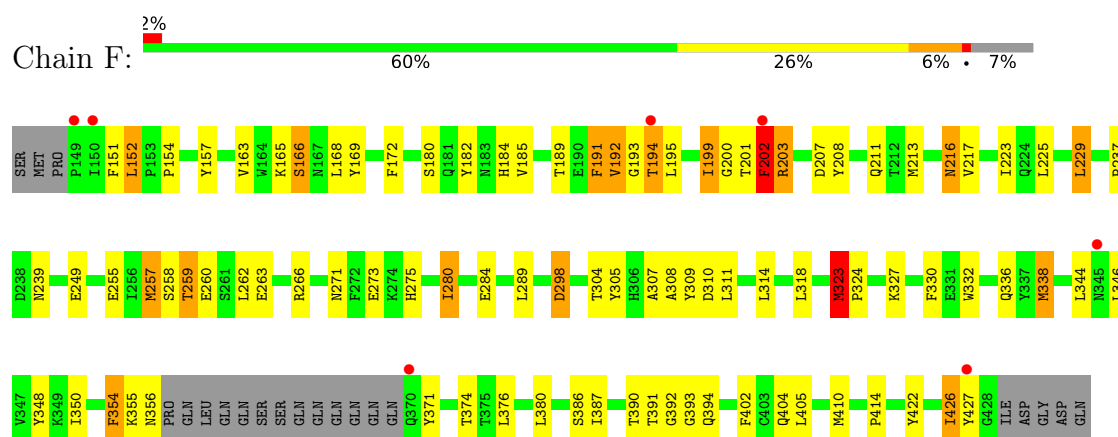


• Molecule 1: POLY(A) RIBONUCLEASE POP2

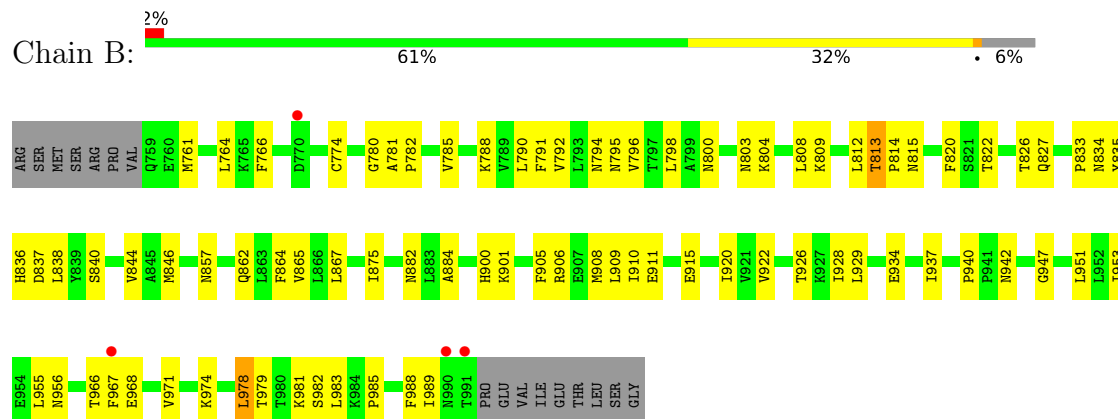




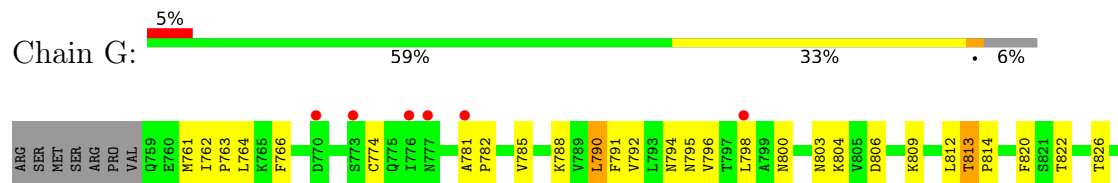
• Molecule 1: POLY(A) RIBONUCLEASE POP2

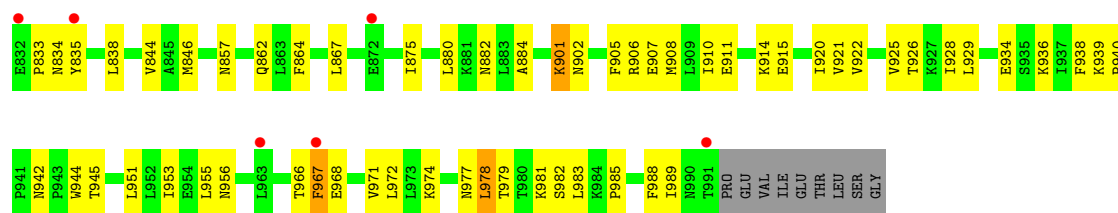


• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1



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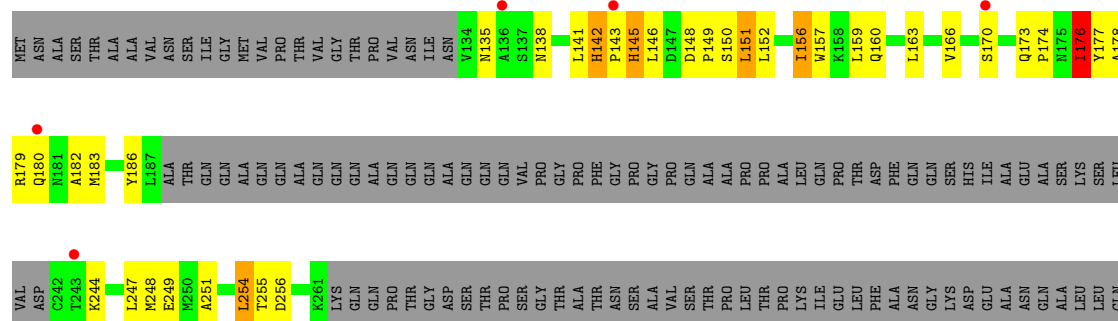
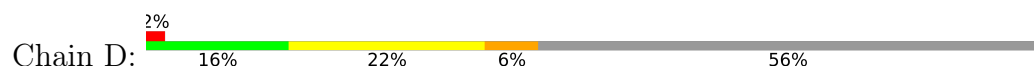
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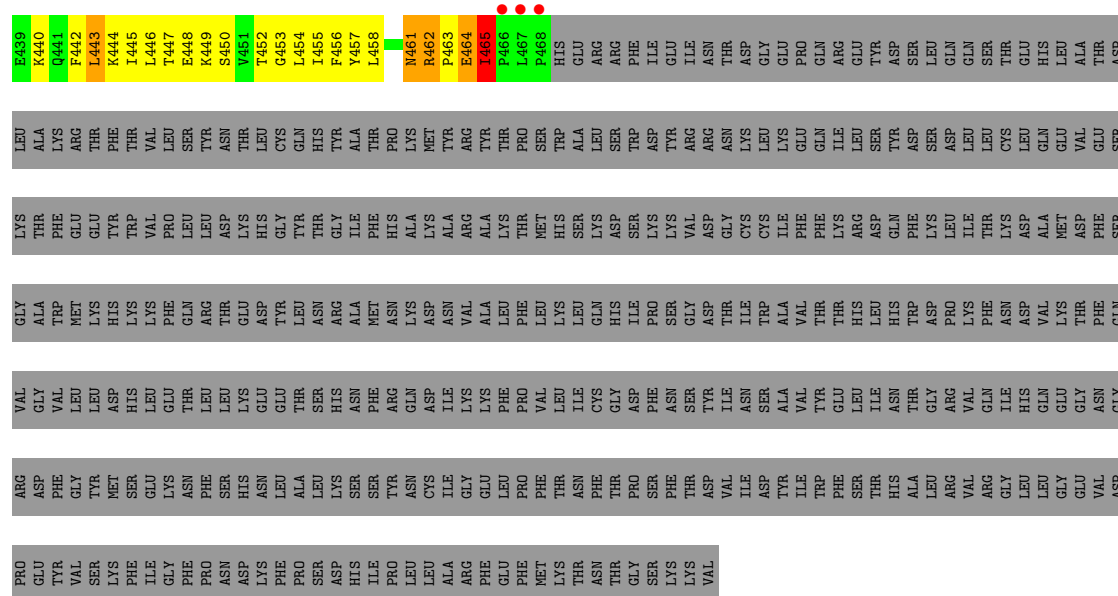


• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

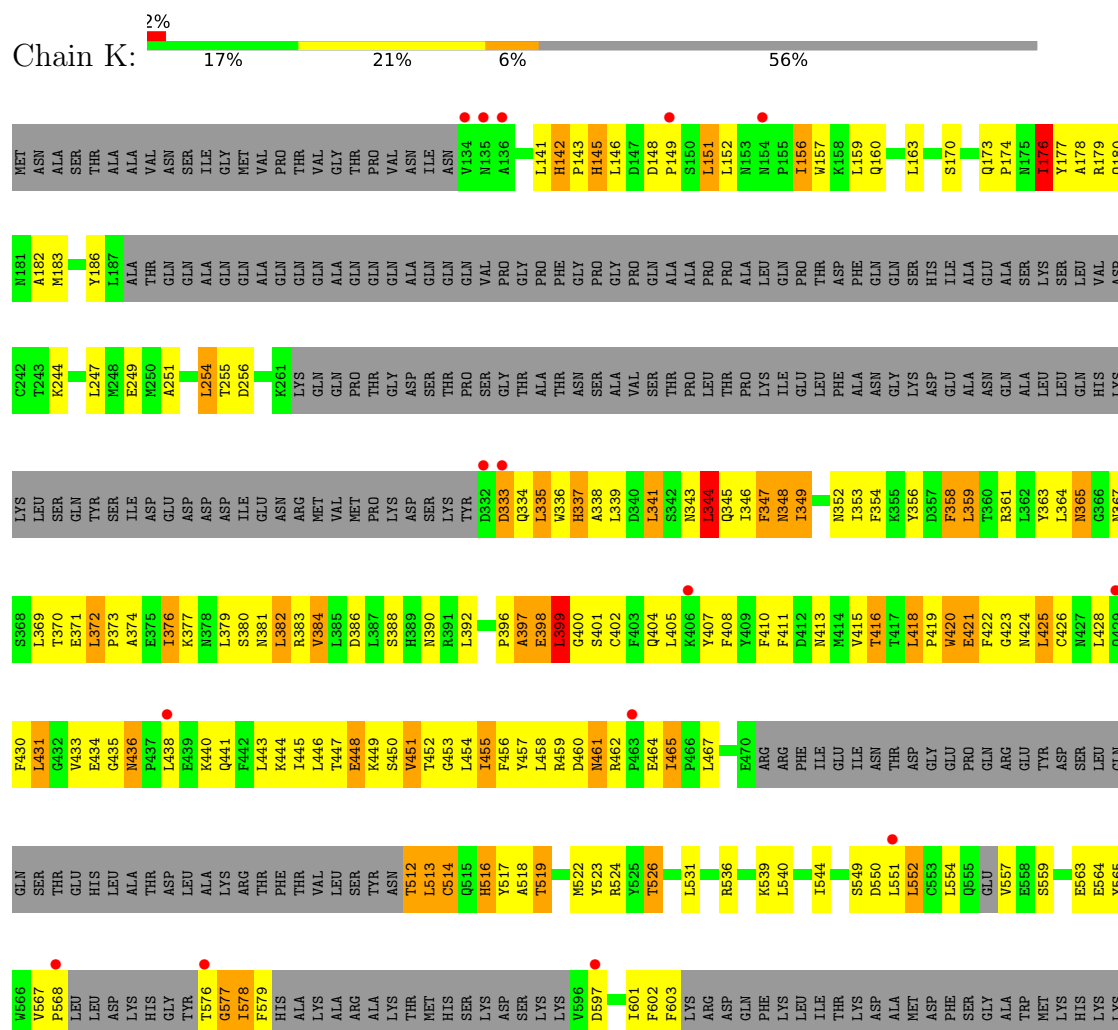


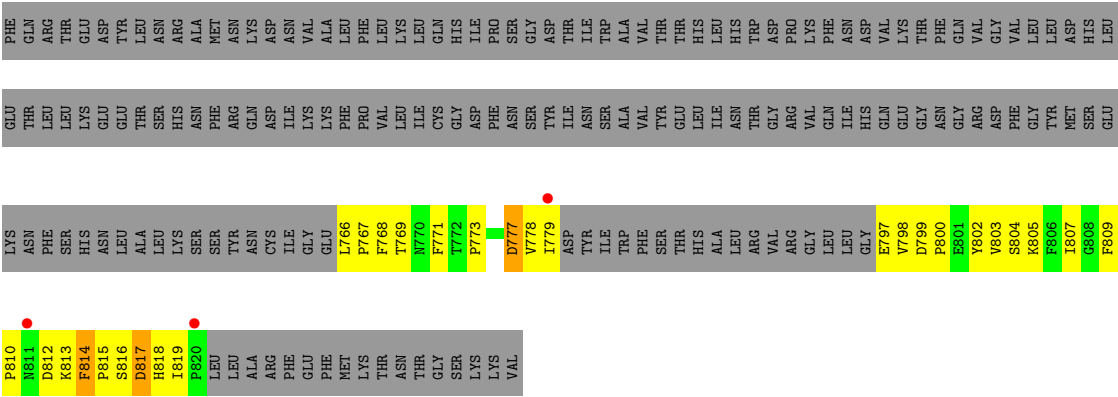
• Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR



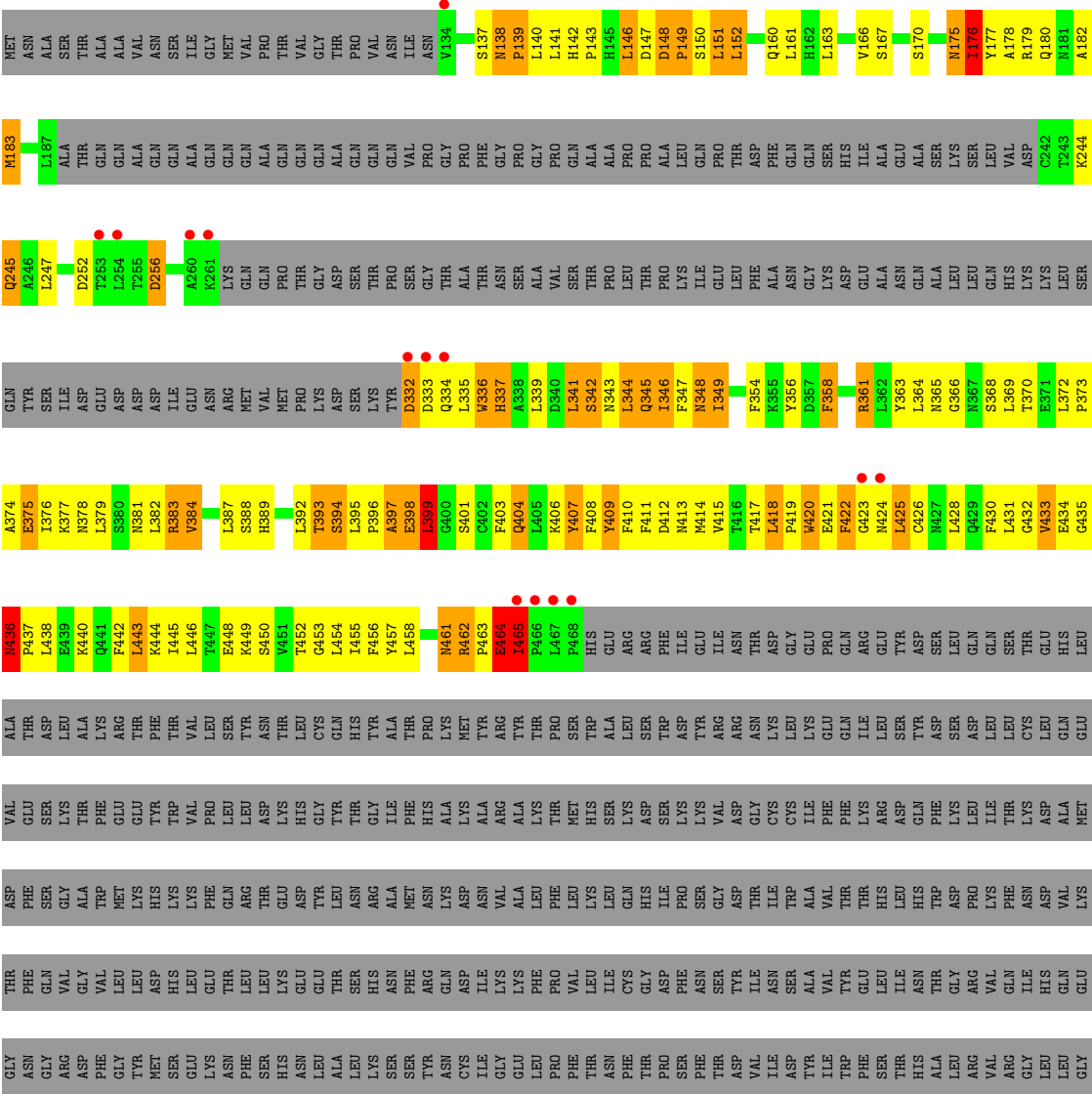


• Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR





● Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR



GLU VAL ASP PRO GLU TYR VAL SER LYS PHE ILE GLY PHE PRO ASN ASP LYS PHE PRO SER ASP HIS ILE PRO LEU LEU ALA ARG PHE GLU PHE MET LYS THR ASN THR GLY SER LYS VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.65Å 122.91Å 126.42Å 89.47° 89.74° 64.22°	Depositor
Resolution (Å)	47.95 – 3.41 47.95 – 3.41	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.95-3.41) 98.5 (47.95-3.41)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.233 , 0.270 0.227 , 0.265	Depositor DCC
R_{free} test set	4942 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.018 for k,h,-l 0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24298	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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	0.67	0/2231	1.01	11/3028 (0.4%)
1	C	0.64	0/2235	1.01	9/3032 (0.3%)
1	E	0.64	0/2235	1.00	8/3033 (0.3%)
1	F	0.65	1/2231 (0.0%)	0.98	7/3028 (0.2%)
2	B	0.54	0/1908	0.92	2/2588 (0.1%)
2	G	0.53	0/1908	0.91	1/2588 (0.0%)
2	H	0.53	0/1908	0.92	2/2588 (0.1%)
2	I	0.53	0/1908	0.90	1/2588 (0.0%)
3	D	0.69	1/2520 (0.0%)	1.19	30/3446 (0.9%)
3	J	0.81	3/1640 (0.2%)	1.50	24/2240 (1.1%)
3	K	0.70	3/2535 (0.1%)	1.20	30/3463 (0.9%)
3	L	0.83	3/1640 (0.2%)	1.56	30/2240 (1.3%)
All	All	0.65	11/24899 (0.0%)	1.10	155/33862 (0.5%)

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	C	0	1
1	E	0	1
3	D	0	1
3	J	0	1
3	K	0	1
3	L	0	2
All	All	0	8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	462	ARG	C-N	7.32	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	462	ARG	C-N	7.11	1.50	1.33
3	L	332	ASP	CA-CB	6.55	1.66	1.53
3	L	361	ARG	CA-C	6.45	1.58	1.52
3	K	334	GLN	CA-C	5.79	1.60	1.52
1	F	194	THR	CA-CB	5.71	1.60	1.52
3	J	361	ARG	CA-C	5.29	1.57	1.52
3	K	333	ASP	CA-C	5.14	1.59	1.52
3	D	352	ASN	CG-ND2	-5.09	1.22	1.33
3	J	332	ASP	CA-CB	5.06	1.63	1.53
3	K	333	ASP	N-CA	5.03	1.52	1.46

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	462	ARG	O-C-N	27.71	145.96	121.30
3	J	462	ARG	O-C-N	27.41	145.70	121.30
3	L	465	ILE	CA-C-N	15.11	136.09	119.92
3	L	465	ILE	C-N-CA	15.11	136.09	119.92
3	J	397	ALA	N-CA-C	-12.97	94.10	110.19
3	L	397	ALA	N-CA-C	-12.56	94.96	110.41
3	J	399	LEU	N-CA-C	-10.06	101.00	113.18
3	K	462	ARG	CA-C-N	-9.99	110.29	120.98
3	K	462	ARG	C-N-CA	-9.99	110.29	120.98
3	L	399	LEU	N-CA-C	-9.88	101.22	113.18
3	J	462	ARG	CA-C-N	-9.66	107.76	119.84
3	J	462	ARG	C-N-CA	-9.66	107.76	119.84
3	K	399	LEU	N-CA-C	-9.28	101.22	112.54
3	J	465	ILE	CA-C-N	9.10	130.68	120.85
3	J	465	ILE	C-N-CA	9.10	130.68	120.85
3	K	465	ILE	CA-C-N	8.90	130.97	119.84
3	K	465	ILE	C-N-CA	8.90	130.97	119.84
3	L	462	ARG	CA-C-N	-8.90	108.71	119.84
3	L	462	ARG	C-N-CA	-8.90	108.71	119.84
3	L	151	LEU	N-CA-C	-8.77	102.60	113.38
3	D	465	ILE	CA-C-N	8.73	130.75	119.84
3	D	465	ILE	C-N-CA	8.73	130.75	119.84
3	D	399	LEU	N-CA-C	-8.70	101.93	112.54
3	J	151	LEU	N-CA-C	-8.55	102.86	113.38
3	K	333	ASP	N-CA-C	8.53	121.46	107.73
3	D	333	ASP	N-CA-C	8.44	121.31	107.73
3	D	462	ARG	CA-C-N	-7.68	110.24	119.84
3	D	462	ARG	C-N-CA	-7.68	110.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	151	LEU	N-CA-C	-7.25	104.03	113.17
3	L	146	LEU	N-CA-C	-7.22	102.80	111.69
3	L	433	VAL	N-CA-C	7.00	119.62	112.90
3	J	433	VAL	N-CA-C	6.96	119.59	112.90
3	J	348	ASN	N-CA-C	6.89	119.64	109.24
3	J	337	HIS	N-CA-C	6.84	122.47	113.30
3	J	146	LEU	N-CA-C	-6.79	103.33	111.69
3	K	151	LEU	N-CA-C	-6.78	104.63	113.17
3	L	348	ASN	N-CA-C	6.74	119.58	108.99
1	F	202	PHE	CB-CA-C	-6.58	107.14	116.34
3	D	335	LEU	N-CA-C	6.52	124.68	110.80
2	B	766	PHE	N-CA-C	6.51	120.92	112.92
1	E	202	PHE	CB-CA-C	-6.50	107.25	116.34
1	C	202	PHE	N-CA-C	6.46	117.56	108.00
3	K	335	LEU	N-CA-C	6.38	124.38	110.80
3	L	361	ARG	N-CA-C	6.33	120.77	111.34
3	D	348	ASN	N-CA-C	6.32	118.46	108.79
1	A	201	THR	N-CA-C	6.29	120.78	111.04
3	K	348	ASN	N-CA-C	6.28	118.40	108.79
3	K	337	HIS	N-CA-C	6.27	121.71	113.30
3	K	462	ARG	N-CA-C	-6.25	95.99	109.81
3	D	418	LEU	CA-C-N	6.25	125.94	119.82
3	D	418	LEU	C-N-CA	6.25	125.94	119.82
3	D	462	ARG	N-CA-C	-6.25	96.01	109.81
3	K	397	ALA	N-CA-C	-6.22	100.08	109.60
3	L	465	ILE	N-CA-C	6.21	122.29	108.88
1	A	153	PRO	O-C-N	6.20	124.16	121.31
3	K	418	LEU	CA-C-N	6.15	125.84	119.82
3	K	418	LEU	C-N-CA	6.15	125.84	119.82
3	K	513	LEU	N-CA-C	6.08	118.03	110.91
3	K	176	ILE	CB-CA-C	-6.04	103.97	111.70
2	G	766	PHE	N-CA-C	5.99	120.29	112.92
3	D	336	TRP	N-CA-C	5.99	119.04	110.24
2	H	766	PHE	N-CA-C	5.96	120.69	113.17
1	A	202	PHE	N-CA-C	5.95	116.81	108.00
3	L	176	ILE	CB-CA-C	-5.95	104.27	111.88
1	C	202	PHE	CB-CA-C	-5.94	108.02	116.34
3	K	146	LEU	N-CA-C	-5.94	106.03	113.28
3	D	397	ALA	N-CA-C	-5.92	100.55	109.60
3	K	578	ILE	N-CA-C	5.92	116.15	107.75
3	D	349	ILE	N-CA-C	5.87	116.58	108.12
1	F	202	PHE	N-CA-C	5.87	116.68	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	336	TRP	N-CA-C	5.86	118.85	110.24
3	D	513	LEU	N-CA-C	5.85	117.75	110.91
1	C	306	HIS	N-CA-C	-5.84	104.08	110.91
1	A	165	LYS	N-CA-C	-5.84	104.83	111.07
1	C	201	THR	N-CA-C	5.84	120.09	111.04
1	A	382	LEU	CA-C-N	5.83	126.15	119.92
1	A	382	LEU	C-N-CA	5.83	126.15	119.92
3	J	342	SER	N-CA-C	5.82	118.78	110.10
3	J	246	ALA	N-CA-C	-5.80	105.04	111.36
1	E	202	PHE	N-CA-C	5.75	116.51	108.00
1	A	202	PHE	CB-CA-C	-5.74	108.30	116.34
2	I	766	PHE	N-CA-C	5.71	120.37	113.17
3	L	337	HIS	N-CA-C	5.71	120.94	113.30
3	L	418	LEU	CA-C-N	5.70	126.97	119.84
3	L	418	LEU	C-N-CA	5.70	126.97	119.84
3	D	337	HIS	N-CA-C	5.69	120.93	113.30
3	J	361	ARG	N-CA-C	5.69	119.82	111.34
1	F	216	ASN	N-CA-C	5.69	117.56	111.36
3	D	365	ASN	N-CA-C	5.67	118.06	110.35
1	A	306	HIS	N-CA-C	-5.67	104.28	110.91
3	D	420	TRP	N-CA-C	-5.67	98.50	108.08
3	K	421	GLU	N-CA-C	-5.61	98.86	110.80
3	K	349	ILE	N-CA-C	5.60	116.18	108.12
3	L	336	TRP	N-CA-C	5.59	118.69	110.30
1	C	153	PRO	O-C-N	5.59	123.88	121.31
1	E	203	ARG	N-CA-C	-5.56	100.56	108.23
3	L	149	PRO	CA-C-N	-5.54	114.26	122.41
3	L	149	PRO	C-N-CA	-5.54	114.26	122.41
1	E	306	HIS	N-CA-C	-5.54	104.43	110.91
3	L	334	GLN	CA-C-N	5.52	132.08	121.54
3	L	334	GLN	C-N-CA	5.52	132.08	121.54
3	K	420	TRP	N-CA-C	-5.48	98.82	108.08
3	D	342	SER	N-CA-C	5.47	118.17	109.96
1	E	201	THR	N-CA-C	5.46	119.51	111.04
1	F	203	ARG	N-CA-C	-5.45	100.71	108.23
3	K	352	ASN	N-CA-C	5.44	117.91	111.33
3	K	799	ASP	CA-C-N	5.44	125.05	119.56
3	K	799	ASP	C-N-CA	5.44	125.05	119.56
3	K	365	ASN	N-CA-C	5.43	117.73	110.35
1	F	392	GLY	N-CA-C	-5.40	106.23	112.50
3	D	814	PHE	CA-C-N	-5.37	113.13	119.84
3	D	814	PHE	C-N-CA	-5.37	113.13	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	436	ASN	N-CA-C	-5.35	99.78	109.09
3	K	814	PHE	CA-C-N	-5.34	113.16	119.84
3	K	814	PHE	C-N-CA	-5.34	113.16	119.84
1	E	323	MET	CA-C-N	5.34	125.63	119.92
1	E	323	MET	C-N-CA	5.34	125.63	119.92
3	D	146	LEU	N-CA-C	-5.33	106.78	113.28
3	D	421	GLU	N-CA-C	-5.32	99.47	110.80
3	L	342	SER	N-CA-C	5.32	118.02	110.10
3	D	799	ASP	CA-C-N	5.30	124.91	119.56
3	D	799	ASP	C-N-CA	5.30	124.91	119.56
3	D	813	LYS	N-CA-C	5.29	119.84	113.17
3	K	577	GLY	N-CA-C	5.28	120.09	111.27
3	J	334	GLN	CA-C-N	5.27	131.60	121.54
3	J	334	GLN	C-N-CA	5.27	131.60	121.54
1	C	323	MET	CA-C-N	5.25	125.53	119.92
1	C	323	MET	C-N-CA	5.25	125.53	119.92
3	J	176	ILE	CB-CA-C	-5.23	105.18	111.88
2	H	982	SER	N-CA-C	5.22	116.97	111.28
3	D	598	GLY	N-CA-C	5.20	117.77	110.38
1	E	392	GLY	N-CA-C	-5.19	106.47	112.50
3	J	149	PRO	CA-C-N	-5.17	114.81	122.41
3	J	149	PRO	C-N-CA	-5.17	114.81	122.41
3	K	813	LYS	N-CA-C	5.16	119.67	113.17
1	C	216	ASN	N-CA-C	5.16	116.98	111.36
3	L	148	ASP	N-CA-C	5.15	119.17	112.17
3	L	166	VAL	CB-CA-C	-5.14	105.20	112.14
3	J	148	ASP	N-CA-C	5.14	119.16	112.17
3	L	420	TRP	N-CA-C	-5.14	99.86	110.80
3	J	362	LEU	N-CA-C	5.13	121.73	110.80
1	C	167	ASN	N-CA-C	5.12	119.22	112.92
1	F	323	MET	CA-C-N	5.12	125.40	119.92
1	F	323	MET	C-N-CA	5.12	125.40	119.92
1	A	323	MET	CA-C-N	5.12	125.40	119.92
1	A	323	MET	C-N-CA	5.12	125.40	119.92
2	B	780	GLY	N-CA-C	-5.12	104.37	112.66
3	J	252	ASP	N-CA-C	5.11	117.59	111.71
3	L	409	TYR	CB-CA-C	-5.10	102.91	110.62
3	L	138	ASN	CA-C-N	5.10	126.21	119.84
3	L	138	ASN	C-N-CA	5.10	126.21	119.84
3	D	176	ILE	CB-CA-C	-5.08	105.20	111.70
1	A	256	ILE	CB-CA-C	-5.07	105.15	111.08
3	L	436	ASN	N-CA-C	-5.06	100.28	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	SER	N-CA-C	-5.04	107.11	113.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	THR	Peptide
1	C	194	THR	Peptide
3	D	344	LEU	Peptide
1	E	194	THR	Peptide
3	J	332	ASP	Peptide
3	K	344	LEU	Peptide
3	L	332	ASP	Peptide
3	L	464	GLU	Mainchain

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	2170	0	2083	99	0
1	C	2174	0	2094	102	0
1	E	2174	0	2089	94	1
1	F	2170	0	2083	81	1
2	B	1869	0	1936	56	0
2	G	1869	0	1936	55	1
2	H	1869	0	1936	64	0
2	I	1869	0	1936	56	1
3	D	2456	0	2268	232	0
3	J	1604	0	1505	150	1
3	K	2470	0	2293	211	0
3	L	1604	0	1505	164	1
All	All	24298	0	23664	1318	3

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 27.

All (1318) 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)
3:D:176:ILE:HD11	3:D:343:ASN:HD22	1.20	1.04
3:J:422:PHE:HD1	3:J:422:PHE:O	1.42	1.00
3:K:176:ILE:HD11	3:K:343:ASN:HD22	1.21	1.00
3:K:567:VAL:HG13	3:K:568:PRO:HD3	1.41	0.99
3:D:424:ASN:HD21	3:D:807:ILE:HG21	1.29	0.98
3:L:422:PHE:HD1	3:L:422:PHE:O	1.43	0.98
3:D:567:VAL:HG13	3:D:568:PRO:HD3	1.42	0.97
3:J:150:SER:HA	3:J:152:LEU:HD12	1.49	0.95
3:K:424:ASN:HD21	3:K:807:ILE:HG21	1.32	0.94
3:L:150:SER:HA	3:L:152:LEU:HD12	1.50	0.94
1:C:287:GLN:NE2	2:H:947:GLY:HA3	1.84	0.91
3:K:445:ILE:O	3:K:449:LYS:HB2	1.73	0.89
3:L:422:PHE:CB	3:L:425:LEU:HG	2.02	0.89
3:J:422:PHE:O	3:J:422:PHE:CD1	2.25	0.88
1:E:197:ARG:HG2	3:L:175:ASN:ND2	1.88	0.88
3:K:422:PHE:HB3	3:K:425:LEU:HG	1.56	0.88
3:D:422:PHE:HB3	3:D:425:LEU:HG	1.56	0.88
1:E:197:ARG:HG2	3:L:175:ASN:HD22	1.36	0.88
1:E:197:ARG:CG	3:L:175:ASN:HD22	1.84	0.88
3:J:422:PHE:CB	3:J:425:LEU:HG	2.04	0.88
3:D:176:ILE:HD11	3:D:343:ASN:ND2	1.90	0.87
3:D:445:ILE:O	3:D:449:LYS:HB2	1.75	0.87
3:K:579:PHE:HD1	3:K:579:PHE:O	1.55	0.86
3:K:176:ILE:HD11	3:K:343:ASN:ND2	1.91	0.86
3:L:422:PHE:O	3:L:422:PHE:CD1	2.27	0.86
3:D:422:PHE:HA	3:D:424:ASN:N	1.90	0.86
3:D:392:LEU:HB2	3:D:413:ASN:HD22	1.41	0.86
3:D:163:LEU:HD11	3:D:249:GLU:HA	1.58	0.85
3:K:163:LEU:HD11	3:K:249:GLU:HA	1.58	0.85
3:K:392:LEU:HB2	3:K:413:ASN:HD22	1.42	0.85
3:D:567:VAL:HG13	3:D:568:PRO:CD	2.07	0.84
3:K:579:PHE:O	3:K:579:PHE:CD1	2.31	0.84
3:K:567:VAL:HG13	3:K:568:PRO:CD	2.08	0.84
3:K:349:ILE:HG21	3:K:353:ILE:HD11	1.59	0.83
1:F:202:PHE:CE2	1:F:208:TYR:HD1	1.96	0.83
3:J:170:SER:HB3	3:J:176:ILE:HD13	1.61	0.83
1:C:203:ARG:HH22	3:K:333:ASP:CB	1.92	0.82
1:A:426:ILE:HG22	1:A:427:TYR:H	1.44	0.82
1:C:169:TYR:OH	1:C:284:GLU:OE1	1.98	0.82
3:K:424:ASN:HD21	3:K:807:ILE:CG2	1.94	0.81
1:E:169:TYR:OH	1:E:284:GLU:OE1	1.99	0.80
3:D:424:ASN:HD21	3:D:807:ILE:CG2	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:422:PHE:HA	3:K:424:ASN:N	1.95	0.80
3:J:419:PRO:HD2	3:J:422:PHE:CE1	2.14	0.80
1:A:169:TYR:OH	1:A:284:GLU:OE1	1.99	0.80
3:L:170:SER:HB3	3:L:176:ILE:HD13	1.63	0.80
3:D:418:LEU:HB3	3:D:422:PHE:HE1	1.46	0.80
3:L:137:SER:O	3:L:139:PRO:HD3	1.80	0.80
3:D:766:LEU:HG	3:D:767:PRO:HD2	1.62	0.80
3:J:449:LYS:HB3	3:J:453:GLY:HA3	1.64	0.80
3:K:418:LEU:HB3	3:K:422:PHE:HE1	1.47	0.80
3:D:349:ILE:HG21	3:D:353:ILE:HD11	1.62	0.79
1:F:169:TYR:OH	1:F:284:GLU:OE1	2.00	0.79
3:D:397:ALA:O	3:D:399:LEU:N	2.15	0.79
1:E:305:TYR:OH	1:E:371:TYR:O	1.99	0.79
1:A:287:GLN:NE2	2:B:947:GLY:HA3	1.97	0.79
3:J:137:SER:O	3:J:139:PRO:HD3	1.82	0.79
1:E:202:PHE:CE2	1:E:208:TYR:HD1	2.01	0.78
1:E:213:MET:HG3	1:E:309:TYR:CD1	2.18	0.78
1:F:305:TYR:OH	1:F:371:TYR:O	2.01	0.78
1:C:305:TYR:OH	1:C:371:TYR:O	2.01	0.78
1:F:194:THR:HG23	1:F:194:THR:O	1.81	0.78
3:L:150:SER:HA	3:L:152:LEU:CD1	2.12	0.78
1:A:305:TYR:OH	1:A:371:TYR:O	2.02	0.78
1:C:426:ILE:HG22	1:C:427:TYR:H	1.48	0.78
1:F:213:MET:HG3	1:F:309:TYR:CD1	2.19	0.78
3:J:150:SER:HA	3:J:152:LEU:CD1	2.13	0.77
1:E:426:ILE:HG22	1:E:427:TYR:H	1.49	0.77
3:K:397:ALA:O	3:K:399:LEU:N	2.17	0.77
3:L:422:PHE:HB2	3:L:425:LEU:HG	1.65	0.76
3:K:399:LEU:O	3:K:402:CYS:HB2	1.86	0.76
1:C:202:PHE:CE2	1:C:208:TYR:HD1	2.04	0.76
3:L:376:ILE:HD12	3:L:379:LEU:HD12	1.66	0.76
1:A:203:ARG:HH22	3:D:333:ASP:CB	1.99	0.76
3:D:372:LEU:HD21	3:D:376:ILE:HD13	1.68	0.76
3:L:148:ASP:HB3	3:L:149:PRO:C	2.10	0.76
3:D:577:GLY:C	3:D:578:ILE:HD12	2.11	0.76
3:L:419:PRO:HD2	3:L:422:PHE:CE1	2.20	0.75
3:L:449:LYS:HB3	3:L:453:GLY:HA3	1.68	0.75
3:K:766:LEU:HG	3:K:767:PRO:HD2	1.67	0.75
3:D:399:LEU:O	3:D:402:CYS:HB2	1.87	0.75
1:A:189:THR:OG1	1:A:310:ASP:OD1	2.04	0.75
2:I:790:LEU:O	2:I:794:ASN:ND2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:148:ASP:HB3	3:J:149:PRO:C	2.10	0.75
3:J:422:PHE:HB3	3:J:425:LEU:HG	1.66	0.75
3:K:773:PRO:HD3	3:K:807:ILE:O	1.87	0.75
3:K:349:ILE:HG21	3:K:353:ILE:CD1	2.15	0.75
1:C:189:THR:OG1	1:C:310:ASP:OD1	2.04	0.75
1:F:426:ILE:HG22	1:F:427:TYR:H	1.52	0.74
3:D:349:ILE:HG21	3:D:353:ILE:CD1	2.16	0.74
2:H:812:LEU:HD23	2:H:846:MET:HE2	1.68	0.74
3:J:422:PHE:HA	3:J:424:ASN:N	2.03	0.74
2:B:812:LEU:HD23	2:B:846:MET:HE2	1.70	0.74
3:L:383:ARG:CZ	3:L:404:GLN:HG2	2.18	0.74
3:D:773:PRO:HD3	3:D:807:ILE:O	1.88	0.74
1:E:203:ARG:HH22	3:L:333:ASP:CB	2.00	0.73
3:J:422:PHE:HB2	3:J:425:LEU:HG	1.69	0.73
3:D:397:ALA:O	3:D:398:GLU:HG2	1.88	0.73
1:F:189:THR:OG1	1:F:310:ASP:OD1	2.05	0.73
1:F:202:PHE:CE2	1:F:208:TYR:CD1	2.76	0.73
3:J:442:PHE:HE1	3:J:458:LEU:HD21	1.53	0.73
3:L:422:PHE:HB3	3:L:425:LEU:HG	1.68	0.73
1:E:195:LEU:HA	1:E:216:ASN:OD1	1.88	0.73
3:K:428:LEU:HD21	3:K:431:LEU:HB2	1.69	0.73
1:F:191:PHE:CZ	1:F:309:TYR:HD2	2.05	0.73
3:J:383:ARG:CZ	3:J:404:GLN:HG2	2.19	0.73
3:K:397:ALA:O	3:K:398:GLU:HG2	1.89	0.73
1:A:191:PHE:CZ	1:A:309:TYR:HD2	2.07	0.73
1:A:195:LEU:HA	1:A:216:ASN:OD1	1.88	0.73
3:K:422:PHE:HB2	3:K:425:LEU:HD11	1.70	0.73
3:D:446:LEU:HD12	3:D:450:SER:O	1.87	0.72
3:D:766:LEU:CG	3:D:767:PRO:HD2	2.18	0.72
3:K:372:LEU:HD21	3:K:376:ILE:HD13	1.71	0.72
3:J:420:TRP:CE2	3:J:463:PRO:HD3	2.24	0.72
3:L:442:PHE:HE1	3:L:458:LEU:HD21	1.53	0.72
3:D:578:ILE:HG22	3:D:579:PHE:N	2.04	0.72
1:E:191:PHE:CZ	1:E:309:TYR:HD2	2.06	0.71
3:K:422:PHE:HB3	3:K:425:LEU:CG	2.19	0.71
3:L:422:PHE:HA	3:L:424:ASN:N	2.06	0.71
3:D:578:ILE:HG22	3:D:579:PHE:H	1.56	0.71
1:E:189:THR:OG1	1:E:310:ASP:OD1	2.06	0.71
1:E:202:PHE:CE2	1:E:208:TYR:CD1	2.78	0.71
1:A:202:PHE:CE2	1:A:208:TYR:HD1	2.09	0.71
2:B:790:LEU:O	2:B:794:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:397:ALA:O	3:J:398:GLU:HG2	1.91	0.71
3:L:143:PRO:HG3	3:L:443:LEU:HD11	1.71	0.71
1:C:176:ARG:HD3	2:H:900:HIS:HB3	1.73	0.71
3:K:411:PHE:HD1	3:K:434:GLU:O	1.74	0.71
1:C:287:GLN:HE22	2:H:947:GLY:HA3	1.53	0.71
2:H:790:LEU:O	2:H:794:ASN:ND2	2.24	0.70
2:G:790:LEU:O	2:G:794:ASN:ND2	2.23	0.70
1:C:257:MET:HE1	1:C:262:LEU:HD13	1.72	0.70
3:D:422:PHE:HB2	3:D:425:LEU:HD11	1.72	0.70
3:D:428:LEU:HD21	3:D:431:LEU:HB2	1.72	0.70
3:D:440:LYS:O	3:D:444:LYS:HG3	1.91	0.70
3:K:461:ASN:OD1	3:K:461:ASN:N	2.24	0.70
1:C:191:PHE:CZ	1:C:309:TYR:HD2	2.10	0.70
3:D:397:ALA:C	3:D:399:LEU:H	1.99	0.70
3:D:411:PHE:HD1	3:D:434:GLU:O	1.75	0.70
3:D:529:TRP:HB3	2:H:913:TYR:CE2	2.27	0.70
1:A:257:MET:HE1	1:A:262:LEU:HD13	1.72	0.70
3:D:766:LEU:HD21	3:D:797:GLU:N	2.07	0.70
2:G:833:PRO:HD3	2:G:882:ASN:ND2	2.07	0.70
2:G:812:LEU:HD23	2:G:846:MET:HE2	1.74	0.69
3:D:422:PHE:CB	3:D:425:LEU:HG	2.22	0.69
2:I:812:LEU:HD23	2:I:846:MET:HE2	1.73	0.69
3:L:383:ARG:NH1	3:L:404:GLN:HG2	2.06	0.69
3:L:419:PRO:O	3:L:420:TRP:HB2	1.92	0.69
1:C:195:LEU:HA	1:C:216:ASN:OD1	1.91	0.69
3:D:422:PHE:HB3	3:D:425:LEU:CG	2.21	0.69
3:J:383:ARG:NH1	3:J:404:GLN:HG2	2.06	0.69
3:D:579:PHE:CZ	3:D:598:GLY:HA3	2.27	0.69
3:L:397:ALA:O	3:L:398:GLU:HG2	1.93	0.69
3:L:433:VAL:O	3:L:435:GLY:HA2	1.91	0.69
3:D:428:LEU:HB3	3:D:455:ILE:HD11	1.74	0.69
3:K:422:PHE:CB	3:K:425:LEU:HG	2.22	0.69
3:J:358:PHE:HD1	3:J:358:PHE:H	1.40	0.68
3:K:397:ALA:C	3:K:399:LEU:H	2.01	0.68
1:C:213:MET:HG3	1:C:309:TYR:CD1	2.28	0.68
3:J:376:ILE:HD12	3:J:379:LEU:HD12	1.73	0.68
3:K:766:LEU:CG	3:K:767:PRO:HD2	2.23	0.68
3:K:440:LYS:O	3:K:444:LYS:HG3	1.93	0.68
2:G:967:PHE:O	2:G:971:VAL:HG23	1.93	0.68
1:C:305:TYR:HD1	1:C:344:LEU:HB3	1.57	0.68
3:D:344:LEU:O	3:D:346:ILE:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:347:PHE:HD1	3:L:368:SER:HB2	1.58	0.68
3:D:422:PHE:HA	3:D:424:ASN:H	1.57	0.68
3:D:461:ASN:OD1	3:D:461:ASN:N	2.27	0.68
3:L:374:ALA:HB1	3:L:398:GLU:OE2	1.93	0.68
3:J:244:LYS:O	3:J:247:LEU:N	2.26	0.67
3:D:361:ARG:HA	3:D:384:VAL:HG23	1.77	0.67
3:J:374:ALA:HB1	3:J:398:GLU:OE2	1.94	0.67
3:K:428:LEU:HB3	3:K:455:ILE:HD11	1.77	0.67
3:K:344:LEU:O	3:K:346:ILE:HG13	1.94	0.67
3:L:354:PHE:CZ	3:L:373:PRO:HG2	2.29	0.66
2:H:884:ALA:HB1	2:H:928:ILE:HG13	1.77	0.66
1:E:305:TYR:HD1	1:E:344:LEU:HB3	1.58	0.66
3:J:347:PHE:HD1	3:J:368:SER:HB2	1.59	0.66
3:K:446:LEU:HD12	3:K:450:SER:O	1.95	0.66
1:A:176:ARG:HD3	2:B:900:HIS:HB3	1.77	0.66
3:D:335:LEU:O	3:D:337:HIS:CE1	2.49	0.66
3:L:244:LYS:O	3:L:247:LEU:N	2.28	0.66
2:H:781:ALA:HB1	2:H:785:VAL:HB	1.78	0.66
3:K:335:LEU:O	3:K:337:HIS:CE1	2.49	0.65
3:K:361:ARG:HA	3:K:384:VAL:HG23	1.78	0.65
3:D:142:HIS:CD2	3:D:142:HIS:H	2.12	0.65
3:J:396:PRO:HD2	3:J:399:LEU:HD12	1.77	0.65
3:K:142:HIS:CD2	3:K:142:HIS:H	2.13	0.65
3:L:396:PRO:HD2	3:L:399:LEU:HD12	1.78	0.65
1:E:194:THR:O	1:E:194:THR:HG23	1.97	0.65
3:L:345:GLN:N	3:L:345:GLN:OE1	2.30	0.65
3:L:358:PHE:HD1	3:L:358:PHE:H	1.44	0.65
3:K:540:LEU:HD23	3:K:815:PRO:HG2	1.79	0.65
3:J:346:ILE:O	3:J:346:ILE:HG22	1.95	0.65
3:K:766:LEU:HD21	3:K:797:GLU:N	2.12	0.65
3:D:251:ALA:O	3:D:254:LEU:N	2.29	0.64
2:I:967:PHE:O	2:I:971:VAL:HG23	1.97	0.64
1:A:213:MET:HG3	1:A:309:TYR:CD1	2.32	0.64
3:D:346:ILE:HB	3:D:367:ASN:HD22	1.63	0.64
2:H:833:PRO:HD3	2:H:882:ASN:ND2	2.11	0.64
3:J:354:PHE:CZ	3:J:373:PRO:HG2	2.32	0.64
3:L:420:TRP:CE2	3:L:463:PRO:HD3	2.32	0.64
1:A:287:GLN:HE22	2:B:947:GLY:HA3	1.62	0.64
1:A:305:TYR:HD1	1:A:344:LEU:HB3	1.61	0.64
3:D:157:TRP:HZ3	3:D:443:LEU:HD22	1.62	0.64
3:J:419:PRO:HD2	3:J:422:PHE:HE1	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:160:GLN:HE22	3:J:432:GLY:HA2	1.63	0.64
2:B:922:VAL:O	2:B:926:THR:HG23	1.98	0.64
3:L:346:ILE:O	3:L:346:ILE:HG22	1.96	0.64
3:J:440:LYS:HA	3:J:443:LEU:HB2	1.79	0.64
2:B:833:PRO:HD3	2:B:882:ASN:ND2	2.13	0.64
2:I:833:PRO:HD3	2:I:882:ASN:ND2	2.13	0.64
3:J:433:VAL:O	3:J:435:GLY:HA2	1.98	0.63
3:K:183:MET:O	3:K:186:TYR:HB3	1.98	0.63
3:L:440:LYS:HA	3:L:443:LEU:HB2	1.79	0.63
3:J:143:PRO:HG3	3:J:443:LEU:HD11	1.78	0.63
3:K:518:ALA:O	3:K:531:LEU:HD11	1.97	0.63
2:G:922:VAL:O	2:G:926:THR:HG23	1.98	0.63
3:L:160:GLN:HE22	3:L:432:GLY:HA2	1.64	0.63
1:C:191:PHE:HD1	1:C:191:PHE:N	1.96	0.63
3:D:766:LEU:CD1	3:D:767:PRO:HD2	2.29	0.63
3:K:550:ASP:O	3:K:603:PHE:HA	1.98	0.63
3:D:183:MET:O	3:D:186:TYR:HB3	1.98	0.63
3:D:518:ALA:O	3:D:531:LEU:HD11	1.97	0.63
1:F:151:PHE:CD1	1:F:151:PHE:C	2.75	0.63
3:K:513:LEU:HD12	3:K:816:SER:HA	1.80	0.63
3:L:417:THR:HG23	3:L:442:PHE:CE2	2.34	0.63
2:B:875:ILE:HD12	2:B:920:ILE:HG12	1.79	0.63
1:E:257:MET:HE1	1:E:262:LEU:HD13	1.79	0.63
1:F:191:PHE:N	1:F:191:PHE:HD1	1.96	0.63
3:J:403:PHE:CD1	3:J:404:GLN:N	2.67	0.63
2:I:781:ALA:HB1	2:I:785:VAL:HB	1.78	0.63
1:F:257:MET:HE1	1:F:262:LEU:HD13	1.80	0.63
1:C:355:LYS:O	1:C:355:LYS:HG3	1.97	0.63
3:D:540:LEU:HD23	3:D:815:PRO:HG2	1.81	0.62
2:I:956:ASN:HD21	2:I:966:THR:HG23	1.63	0.62
2:B:884:ALA:HB1	2:B:928:ILE:HG13	1.81	0.62
1:C:202:PHE:CE2	1:C:208:TYR:CD1	2.85	0.62
3:K:148:ASP:HB3	3:K:149:PRO:C	2.24	0.62
2:B:781:ALA:HB1	2:B:785:VAL:HB	1.82	0.62
1:C:151:PHE:CD1	1:C:151:PHE:C	2.76	0.62
3:K:766:LEU:CD1	3:K:767:PRO:HD2	2.30	0.62
3:D:179:ARG:O	3:D:182:ALA:HB3	1.99	0.62
3:D:349:ILE:HD11	3:D:369:LEU:HD21	1.81	0.62
3:D:578:ILE:CG2	3:D:579:PHE:H	2.12	0.62
1:E:197:ARG:HG3	3:L:175:ASN:HD22	1.63	0.62
3:J:397:ALA:C	3:J:399:LEU:H	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:419:PRO:HD2	3:D:422:PHE:CZ	2.34	0.62
3:K:157:TRP:HZ3	3:K:443:LEU:HD22	1.64	0.62
3:K:419:PRO:HD2	3:K:422:PHE:CE1	2.35	0.62
3:K:422:PHE:HA	3:K:424:ASN:H	1.64	0.62
3:K:766:LEU:HD11	3:K:797:GLU:CB	2.29	0.62
2:B:967:PHE:O	2:B:971:VAL:HG23	2.00	0.62
3:J:419:PRO:HD2	3:J:422:PHE:CZ	2.33	0.62
3:K:433:VAL:O	3:K:435:GLY:HA2	1.99	0.62
3:D:513:LEU:HD12	3:D:816:SER:HA	1.82	0.62
1:E:151:PHE:CD1	1:E:151:PHE:C	2.77	0.62
3:K:577:GLY:HA3	3:K:602:PHE:CD1	2.34	0.62
3:D:464:GLU:O	3:D:465:ILE:HD13	1.99	0.62
1:C:192:VAL:HG11	1:C:257:MET:HG2	1.82	0.61
3:D:160:GLN:NE2	3:D:430:PHE:CE1	2.68	0.61
3:D:433:VAL:O	3:D:435:GLY:HA2	2.00	0.61
1:A:192:VAL:HG11	1:A:257:MET:HG2	1.82	0.61
3:L:403:PHE:CD1	3:L:404:GLN:N	2.69	0.61
1:A:151:PHE:CD1	1:A:151:PHE:C	2.78	0.61
3:K:420:TRP:CZ3	3:K:461:ASN:O	2.54	0.61
1:C:191:PHE:N	1:C:191:PHE:CD1	2.67	0.61
3:D:148:ASP:HB3	3:D:149:PRO:C	2.25	0.61
1:F:195:LEU:HA	1:F:216:ASN:OD1	2.01	0.61
1:F:305:TYR:HD1	1:F:344:LEU:HB3	1.63	0.61
1:F:154:PRO:HG2	1:F:157:TYR:CD1	2.36	0.61
2:I:884:ALA:HB1	2:I:928:ILE:HG13	1.82	0.61
3:K:449:LYS:HB3	3:K:453:GLY:HA3	1.83	0.61
1:F:192:VAL:HG11	1:F:257:MET:HG2	1.83	0.61
2:H:967:PHE:O	2:H:971:VAL:HG23	2.01	0.61
3:L:379:LEU:O	3:L:382:LEU:HB2	2.01	0.61
3:D:419:PRO:HD2	3:D:422:PHE:CE1	2.36	0.61
3:D:420:TRP:CZ3	3:D:461:ASN:O	2.54	0.61
3:J:396:PRO:O	3:J:399:LEU:HB2	2.00	0.61
3:K:251:ALA:O	3:K:254:LEU:N	2.33	0.61
3:K:419:PRO:HD2	3:K:422:PHE:CZ	2.36	0.61
3:K:769:THR:HG23	3:K:778:VAL:HG13	1.82	0.61
3:L:423:GLY:HA3	3:L:455:ILE:HG23	1.81	0.60
2:H:875:ILE:HD12	2:H:920:ILE:HG12	1.81	0.60
3:K:512:THR:CG2	3:K:512:THR:O	2.48	0.60
3:L:396:PRO:O	3:L:399:LEU:HB2	2.00	0.60
1:F:193:GLY:C	1:F:195:LEU:HD23	2.26	0.60
2:I:922:VAL:O	2:I:926:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:345:GLN:N	3:J:345:GLN:OE1	2.34	0.60
1:E:191:PHE:HD1	1:E:191:PHE:N	1.99	0.60
3:K:349:ILE:HD11	3:K:369:LEU:HD21	1.83	0.60
3:K:420:TRP:O	3:K:422:PHE:O	2.19	0.60
3:D:440:LYS:HA	3:D:443:LEU:HD12	1.83	0.60
1:F:207:ASP:O	1:F:211:GLN:HG2	2.02	0.60
2:G:781:ALA:HB1	2:G:785:VAL:HB	1.83	0.60
3:D:449:LYS:HB3	3:D:453:GLY:HA3	1.84	0.60
1:F:191:PHE:HD1	1:F:191:PHE:H	1.48	0.60
3:L:397:ALA:O	3:L:398:GLU:CG	2.49	0.60
3:D:766:LEU:HD11	3:D:797:GLU:CB	2.31	0.60
3:K:411:PHE:CD1	3:K:434:GLU:O	2.54	0.60
2:G:956:ASN:HD21	2:G:966:THR:HG23	1.66	0.59
3:J:421:GLU:C	3:J:424:ASN:HB2	2.27	0.59
2:H:922:VAL:O	2:H:926:THR:HG23	2.03	0.59
2:B:782:PRO:HG2	2:B:785:VAL:HG23	1.82	0.59
3:K:440:LYS:HA	3:K:443:LEU:HD12	1.84	0.59
3:K:346:ILE:HB	3:K:367:ASN:HD22	1.67	0.59
1:F:191:PHE:N	1:F:191:PHE:CD1	2.68	0.59
3:D:180:GLN:OE1	3:D:244:LYS:HA	2.02	0.59
2:B:956:ASN:HD21	2:B:966:THR:HG23	1.66	0.59
3:D:411:PHE:CD1	3:D:434:GLU:O	2.55	0.59
3:D:578:ILE:HD12	3:D:578:ILE:N	2.17	0.59
1:A:202:PHE:CE2	1:A:208:TYR:CD1	2.89	0.59
3:D:346:ILE:HB	3:D:367:ASN:ND2	2.17	0.59
3:D:424:ASN:ND2	3:D:807:ILE:HG21	2.11	0.59
3:D:457:TYR:CD1	3:D:457:TYR:C	2.80	0.59
3:D:769:THR:HG23	3:D:778:VAL:HG13	1.83	0.59
2:H:782:PRO:HG2	2:H:785:VAL:HG23	1.83	0.59
3:K:464:GLU:O	3:K:465:ILE:HD13	2.02	0.59
3:L:419:PRO:HD2	3:L:422:PHE:HE1	1.66	0.59
3:L:433:VAL:HB	3:L:438:LEU:HD11	1.85	0.59
1:E:202:PHE:CE1	3:L:336:TRP:HB3	2.38	0.58
1:F:191:PHE:HZ	1:F:309:TYR:HD2	1.51	0.58
3:D:512:THR:CG2	3:D:512:THR:O	2.51	0.58
3:D:768:PHE:CE2	3:D:771:PHE:HB2	2.38	0.58
2:H:956:ASN:HD21	2:H:966:THR:HG23	1.66	0.58
1:A:191:PHE:N	1:A:191:PHE:HD1	2.01	0.58
1:A:199:ILE:HB	3:D:338:ALA:HB3	1.84	0.58
2:B:953:ILE:HG22	2:B:985:PRO:HB3	1.86	0.58
3:K:422:PHE:HB2	3:K:425:LEU:CD1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:457:TYR:CD1	3:K:457:TYR:C	2.81	0.58
3:K:516:HIS:O	3:K:516:HIS:ND1	2.37	0.58
3:L:177:TYR:CD2	3:L:363:TYR:CZ	2.91	0.58
3:D:423:GLY:H	3:D:458:LEU:HB2	1.67	0.58
2:G:834:ASN:HB2	2:G:835:TYR:CD1	2.39	0.58
3:K:347:PHE:H	3:K:347:PHE:HD1	1.50	0.58
2:B:955:LEU:HD23	2:B:989:ILE:HG13	1.85	0.58
3:J:417:THR:HG23	3:J:442:PHE:CE2	2.39	0.58
3:J:428:LEU:HD21	3:J:431:LEU:HB2	1.85	0.58
3:L:179:ARG:O	3:L:182:ALA:HB3	2.04	0.58
3:L:421:GLU:C	3:L:424:ASN:HB2	2.29	0.58
3:L:422:PHE:CB	3:L:425:LEU:CG	2.80	0.58
3:K:539:LYS:CB	3:K:815:PRO:HG3	2.33	0.58
2:H:955:LEU:HD23	2:H:989:ILE:HG13	1.85	0.58
1:A:298:ASP:OD1	1:A:298:ASP:N	2.35	0.58
1:E:191:PHE:HZ	1:E:309:TYR:HD2	1.51	0.58
3:J:177:TYR:CD2	3:J:363:TYR:CZ	2.92	0.58
3:K:512:THR:O	3:K:512:THR:HG23	2.04	0.58
1:A:191:PHE:N	1:A:191:PHE:CD1	2.72	0.57
3:D:455:ILE:HG22	3:D:456:PHE:N	2.19	0.57
3:J:433:VAL:HB	3:J:438:LEU:HD11	1.86	0.57
3:K:766:LEU:HD12	3:K:767:PRO:HD2	1.86	0.57
3:D:802:TYR:O	3:D:804:SER:O	2.21	0.57
1:E:191:PHE:N	1:E:191:PHE:CD1	2.70	0.57
3:J:179:ARG:O	3:J:182:ALA:HB3	2.05	0.57
2:G:798:LEU:HD12	2:G:838:LEU:HD13	1.85	0.57
1:C:199:ILE:HG22	1:C:200:GLY:H	1.69	0.57
2:G:800:ASN:ND2	2:G:804:LYS:HG3	2.20	0.57
1:A:257:MET:O	3:D:347:PHE:CD1	2.58	0.57
1:C:191:PHE:HD1	1:C:191:PHE:H	1.51	0.57
3:D:422:PHE:HB2	3:D:425:LEU:CD1	2.32	0.57
3:K:388:SER:HA	3:K:411:PHE:H	1.69	0.57
3:D:578:ILE:CG2	3:D:579:PHE:N	2.67	0.57
3:D:768:PHE:CD2	3:D:771:PHE:HB2	2.40	0.57
3:D:766:LEU:HD12	3:D:767:PRO:HD2	1.87	0.57
3:J:396:PRO:C	3:J:397:ALA:O	2.37	0.57
3:K:180:GLN:OE1	3:K:244:LYS:HA	2.04	0.57
3:D:354:PHE:CE2	3:D:373:PRO:HG2	2.40	0.57
3:D:539:LYS:CB	3:D:815:PRO:HG3	2.34	0.57
3:J:419:PRO:O	3:J:421:GLU:HG2	2.05	0.57
3:L:140:LEU:HG	3:L:437:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:422:PHE:CA	3:D:424:ASN:H	2.18	0.56
2:H:812:LEU:HD21	2:H:820:PHE:HD2	1.70	0.56
3:K:143:PRO:HD2	3:K:157:TRP:CH2	2.40	0.56
3:K:179:ARG:O	3:K:182:ALA:HB3	2.05	0.56
3:K:369:LEU:HD13	3:K:390:ASN:OD1	2.05	0.56
3:K:422:PHE:CD2	3:K:425:LEU:HD21	2.41	0.56
1:E:191:PHE:HD1	1:E:191:PHE:H	1.52	0.56
3:K:436:ASN:O	3:K:438:LEU:N	2.38	0.56
1:A:257:MET:O	3:D:347:PHE:HD1	1.88	0.56
3:D:444:LYS:HB3	2:H:963:LEU:HD12	1.87	0.56
2:G:910:ILE:HD11	2:G:988:PHE:HB3	1.88	0.56
2:I:875:ILE:HD12	2:I:920:ILE:HG12	1.88	0.56
3:K:354:PHE:CE2	3:K:373:PRO:HG2	2.41	0.56
3:D:447:THR:O	3:D:448:GLU:CD	2.49	0.56
2:G:782:PRO:HG2	2:G:785:VAL:HG23	1.86	0.56
2:G:834:ASN:HB2	2:G:835:TYR:CE1	2.41	0.56
2:G:884:ALA:HB1	2:G:928:ILE:HG13	1.87	0.56
3:J:397:ALA:O	3:J:398:GLU:CG	2.53	0.56
1:C:354:PHE:HD2	1:C:414:PRO:HB2	1.71	0.56
1:E:193:GLY:C	1:E:195:LEU:HD23	2.30	0.56
3:K:455:ILE:HG22	3:K:456:PHE:N	2.20	0.56
3:L:384:VAL:HG22	3:L:407:TYR:HB2	1.88	0.56
3:D:388:SER:HA	3:D:411:PHE:H	1.71	0.56
2:I:910:ILE:HD11	2:I:988:PHE:HB3	1.88	0.56
1:C:199:ILE:HB	3:K:338:ALA:HB3	1.87	0.56
3:D:523:TYR:CD1	3:D:523:TYR:N	2.72	0.56
1:F:194:THR:O	1:F:194:THR:CG2	2.52	0.56
3:L:422:PHE:HB2	3:L:425:LEU:CG	2.34	0.56
3:J:379:LEU:O	3:J:382:LEU:HB2	2.06	0.56
3:J:423:GLY:HA3	3:J:455:ILE:HG23	1.86	0.56
3:K:802:TYR:O	3:K:804:SER:O	2.24	0.56
2:G:867:LEU:HD13	2:G:908:MET:HE1	1.88	0.55
3:D:392:LEU:HD12	3:D:413:ASN:ND2	2.21	0.55
3:D:415:VAL:H	3:D:436:ASN:HB3	1.71	0.55
1:E:354:PHE:HD1	1:E:354:PHE:N	2.04	0.55
3:K:447:THR:O	3:K:448:GLU:CD	2.50	0.55
1:A:207:ASP:O	1:A:211:GLN:HG2	2.06	0.55
2:G:875:ILE:HD12	2:G:920:ILE:HG12	1.88	0.55
3:K:160:GLN:NE2	3:K:430:PHE:CE1	2.73	0.55
3:K:381:ASN:O	3:K:383:ARG:NH1	2.39	0.55
3:K:768:PHE:CE2	3:K:771:PHE:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:416:THR:O	3:D:438:LEU:HD23	2.06	0.55
1:E:192:VAL:HG11	1:E:257:MET:HG2	1.89	0.55
1:E:213:MET:HG3	1:E:309:TYR:CE1	2.41	0.55
3:J:419:PRO:CD	3:J:422:PHE:CE1	2.89	0.55
1:E:354:PHE:HD2	1:E:414:PRO:HB2	1.72	0.55
2:H:940:PRO:HA	2:H:942:ASN:H	1.72	0.55
3:K:142:HIS:CD2	3:K:142:HIS:N	2.75	0.55
3:K:423:GLY:H	3:K:458:LEU:HB2	1.71	0.55
3:L:419:PRO:HD2	3:L:422:PHE:CZ	2.40	0.55
3:D:142:HIS:CD2	3:D:142:HIS:N	2.75	0.55
3:D:436:ASN:O	3:D:438:LEU:N	2.39	0.55
2:G:955:LEU:HD23	2:G:989:ILE:HG13	1.88	0.55
2:I:782:PRO:HG2	2:I:785:VAL:HG23	1.87	0.55
2:I:850:LEU:HD11	2:I:854:PHE:CE2	2.42	0.55
3:J:384:VAL:HG22	3:J:407:TYR:HB2	1.89	0.55
1:A:354:PHE:HD1	1:A:354:PHE:N	2.04	0.55
1:C:344:LEU:HD13	1:C:402:PHE:HB2	1.88	0.55
3:D:369:LEU:HD13	3:D:390:ASN:OD1	2.07	0.55
3:D:397:ALA:C	3:D:399:LEU:N	2.63	0.55
1:F:354:PHE:HD1	1:F:354:PHE:N	2.05	0.55
3:D:143:PRO:HD2	3:D:157:TRP:CH2	2.42	0.55
3:D:512:THR:O	3:D:512:THR:HG23	2.07	0.55
1:E:154:PRO:HG2	1:E:157:TYR:CD1	2.42	0.55
2:H:951:LEU:HD13	2:H:988:PHE:HD2	1.72	0.55
3:K:174:PRO:O	3:K:179:ARG:NH2	2.39	0.55
3:K:415:VAL:H	3:K:436:ASN:HB3	1.72	0.55
1:A:387:ILE:O	1:A:393:GLY:HA3	2.07	0.55
1:F:213:MET:HG3	1:F:309:TYR:CE1	2.42	0.55
1:F:344:LEU:HD13	1:F:402:PHE:HB2	1.89	0.55
2:H:798:LEU:HD12	2:H:838:LEU:HD13	1.89	0.55
3:D:160:GLN:NE2	3:D:430:PHE:HE1	2.05	0.55
3:D:367:ASN:HB2	3:D:369:LEU:HD13	1.88	0.55
2:I:798:LEU:HD12	2:I:838:LEU:HD13	1.87	0.55
2:I:834:ASN:HB2	2:I:835:TYR:CD1	2.42	0.55
3:K:346:ILE:HB	3:K:367:ASN:ND2	2.21	0.55
1:A:354:PHE:N	1:A:354:PHE:CD1	2.73	0.54
3:J:148:ASP:HB3	3:J:149:PRO:O	2.06	0.54
3:L:397:ALA:C	3:L:399:LEU:H	2.15	0.54
1:A:199:ILE:HG22	1:A:200:GLY:H	1.72	0.54
3:D:347:PHE:HD1	3:D:347:PHE:H	1.53	0.54
2:H:834:ASN:HB2	2:H:835:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:396:PRO:C	3:L:397:ALA:O	2.40	0.54
1:A:191:PHE:CZ	1:A:309:TYR:CD2	2.94	0.54
1:E:348:TYR:CE1	1:E:376:LEU:HD13	2.43	0.54
1:F:354:PHE:HD2	1:F:414:PRO:HB2	1.72	0.54
2:H:800:ASN:ND2	2:H:804:LYS:HG3	2.22	0.54
3:K:443:LEU:O	3:K:447:THR:HG23	2.07	0.54
1:F:154:PRO:HG2	1:F:157:TYR:CE1	2.42	0.54
2:G:953:ILE:HG22	2:G:985:PRO:HB3	1.89	0.54
3:K:424:ASN:ND2	3:K:807:ILE:HG21	2.14	0.54
2:B:826:THR:HG22	2:B:862:GLN:OE1	2.08	0.54
1:E:354:PHE:N	1:E:354:PHE:CD1	2.74	0.54
1:F:151:PHE:C	1:F:151:PHE:HD1	2.14	0.54
3:J:420:TRP:CE2	3:J:463:PRO:CD	2.89	0.54
3:L:393:THR:HA	3:L:414:MET:O	2.07	0.54
3:L:418:LEU:HD11	3:L:454:LEU:HD21	1.90	0.54
3:K:367:ASN:HB2	3:K:369:LEU:HD13	1.90	0.54
3:K:416:THR:O	3:K:438:LEU:HD23	2.07	0.54
2:B:910:ILE:HD11	2:B:988:PHE:HB3	1.88	0.54
2:B:940:PRO:HA	2:B:942:ASN:H	1.73	0.54
1:E:207:ASP:O	1:E:211:GLN:HG2	2.08	0.54
2:I:800:ASN:ND2	2:I:804:LYS:HG3	2.23	0.54
2:I:907:GLU:OE1	2:I:907:GLU:N	2.30	0.54
3:K:156:ILE:HG21	3:K:447:THR:HA	1.88	0.54
3:K:540:LEU:CD2	3:K:815:PRO:HG2	2.38	0.54
3:D:381:ASN:O	3:D:383:ARG:NH1	2.41	0.54
3:K:143:PRO:HD2	3:K:157:TRP:CZ2	2.42	0.54
1:A:354:PHE:HD2	1:A:414:PRO:HB2	1.73	0.54
3:D:420:TRP:O	3:D:422:PHE:O	2.26	0.54
1:C:151:PHE:C	1:C:151:PHE:HD1	2.15	0.54
3:D:341:LEU:HB2	3:D:364:LEU:HD23	1.88	0.54
1:F:199:ILE:HG22	1:F:200:GLY:H	1.70	0.54
1:F:354:PHE:N	1:F:354:PHE:CD1	2.75	0.54
3:K:397:ALA:C	3:K:399:LEU:N	2.65	0.54
3:K:817:ASP:OD1	3:K:817:ASP:N	2.37	0.53
2:B:956:ASN:OD1	2:B:966:THR:HG23	2.08	0.53
3:D:152:LEU:HD12	3:D:152:LEU:H	1.72	0.53
1:F:376:LEU:HD11	1:F:405:LEU:HD22	1.89	0.53
1:F:387:ILE:O	1:F:393:GLY:HA3	2.07	0.53
3:J:140:LEU:HG	3:J:437:PRO:HB3	1.89	0.53
3:J:252:ASP:O	3:J:256:ASP:HB2	2.08	0.53
3:J:335:LEU:O	3:J:337:HIS:ND1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:422:PHE:HB3	3:K:425:LEU:CD2	2.38	0.53
3:K:567:VAL:CG1	3:K:568:PRO:CD	2.84	0.53
3:L:138:ASN:HB3	3:L:141:LEU:HD23	1.90	0.53
2:B:813:THR:HG22	2:B:814:PRO:HD2	1.91	0.53
1:C:354:PHE:CD1	1:C:354:PHE:N	2.75	0.53
3:D:567:VAL:CG1	3:D:568:PRO:CD	2.84	0.53
1:A:199:ILE:HD13	3:D:178:ALA:HA	1.91	0.53
2:B:800:ASN:ND2	2:B:804:LYS:HG3	2.24	0.53
2:H:971:VAL:O	2:H:974:LYS:HB3	2.08	0.53
2:I:812:LEU:HD21	2:I:820:PHE:HD2	1.73	0.53
3:K:422:PHE:CB	3:K:425:LEU:CG	2.85	0.53
3:J:393:THR:HA	3:J:414:MET:O	2.07	0.53
3:K:346:ILE:H	3:K:367:ASN:HB3	1.73	0.53
3:K:523:TYR:CD1	3:K:523:TYR:N	2.74	0.53
1:A:273:GLU:OE1	1:A:273:GLU:N	2.40	0.53
2:B:834:ASN:HB2	2:B:835:TYR:CD1	2.44	0.53
2:H:953:ILE:HG22	2:H:985:PRO:HB3	1.91	0.53
3:J:420:TRP:NE1	3:J:463:PRO:CD	2.72	0.53
3:D:346:ILE:H	3:D:367:ASN:HB3	1.73	0.53
3:J:446:LEU:O	3:J:450:SER:HA	2.08	0.53
3:L:148:ASP:HB3	3:L:149:PRO:O	2.08	0.53
3:L:163:LEU:HD12	3:L:430:PHE:CE1	2.43	0.53
3:L:252:ASP:O	3:L:256:ASP:HB2	2.08	0.53
1:A:344:LEU:HD21	1:A:376:LEU:HD23	1.91	0.53
3:D:143:PRO:HD2	3:D:157:TRP:CZ2	2.44	0.53
3:D:422:PHE:CB	3:D:425:LEU:CG	2.86	0.53
2:I:867:LEU:HD23	2:I:920:ILE:HG22	1.91	0.53
3:J:397:ALA:HB1	3:J:421:GLU:HG3	1.90	0.53
3:D:335:LEU:O	3:D:337:HIS:ND1	2.42	0.53
3:K:768:PHE:CD2	3:K:771:PHE:HB2	2.44	0.53
1:A:350:ILE:HD11	1:A:422:TYR:CE2	2.44	0.53
1:C:354:PHE:N	1:C:354:PHE:HD1	2.05	0.53
3:D:540:LEU:CD2	3:D:815:PRO:HG2	2.39	0.52
2:I:826:THR:HG22	2:I:862:GLN:OE1	2.09	0.52
3:L:411:PHE:O	3:L:412:ASP:CB	2.57	0.52
3:D:443:LEU:O	3:D:447:THR:HG23	2.09	0.52
2:H:910:ILE:HD11	2:H:988:PHE:HB3	1.89	0.52
1:A:219:PHE:HE1	3:D:356:TYR:CD1	2.27	0.52
1:A:247:ASN:HB3	1:A:275:HIS:CE1	2.44	0.52
3:D:376:ILE:O	3:D:379:LEU:HB2	2.09	0.52
2:I:978:LEU:HB3	2:I:982:SER:OG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:152:LEU:HD12	3:J:152:LEU:H	1.73	0.52
3:J:344:LEU:O	3:J:346:ILE:HB	2.10	0.52
3:J:419:PRO:O	3:J:420:TRP:HB2	2.09	0.52
3:K:392:LEU:HD12	3:K:413:ASN:ND2	2.24	0.52
2:G:867:LEU:HD23	2:G:920:ILE:HG22	1.92	0.52
1:C:350:ILE:HD11	1:C:422:TYR:CE2	2.45	0.52
3:D:173:GLN:O	3:D:176:ILE:HD13	2.10	0.52
1:F:258:SER:O	1:F:259:THR:C	2.53	0.52
3:L:410:PHE:CZ	3:L:433:VAL:HG12	2.43	0.52
3:L:423:GLY:HA2	3:L:455:ILE:HD12	1.91	0.52
2:H:813:THR:HG22	2:H:814:PRO:HD2	1.92	0.52
3:J:141:LEU:CD1	3:J:437:PRO:HD3	2.40	0.52
3:J:438:LEU:HD13	3:J:443:LEU:HD23	1.92	0.52
1:A:151:PHE:C	1:A:151:PHE:HD1	2.18	0.52
1:F:289:LEU:HD23	1:F:318:LEU:HD21	1.92	0.52
3:J:183:MET:HE3	3:J:183:MET:HA	1.92	0.52
1:C:191:PHE:CZ	1:C:309:TYR:CD2	2.97	0.52
1:E:376:LEU:HD11	1:E:405:LEU:HD22	1.91	0.52
2:H:788:LYS:O	2:H:792:VAL:HG23	2.09	0.52
3:J:410:PHE:CD1	3:J:410:PHE:N	2.77	0.52
3:K:186:TYR:CD1	3:K:186:TYR:C	2.88	0.52
3:K:335:LEU:O	3:K:337:HIS:ND1	2.43	0.52
1:A:191:PHE:HZ	1:A:309:TYR:HD2	1.55	0.52
3:D:423:GLY:C	3:D:425:LEU:N	2.65	0.52
3:J:397:ALA:C	3:J:399:LEU:N	2.66	0.52
3:L:407:TYR:CD1	3:L:407:TYR:N	2.78	0.52
3:K:422:PHE:CA	3:K:424:ASN:H	2.23	0.52
1:C:376:LEU:HD11	1:C:405:LEU:HD22	1.91	0.51
3:K:549:SER:HB3	3:K:552:LEU:CD2	2.40	0.51
1:A:376:LEU:HD11	1:A:405:LEU:HD22	1.91	0.51
3:D:559:SER:O	3:D:563:GLU:HG2	2.11	0.51
1:E:199:ILE:HG22	1:E:200:GLY:H	1.73	0.51
1:F:354:PHE:O	1:F:355:LYS:CB	2.58	0.51
2:I:911:GLU:O	2:I:915:GLU:HG2	2.10	0.51
3:J:403:PHE:HD1	3:J:404:GLN:N	2.09	0.51
3:J:418:LEU:HD11	3:J:454:LEU:HD21	1.92	0.51
3:J:422:PHE:HB3	3:J:425:LEU:CG	2.38	0.51
3:K:145:HIS:O	3:K:145:HIS:ND1	2.44	0.51
2:B:971:VAL:O	2:B:974:LYS:HB3	2.10	0.51
3:D:418:LEU:HB3	3:D:422:PHE:CE1	2.37	0.51
3:K:422:PHE:HD2	3:K:425:LEU:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:SER:CA	3:L:152:LEU:HD12	2.33	0.51
3:L:417:THR:HG23	3:L:442:PHE:HE2	1.73	0.51
3:L:446:LEU:O	3:L:450:SER:HA	2.09	0.51
1:A:348:TYR:CE1	1:A:376:LEU:HD13	2.46	0.51
2:B:812:LEU:HD21	2:B:820:PHE:HD2	1.75	0.51
3:J:411:PHE:O	3:J:412:ASP:CB	2.59	0.51
3:K:434:GLU:OE1	3:K:435:GLY:HA3	2.11	0.51
3:L:428:LEU:HD21	3:L:431:LEU:HB2	1.91	0.51
1:C:154:PRO:HG2	1:C:157:TYR:CD1	2.45	0.51
1:C:387:ILE:O	1:C:393:GLY:HA3	2.10	0.51
1:F:225:LEU:C	1:F:225:LEU:HD23	2.35	0.51
3:L:141:LEU:CD1	3:L:437:PRO:HD3	2.41	0.51
3:L:422:PHE:HB3	3:L:425:LEU:CG	2.38	0.51
2:H:812:LEU:HD23	2:H:846:MET:CE	2.40	0.51
3:L:403:PHE:HD1	3:L:404:GLN:N	2.09	0.51
1:C:193:GLY:C	1:C:195:LEU:HD23	2.35	0.51
1:E:151:PHE:C	1:E:151:PHE:HD1	2.16	0.51
3:K:341:LEU:HB2	3:K:364:LEU:HD23	1.91	0.51
3:K:451:VAL:HG12	3:K:452:THR:N	2.25	0.51
3:D:186:TYR:CD1	3:D:186:TYR:C	2.88	0.51
1:F:346:LEU:C	1:F:346:LEU:HD23	2.36	0.51
2:H:909:LEU:HD12	2:H:951:LEU:HD23	1.92	0.51
3:J:422:PHE:CD1	3:J:422:PHE:C	2.88	0.51
2:B:798:LEU:HD12	2:B:838:LEU:HD13	1.93	0.51
1:C:194:THR:HG23	1:C:194:THR:O	2.11	0.51
3:D:145:HIS:O	3:D:145:HIS:ND1	2.44	0.51
3:D:421:GLU:O	3:D:424:ASN:HB2	2.11	0.51
3:K:418:LEU:HB3	3:K:422:PHE:CE1	2.38	0.51
3:L:410:PHE:HE1	3:L:431:LEU:HD11	1.76	0.51
3:L:420:TRP:CE2	3:L:463:PRO:CD	2.94	0.51
1:A:391:THR:O	1:A:394:GLN:HB2	2.11	0.51
2:I:867:LEU:HD13	2:I:908:MET:HE1	1.92	0.51
2:I:953:ILE:HG22	2:I:985:PRO:HB3	1.92	0.51
3:J:407:TYR:N	3:J:407:TYR:CD1	2.79	0.51
3:J:461:ASN:N	3:J:461:ASN:OD1	2.42	0.51
3:L:183:MET:HE3	3:L:183:MET:HA	1.93	0.51
1:C:344:LEU:HD21	1:C:376:LEU:HD23	1.93	0.50
3:L:419:PRO:CD	3:L:422:PHE:CE1	2.93	0.50
3:D:526:THR:HB	3:D:810:PRO:O	2.11	0.50
3:L:410:PHE:CD1	3:L:410:PHE:N	2.78	0.50
1:C:252:PRO:HB3	1:C:257:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:174:PRO:O	3:D:179:ARG:NH2	2.45	0.50
1:E:273:GLU:N	1:E:273:GLU:OE1	2.43	0.50
3:J:423:GLY:HA2	3:J:455:ILE:HD12	1.93	0.50
3:K:423:GLY:C	3:K:425:LEU:N	2.67	0.50
3:L:152:LEU:HD12	3:L:152:LEU:H	1.76	0.50
1:C:182:TYR:CZ	1:C:237:PRO:HD3	2.46	0.50
3:D:549:SER:HB3	3:D:552:LEU:CD2	2.41	0.50
1:E:154:PRO:HG2	1:E:157:TYR:CE1	2.46	0.50
3:J:163:LEU:HD12	3:J:430:PHE:CE1	2.46	0.50
3:K:451:VAL:O	3:K:454:LEU:N	2.44	0.50
3:L:422:PHE:CD1	3:L:422:PHE:C	2.89	0.50
3:L:461:ASN:N	3:L:461:ASN:OD1	2.44	0.50
2:B:951:LEU:HD13	2:B:988:PHE:HD2	1.76	0.50
1:C:311:LEU:HD21	1:C:338:MET:HE1	1.94	0.50
3:D:422:PHE:CD2	3:D:425:LEU:HD21	2.47	0.50
3:D:800:PRO:HA	3:D:803:VAL:HG22	1.93	0.50
1:E:199:ILE:HD13	3:L:178:ALA:HA	1.93	0.50
2:G:812:LEU:HD21	2:G:820:PHE:HD2	1.76	0.50
2:H:826:THR:HG22	2:H:862:GLN:OE1	2.12	0.50
3:J:444:LYS:HE3	3:J:448:GLU:OE2	2.10	0.50
1:A:219:PHE:CE2	3:D:353:ILE:HG22	2.46	0.50
1:C:199:ILE:HD13	3:K:178:ALA:HA	1.94	0.50
1:C:355:LYS:HB2	1:C:355:LYS:NZ	2.26	0.50
3:D:451:VAL:HG12	3:D:452:THR:N	2.26	0.50
1:E:193:GLY:C	1:E:195:LEU:CD2	2.85	0.50
1:E:304:THR:HB	1:E:307:ALA:HB2	1.94	0.50
1:E:354:PHE:O	1:E:355:LYS:CB	2.59	0.50
3:K:160:GLN:NE2	3:K:430:PHE:HE1	2.09	0.50
3:L:335:LEU:O	3:L:337:HIS:ND1	2.44	0.50
1:C:219:PHE:HE1	3:K:356:TYR:CD1	2.30	0.50
2:G:911:GLU:O	2:G:915:GLU:HG2	2.12	0.50
2:I:955:LEU:HD23	2:I:989:ILE:HG13	1.93	0.50
3:K:559:SER:O	3:K:563:GLU:HG2	2.12	0.50
1:F:402:PHE:CD1	1:F:402:PHE:C	2.90	0.50
3:J:375:GLU:C	3:J:377:LYS:N	2.69	0.50
3:D:817:ASP:OD1	3:D:817:ASP:N	2.39	0.50
1:F:273:GLU:OE1	1:F:273:GLU:N	2.44	0.50
3:J:345:GLN:CD	3:J:345:GLN:H	2.19	0.50
3:L:163:LEU:HD12	3:L:430:PHE:CZ	2.46	0.50
3:L:422:PHE:HB2	3:L:425:LEU:CD1	2.42	0.50
1:C:207:ASP:O	1:C:211:GLN:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:PHE:HZ	1:F:309:TYR:CD2	2.29	0.49
3:L:344:LEU:O	3:L:346:ILE:HB	2.12	0.49
1:F:298:ASP:OD1	1:F:298:ASP:N	2.34	0.49
3:K:428:LEU:HB3	3:K:455:ILE:CD1	2.41	0.49
3:K:800:PRO:HA	3:K:803:VAL:HG22	1.92	0.49
2:B:812:LEU:HD23	2:B:846:MET:CE	2.41	0.49
1:E:258:SER:O	1:E:259:THR:C	2.55	0.49
1:E:298:ASP:OD1	1:E:298:ASP:N	2.35	0.49
1:E:387:ILE:O	1:E:393:GLY:HA3	2.12	0.49
3:K:421:GLU:O	3:K:424:ASN:HB2	2.12	0.49
3:K:526:THR:HB	3:K:810:PRO:O	2.12	0.49
3:L:345:GLN:H	3:L:345:GLN:CD	2.19	0.49
2:B:956:ASN:ND2	2:B:966:THR:HG23	2.26	0.49
1:C:298:ASP:OD1	1:C:298:ASP:N	2.36	0.49
1:E:350:ILE:HD11	1:E:422:TYR:CE2	2.47	0.49
2:H:867:LEU:HD23	2:H:920:ILE:HG22	1.95	0.49
3:K:173:GLN:O	3:K:176:ILE:HD13	2.12	0.49
3:K:459:ARG:NE	3:K:460:ASP:OD1	2.44	0.49
3:L:374:ALA:CB	3:L:398:GLU:OE2	2.59	0.49
3:J:417:THR:HG23	3:J:442:PHE:HE2	1.77	0.49
3:J:442:PHE:CE1	3:J:458:LEU:HD21	2.42	0.49
3:L:177:TYR:CD2	3:L:363:TYR:CE1	3.00	0.49
3:L:342:SER:HA	3:L:365:ASN:O	2.13	0.49
3:L:397:ALA:HB1	3:L:421:GLU:HG3	1.93	0.49
2:B:796:VAL:HG13	2:B:838:LEU:HD21	1.95	0.49
1:C:163:VAL:HG12	1:C:280:ILE:HD11	1.94	0.49
3:D:434:GLU:OE1	3:D:435:GLY:HA3	2.13	0.49
2:G:826:THR:HG22	2:G:862:GLN:OE1	2.12	0.49
3:J:343:ASN:HA	3:J:366:GLY:O	2.12	0.49
3:L:347:PHE:CD1	3:L:368:SER:HB2	2.44	0.49
1:C:191:PHE:HZ	1:C:309:TYR:HD2	1.58	0.49
3:D:519:THR:HG23	3:D:522:MET:CE	2.43	0.49
1:F:350:ILE:HD11	1:F:422:TYR:CE2	2.47	0.49
3:K:519:THR:HG23	3:K:522:MET:CE	2.43	0.49
3:L:388:SER:HB3	3:L:389:HIS:CD2	2.48	0.49
1:C:154:PRO:HG2	1:C:157:TYR:CE1	2.48	0.49
3:K:441:GLN:O	3:K:445:ILE:HG12	2.13	0.49
3:D:156:ILE:HG21	3:D:447:THR:HA	1.94	0.49
3:D:446:LEU:HA	3:D:450:SER:O	2.13	0.49
1:E:191:PHE:HZ	1:E:309:TYR:CD2	2.30	0.49
2:H:796:VAL:HG13	2:H:838:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:940:PRO:HA	2:H:942:ASN:N	2.28	0.49
2:H:981:LYS:HE2	2:H:981:LYS:HA	1.95	0.49
3:J:177:TYR:CD2	3:J:363:TYR:CE1	3.00	0.49
3:K:177:TYR:CD2	3:K:363:TYR:CE1	3.01	0.49
3:K:376:ILE:O	3:K:379:LEU:HB2	2.13	0.49
2:G:835:TYR:CD1	2:G:835:TYR:N	2.81	0.48
3:L:410:PHE:O	3:L:410:PHE:CD2	2.66	0.48
3:L:444:LYS:HE3	3:L:448:GLU:OE2	2.13	0.48
1:C:151:PHE:HD1	1:C:152:LEU:N	2.10	0.48
1:C:380:LEU:HD23	1:C:380:LEU:HA	1.66	0.48
1:E:193:GLY:O	1:E:195:LEU:HG	2.13	0.48
1:E:323:MET:HE1	1:E:330:PHE:CD1	2.49	0.48
1:F:191:PHE:CZ	1:F:309:TYR:CD2	2.92	0.48
3:L:375:GLU:CD	3:L:375:GLU:H	2.20	0.48
3:D:555:GLN:C	3:D:599:CYS:SG	2.96	0.48
2:H:956:ASN:ND2	2:H:966:THR:HG23	2.28	0.48
2:I:813:THR:HG22	2:I:814:PRO:HD2	1.94	0.48
3:J:374:ALA:CB	3:J:398:GLU:OE2	2.60	0.48
3:J:420:TRP:CD1	3:J:463:PRO:HD2	2.48	0.48
1:C:354:PHE:O	1:C:355:LYS:HG2	2.14	0.48
3:D:422:PHE:HB3	3:D:425:LEU:CD2	2.43	0.48
1:E:307:ALA:HB1	1:E:311:LEU:HG	1.95	0.48
2:B:867:LEU:HD23	2:B:920:ILE:HG22	1.96	0.48
1:F:311:LEU:HD21	1:F:338:MET:HE1	1.96	0.48
2:G:791:PHE:HE1	2:G:795:ASN:ND2	2.11	0.48
3:K:396:PRO:C	3:K:397:ALA:O	2.53	0.48
3:L:161:LEU:HD23	3:L:434:GLU:HG3	1.95	0.48
3:J:163:LEU:HD12	3:J:430:PHE:CZ	2.48	0.48
3:K:420:TRP:C	3:K:422:PHE:O	2.57	0.48
1:A:151:PHE:HD1	1:A:152:LEU:N	2.10	0.48
1:A:307:ALA:HB1	1:A:311:LEU:HG	1.96	0.48
3:D:428:LEU:HB3	3:D:455:ILE:CD1	2.41	0.48
3:L:345:GLN:N	3:L:345:GLN:CD	2.71	0.48
2:B:981:LYS:HE2	2:B:981:LYS:HA	1.96	0.48
1:C:219:PHE:HE1	3:K:356:TYR:CE1	2.32	0.48
1:F:151:PHE:HD1	1:F:152:LEU:N	2.12	0.48
1:F:348:TYR:CE1	1:F:376:LEU:HD13	2.49	0.48
3:J:142:HIS:ND1	3:J:434:GLU:OE2	2.46	0.48
3:K:410:PHE:CG	3:K:410:PHE:O	2.66	0.48
3:K:804:SER:O	3:K:805:LYS:HB2	2.14	0.48
1:F:168:LEU:HD13	1:F:280:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:971:VAL:O	2:I:974:LYS:HB3	2.13	0.48
3:J:345:GLN:N	3:J:345:GLN:CD	2.72	0.48
3:J:347:PHE:CD1	3:J:368:SER:HB2	2.45	0.48
1:A:191:PHE:HD1	1:A:191:PHE:H	1.62	0.48
1:A:304:THR:HB	1:A:307:ALA:HB2	1.95	0.48
2:B:909:LEU:HD12	2:B:951:LEU:HD23	1.96	0.48
2:B:978:LEU:HB3	2:B:982:SER:OG	2.14	0.48
3:K:769:THR:O	3:K:818:HIS:HA	2.14	0.48
1:C:304:THR:HB	1:C:307:ALA:HB2	1.95	0.47
3:K:410:PHE:HE1	3:K:431:LEU:HD11	1.78	0.47
3:K:425:LEU:O	3:K:455:ILE:HD13	2.14	0.47
1:A:163:VAL:HG12	1:A:280:ILE:HD11	1.96	0.47
1:A:194:THR:HG23	1:A:194:THR:O	2.14	0.47
1:A:354:PHE:O	1:A:355:LYS:CB	2.61	0.47
3:D:425:LEU:O	3:D:455:ILE:HD13	2.14	0.47
2:G:981:LYS:HA	2:G:981:LYS:HE2	1.96	0.47
3:J:422:PHE:HB2	3:J:425:LEU:CG	2.40	0.47
1:A:311:LEU:HD21	1:A:338:MET:HE1	1.96	0.47
3:D:396:PRO:C	3:D:397:ALA:O	2.56	0.47
1:F:304:THR:HB	1:F:307:ALA:HB2	1.96	0.47
2:G:788:LYS:O	2:G:792:VAL:HG23	2.13	0.47
2:G:971:VAL:O	2:G:974:LYS:HB3	2.13	0.47
2:H:791:PHE:HE1	2:H:795:ASN:ND2	2.12	0.47
1:C:247:ASN:HB3	1:C:275:HIS:CE1	2.49	0.47
1:C:258:SER:C	1:C:260:GLU:N	2.70	0.47
1:C:273:GLU:N	1:C:273:GLU:OE1	2.47	0.47
3:D:397:ALA:HA	3:D:421:GLU:HG3	1.95	0.47
1:E:151:PHE:HD1	1:E:152:LEU:N	2.12	0.47
3:J:408:PHE:C	3:J:408:PHE:CD1	2.91	0.47
3:D:346:ILE:O	3:D:369:LEU:HD12	2.15	0.47
3:D:441:GLN:O	3:D:445:ILE:HG12	2.15	0.47
1:F:182:TYR:CZ	1:F:237:PRO:HD3	2.50	0.47
1:F:344:LEU:HD21	1:F:376:LEU:HD23	1.95	0.47
1:F:346:LEU:HD23	1:F:346:LEU:O	2.13	0.47
2:I:901:LYS:HG2	2:I:902:ASN:N	2.29	0.47
3:L:372:LEU:HD12	3:L:373:PRO:HD2	1.95	0.47
2:B:809:LYS:HG3	2:B:846:MET:SD	2.54	0.47
1:C:182:TYR:CE2	1:C:237:PRO:HD3	2.50	0.47
3:D:451:VAL:O	3:D:454:LEU:N	2.47	0.47
2:H:764:LEU:HD12	2:H:864:PHE:CD1	2.50	0.47
3:J:413:ASN:O	3:J:436:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:536:ARG:O	3:K:540:LEU:HG	2.15	0.47
3:D:769:THR:O	3:D:818:HIS:HA	2.14	0.47
3:D:812:ASP:OD1	3:D:812:ASP:C	2.58	0.47
1:E:182:TYR:CZ	1:E:237:PRO:HD3	2.50	0.47
1:F:193:GLY:C	1:F:195:LEU:CD2	2.87	0.47
2:G:809:LYS:HG3	2:G:846:MET:SD	2.55	0.47
2:H:834:ASN:HB2	2:H:835:TYR:CE1	2.49	0.47
2:I:788:LYS:O	2:I:792:VAL:HG23	2.14	0.47
2:I:938:PHE:O	2:I:945:THR:OG1	2.22	0.47
3:J:358:PHE:N	3:J:358:PHE:CD1	2.82	0.47
3:J:372:LEU:HD12	3:J:373:PRO:HD2	1.96	0.47
3:J:410:PHE:CZ	3:J:433:VAL:HG12	2.48	0.47
3:J:422:PHE:CB	3:J:425:LEU:CG	2.83	0.47
3:K:143:PRO:HG3	3:K:443:LEU:HD13	1.97	0.47
3:K:458:LEU:O	3:K:459:ARG:C	2.57	0.47
3:L:410:PHE:O	3:L:410:PHE:CG	2.68	0.47
3:L:413:ASN:O	3:L:436:ASN:HB3	2.14	0.47
1:C:179:VAL:HG23	1:C:294:LEU:HD23	1.97	0.47
3:D:436:ASN:OD1	3:D:436:ASN:N	2.48	0.47
3:D:579:PHE:HZ	3:D:598:GLY:HA3	1.79	0.47
3:K:812:ASP:OD1	3:K:812:ASP:C	2.58	0.47
1:A:154:PRO:HG2	1:A:157:TYR:CE1	2.50	0.47
1:A:191:PHE:HZ	1:A:309:TYR:CD2	2.32	0.47
2:B:940:PRO:HA	2:B:942:ASN:N	2.29	0.47
2:G:796:VAL:HG13	2:G:838:LEU:HD21	1.97	0.47
3:K:152:LEU:HD12	3:K:152:LEU:H	1.79	0.47
3:K:244:LYS:CB	3:K:247:LEU:HB2	2.45	0.47
1:A:202:PHE:HB2	1:A:203:ARG:H	1.48	0.47
3:D:173:GLN:CB	3:D:179:ARG:HH12	2.28	0.47
3:D:177:TYR:CD2	3:D:363:TYR:CE1	3.03	0.47
1:E:346:LEU:C	1:E:346:LEU:HD23	2.40	0.47
2:I:940:PRO:HA	2:I:942:ASN:H	1.79	0.47
3:L:438:LEU:HD13	3:L:443:LEU:HD23	1.97	0.47
1:C:219:PHE:CE1	3:K:356:TYR:CE1	3.03	0.46
1:E:191:PHE:CZ	1:E:309:TYR:CD2	2.94	0.46
2:I:981:LYS:HE2	2:I:981:LYS:HA	1.96	0.46
3:K:163:LEU:HD11	3:K:249:GLU:CA	2.40	0.46
3:D:339:LEU:HB2	3:D:359:LEU:HD11	1.97	0.46
3:J:341:LEU:O	3:J:344:LEU:HD11	2.15	0.46
3:J:419:PRO:CD	3:J:422:PHE:HE1	2.28	0.46
3:L:425:LEU:CD1	3:L:428:LEU:HD22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:CD2	3:D:353:ILE:HG22	2.51	0.46
3:D:151:LEU:HB3	3:D:157:TRP:HB3	1.97	0.46
3:D:410:PHE:HE1	3:D:431:LEU:HD11	1.79	0.46
3:D:410:PHE:O	3:D:410:PHE:CG	2.68	0.46
3:D:452:THR:HA	3:D:455:ILE:HB	1.98	0.46
3:D:550:ASP:O	3:D:603:PHE:HA	2.16	0.46
3:J:375:GLU:CD	3:J:375:GLU:H	2.22	0.46
3:K:446:LEU:HA	3:K:450:SER:O	2.16	0.46
3:D:384:VAL:HA	3:D:407:TYR:O	2.15	0.46
2:H:956:ASN:OD1	2:H:966:THR:HG23	2.16	0.46
2:I:956:ASN:ND2	2:I:966:THR:HG23	2.29	0.46
3:J:364:LEU:HD23	3:J:364:LEU:HA	1.76	0.46
3:L:408:PHE:CD1	3:L:408:PHE:C	2.92	0.46
1:A:219:PHE:CE1	3:D:353:ILE:HA	2.51	0.46
1:A:380:LEU:HA	1:A:380:LEU:HD23	1.69	0.46
1:C:391:THR:O	1:C:394:GLN:HB2	2.16	0.46
3:D:465:ILE:HA	3:D:466:PRO:HD2	1.68	0.46
1:E:344:LEU:HD13	1:E:402:PHE:HB2	1.97	0.46
2:G:978:LEU:HB3	2:G:982:SER:OG	2.15	0.46
2:H:867:LEU:HD13	2:H:908:MET:HE1	1.98	0.46
2:H:880:LEU:CD2	2:H:920:ILE:HG23	2.45	0.46
3:J:161:LEU:HD23	3:J:434:GLU:HG3	1.98	0.46
3:K:372:LEU:HB3	3:K:396:PRO:HG3	1.97	0.46
3:L:142:HIS:ND1	3:L:434:GLU:OE2	2.48	0.46
1:A:252:PRO:HB3	1:A:257:MET:CE	2.45	0.46
3:D:434:GLU:HA	3:D:435:GLY:HA2	1.54	0.46
2:I:835:TYR:CD1	2:I:835:TYR:N	2.83	0.46
3:K:151:LEU:HB3	3:K:157:TRP:HB3	1.98	0.46
1:A:323:MET:HE1	1:A:330:PHE:CD1	2.50	0.46
2:B:835:TYR:CD1	2:B:835:TYR:N	2.84	0.46
1:C:258:SER:O	1:C:259:THR:C	2.56	0.46
3:D:522:MET:C	3:D:523:TYR:CD1	2.94	0.46
2:G:940:PRO:HA	2:G:942:ASN:H	1.81	0.46
2:H:979:THR:C	2:H:981:LYS:N	2.74	0.46
2:I:764:LEU:HD12	2:I:864:PHE:CD1	2.51	0.46
3:K:346:ILE:HD12	3:K:367:ASN:ND2	2.30	0.46
3:K:431:LEU:O	3:K:431:LEU:HG	2.16	0.46
2:B:764:LEU:HD12	2:B:864:PHE:CD1	2.51	0.46
1:C:213:MET:HG3	1:C:309:TYR:CE1	2.50	0.46
3:D:374:ALA:C	3:D:376:ILE:N	2.73	0.46
3:J:388:SER:HB3	3:J:389:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLY:C	1:A:195:LEU:HD23	2.40	0.46
1:A:258:SER:C	1:A:260:GLU:N	2.73	0.46
1:C:390:THR:HG1	1:C:393:GLY:H	1.57	0.46
3:D:383:ARG:HA	3:D:405:LEU:HA	1.97	0.46
3:D:456:PHE:O	3:D:457:TYR:C	2.56	0.46
1:F:184:HIS:O	1:F:229:LEU:HA	2.16	0.46
2:H:820:PHE:CD1	2:H:820:PHE:C	2.92	0.46
3:J:138:ASN:HB3	3:J:141:LEU:HD23	1.97	0.46
3:K:397:ALA:HA	3:K:421:GLU:HG3	1.98	0.46
3:D:143:PRO:HG3	3:D:443:LEU:HD13	1.98	0.45
2:I:834:ASN:HB2	2:I:835:TYR:CE1	2.51	0.45
3:K:356:TYR:CD2	3:K:358:PHE:HE1	2.33	0.45
2:B:788:LYS:O	2:B:792:VAL:HG23	2.16	0.45
2:B:834:ASN:HB2	2:B:835:TYR:CE1	2.51	0.45
1:C:201:THR:C	1:C:202:PHE:CG	2.93	0.45
1:A:344:LEU:HD13	1:A:402:PHE:HB2	1.97	0.45
1:C:380:LEU:HD22	1:C:404:GLN:HG2	1.98	0.45
3:D:372:LEU:HB3	3:D:396:PRO:HG3	1.98	0.45
1:E:219:PHE:CZ	3:L:356:TYR:CE2	3.04	0.45
1:E:344:LEU:HD21	1:E:376:LEU:HD23	1.97	0.45
1:E:390:THR:HG1	1:E:393:GLY:H	1.61	0.45
2:H:911:GLU:O	2:H:915:GLU:HG2	2.15	0.45
3:J:379:LEU:HD23	3:J:379:LEU:HA	1.74	0.45
3:K:434:GLU:HA	3:K:435:GLY:HA2	1.55	0.45
3:L:376:ILE:O	3:L:379:LEU:HB2	2.16	0.45
1:A:225:LEU:C	1:A:225:LEU:HD23	2.41	0.45
1:C:165:LYS:NZ	1:C:165:LYS:HB3	2.30	0.45
3:D:405:LEU:HD13	3:D:408:PHE:HB2	1.98	0.45
1:E:380:LEU:HD22	1:E:404:GLN:HG2	1.98	0.45
3:J:372:LEU:HA	3:J:373:PRO:HD2	1.87	0.45
3:J:374:ALA:C	3:J:376:ILE:N	2.74	0.45
3:L:167:SER:O	3:L:170:SER:HB2	2.17	0.45
3:L:383:ARG:HG2	3:L:406:LYS:HG3	1.99	0.45
3:D:458:LEU:O	3:D:459:ARG:C	2.59	0.45
3:D:522:MET:C	3:D:523:TYR:HD1	2.24	0.45
3:D:799:ASP:O	3:D:802:TYR:HB3	2.17	0.45
1:E:402:PHE:CD1	1:E:402:PHE:C	2.94	0.45
1:F:307:ALA:HB1	1:F:311:LEU:HG	1.99	0.45
1:F:323:MET:HE1	1:F:330:PHE:CD1	2.52	0.45
2:H:921:VAL:O	2:H:924:PHE:HB3	2.17	0.45
2:H:978:LEU:HB3	2:H:982:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:403:PHE:CD1	3:L:403:PHE:C	2.95	0.45
1:A:154:PRO:HG2	1:A:157:TYR:CD1	2.51	0.45
1:C:168:LEU:HD13	1:C:280:ILE:HD12	1.99	0.45
3:D:579:PHE:O	3:D:579:PHE:CD1	2.70	0.45
1:F:258:SER:C	1:F:260:GLU:N	2.73	0.45
2:G:813:THR:HG22	2:G:814:PRO:HD2	1.99	0.45
2:G:951:LEU:HD13	2:G:988:PHE:HD2	1.82	0.45
2:I:791:PHE:HE1	2:I:795:ASN:ND2	2.14	0.45
2:I:951:LEU:HD13	2:I:988:PHE:HD2	1.82	0.45
3:J:163:LEU:HD23	3:J:163:LEU:HA	1.81	0.45
3:K:452:THR:HA	3:K:455:ILE:HB	1.99	0.45
3:L:420:TRP:NE1	3:L:463:PRO:CD	2.80	0.45
1:A:201:THR:O	1:A:202:PHE:CD2	2.70	0.45
1:C:202:PHE:C	1:C:203:ARG:HG3	2.41	0.45
1:C:257:MET:HE1	1:C:262:LEU:CD1	2.43	0.45
1:C:354:PHE:CE2	1:C:415:ASN:ND2	2.85	0.45
2:H:835:TYR:CD1	2:H:835:TYR:N	2.84	0.45
2:H:929:LEU:HD23	2:H:929:LEU:HA	1.61	0.45
2:I:796:VAL:HG13	2:I:838:LEU:HD21	1.99	0.45
3:K:766:LEU:HD12	3:K:766:LEU:HA	1.73	0.45
1:A:179:VAL:HG23	1:A:294:LEU:HD23	1.99	0.45
2:B:791:PHE:HE1	2:B:795:ASN:ND2	2.15	0.45
1:E:225:LEU:HD23	1:E:225:LEU:C	2.42	0.45
2:G:921:VAL:O	2:G:925:VAL:HG23	2.17	0.45
3:J:342:SER:HA	3:J:365:ASN:O	2.17	0.45
3:K:384:VAL:HA	3:K:407:TYR:O	2.16	0.45
1:C:348:TYR:CE1	1:C:376:LEU:HD13	2.52	0.45
2:G:907:GLU:OE1	2:G:907:GLU:N	2.35	0.45
1:C:202:PHE:O	1:C:203:ARG:HG3	2.17	0.45
3:D:431:LEU:O	3:D:431:LEU:HG	2.17	0.45
1:E:263:GLU:OE1	1:E:263:GLU:HA	2.16	0.45
1:F:249:GLU:HA	1:F:275:HIS:O	2.16	0.45
3:L:180:GLN:OE1	3:L:244:LYS:HA	2.17	0.45
1:C:201:THR:O	1:C:202:PHE:CD2	2.70	0.44
1:C:307:ALA:HB1	1:C:311:LEU:HG	1.99	0.44
1:F:257:MET:HE1	1:F:262:LEU:CD1	2.47	0.44
2:I:792:VAL:HG11	2:I:808:LEU:HB2	1.97	0.44
3:L:464:GLU:O	3:L:465:ILE:CB	2.65	0.44
2:B:837:ASP:O	2:B:840:SER:HB3	2.17	0.44
2:B:865:VAL:HG22	1:F:410:MET:HE3	1.98	0.44
2:B:867:LEU:HD13	2:B:908:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:424:ASN:ND2	3:D:807:ILE:CG2	2.73	0.44
3:J:415:VAL:H	3:J:436:ASN:CB	2.30	0.44
3:K:420:TRP:O	3:K:421:GLU:C	2.61	0.44
3:L:379:LEU:HD23	3:L:379:LEU:HA	1.77	0.44
1:A:257:MET:HE1	1:A:262:LEU:CD1	2.43	0.44
3:J:387:LEU:HD13	3:J:392:LEU:HD11	1.98	0.44
3:J:425:LEU:CD1	3:J:428:LEU:HD22	2.47	0.44
3:K:522:MET:C	3:K:523:TYR:CD1	2.96	0.44
3:L:358:PHE:CD1	3:L:358:PHE:N	2.85	0.44
1:C:301:THR:HG23	1:C:340:ASN:OD1	2.17	0.44
3:D:422:PHE:HD2	3:D:425:LEU:HD21	1.82	0.44
3:D:444:LYS:HB3	2:H:963:LEU:CD1	2.46	0.44
1:E:163:VAL:HG12	1:E:280:ILE:HD11	1.97	0.44
1:A:256:ILE:HG12	3:D:349:ILE:HA	2.00	0.44
1:C:168:LEU:HD22	1:C:280:ILE:HG23	1.99	0.44
1:C:191:PHE:HZ	1:C:309:TYR:CD2	2.35	0.44
1:C:258:SER:O	1:C:260:GLU:N	2.50	0.44
1:E:257:MET:HE1	1:E:262:LEU:CD1	2.47	0.44
1:F:391:THR:O	1:F:394:GLN:HB2	2.18	0.44
2:I:929:LEU:HA	2:I:929:LEU:HD23	1.59	0.44
3:J:361:ARG:O	3:J:384:VAL:O	2.35	0.44
3:J:403:PHE:CD1	3:J:403:PHE:C	2.96	0.44
3:K:339:LEU:HB2	3:K:359:LEU:HD11	2.00	0.44
3:K:383:ARG:HA	3:K:405:LEU:HA	1.98	0.44
3:L:361:ARG:O	3:L:384:VAL:O	2.35	0.44
3:L:397:ALA:C	3:L:399:LEU:N	2.74	0.44
3:L:462:ARG:HA	3:L:463:PRO:HD3	1.67	0.44
1:A:249:GLU:HA	1:A:275:HIS:O	2.18	0.44
1:A:380:LEU:HD22	1:A:404:GLN:HG2	2.00	0.44
1:F:199:ILE:HG22	1:F:200:GLY:N	2.32	0.44
2:G:901:LYS:HG2	2:G:902:ASN:N	2.33	0.44
3:J:176:ILE:HD11	3:J:343:ASN:ND2	2.32	0.44
3:J:392:LEU:O	3:J:413:ASN:HB3	2.18	0.44
3:J:418:LEU:CD1	3:J:454:LEU:HD21	2.47	0.44
3:D:354:PHE:HE2	3:D:373:PRO:HG2	1.80	0.44
3:K:374:ALA:C	3:K:376:ILE:N	2.75	0.44
3:L:363:TYR:HE1	3:L:384:VAL:HG11	1.82	0.44
3:D:810:PRO:HB3	3:D:816:SER:N	2.32	0.44
1:E:323:MET:HE2	1:E:324:PRO:HD2	2.00	0.44
3:J:374:ALA:C	3:J:376:ILE:H	2.26	0.44
3:J:445:ILE:CD1	3:J:457:TYR:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:173:GLN:CB	3:K:179:ARG:HH12	2.31	0.44
3:K:346:ILE:O	3:K:369:LEU:HD12	2.18	0.44
1:A:258:SER:O	1:A:259:THR:C	2.58	0.44
2:B:929:LEU:HD23	2:B:929:LEU:HA	1.65	0.44
1:C:336:GLN:HB3	2:H:937:ILE:HD11	1.99	0.44
3:D:441:GLN:HA	3:D:444:LYS:HD2	2.00	0.44
3:J:394:SER:O	3:J:395:LEU:HD23	2.17	0.44
3:K:544:ILE:HG23	3:K:552:LEU:CD1	2.47	0.44
3:D:768:PHE:HA	3:D:778:VAL:HG22	2.00	0.43
1:E:168:LEU:HD13	1:E:280:ILE:HD12	1.99	0.43
1:E:391:THR:O	1:E:394:GLN:HB2	2.18	0.43
3:K:177:TYR:HE1	3:K:365:ASN:HD21	1.65	0.43
3:L:388:SER:CB	3:L:389:HIS:CD2	3.01	0.43
1:A:193:GLY:O	1:A:195:LEU:HG	2.18	0.43
1:A:201:THR:C	1:A:202:PHE:CG	2.96	0.43
2:B:792:VAL:HG11	2:B:808:LEU:HB2	2.00	0.43
3:D:420:TRP:C	3:D:422:PHE:O	2.61	0.43
1:E:219:PHE:HE2	3:L:339:LEU:HD11	1.83	0.43
1:F:185:VAL:HG23	1:F:229:LEU:HD12	2.00	0.43
2:I:809:LYS:HG3	2:I:846:MET:SD	2.58	0.43
3:K:450:SER:OG	3:K:451:VAL:N	2.50	0.43
3:L:346:ILE:HD13	3:L:346:ILE:HG21	1.55	0.43
3:L:407:TYR:N	3:L:407:TYR:HD1	2.16	0.43
2:B:979:THR:C	2:B:981:LYS:N	2.77	0.43
3:D:152:LEU:HD12	3:D:152:LEU:N	2.33	0.43
3:D:160:GLN:NE2	3:D:430:PHE:CZ	2.85	0.43
3:D:392:LEU:CB	3:D:413:ASN:HD22	2.23	0.43
2:G:820:PHE:CD1	2:G:820:PHE:C	2.96	0.43
2:G:938:PHE:O	2:G:945:THR:OG1	2.23	0.43
3:K:551:LEU:HD21	3:K:601:ILE:HG23	2.00	0.43
3:L:368:SER:O	3:L:369:LEU:C	2.61	0.43
1:C:199:ILE:HG22	1:C:200:GLY:N	2.32	0.43
1:C:386:SER:O	1:C:389:THR:HG23	2.18	0.43
3:D:389:HIS:HA	3:D:412:ASP:HB3	2.00	0.43
3:D:441:GLN:O	3:D:444:LYS:HB2	2.18	0.43
3:D:544:ILE:HG23	3:D:552:LEU:CD1	2.48	0.43
2:H:880:LEU:HD22	2:H:920:ILE:HG23	1.99	0.43
3:J:343:ASN:OD1	3:J:366:GLY:HA3	2.17	0.43
3:J:379:LEU:HB3	3:J:382:LEU:HD13	2.00	0.43
3:J:420:TRP:CZ2	3:J:463:PRO:HD3	2.52	0.43
3:K:436:ASN:OD1	3:K:436:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:441:GLN:HA	3:K:444:LYS:HD2	2.00	0.43
3:L:375:GLU:OE1	3:L:375:GLU:N	2.52	0.43
1:A:390:THR:HG1	1:A:393:GLY:H	1.61	0.43
3:D:356:TYR:CD2	3:D:358:PHE:HE1	2.36	0.43
3:D:369:LEU:HD12	3:D:369:LEU:N	2.33	0.43
3:D:766:LEU:HD12	3:D:766:LEU:HA	1.74	0.43
2:G:929:LEU:HA	2:G:929:LEU:HD23	1.55	0.43
3:J:341:LEU:O	3:J:344:LEU:CD1	2.67	0.43
3:K:254:LEU:HD23	3:K:254:LEU:HA	1.70	0.43
3:K:766:LEU:HD12	3:K:767:PRO:CD	2.48	0.43
1:A:165:LYS:NZ	1:A:165:LYS:HB3	2.33	0.43
1:E:332:TRP:CZ2	1:E:336:GLN:HG3	2.54	0.43
2:H:979:THR:C	2:H:981:LYS:H	2.25	0.43
1:C:249:GLU:HA	1:C:275:HIS:O	2.19	0.43
3:D:163:LEU:HD23	3:D:163:LEU:HA	1.78	0.43
1:E:346:LEU:HD23	1:E:346:LEU:O	2.18	0.43
2:I:813:THR:HG22	2:I:814:PRO:CD	2.49	0.43
3:J:180:GLN:OE1	3:J:244:LYS:HA	2.19	0.43
3:K:445:ILE:HG13	3:K:457:TYR:HD2	1.84	0.43
3:L:394:SER:O	3:L:395:LEU:HD23	2.18	0.43
1:E:247:ASN:HB3	1:E:275:HIS:CE1	2.53	0.43
1:E:289:LEU:HD23	1:E:318:LEU:HD21	2.01	0.43
3:J:410:PHE:HE1	3:J:431:LEU:HD11	1.84	0.43
3:K:392:LEU:CB	3:K:413:ASN:HD22	2.24	0.43
3:L:387:LEU:HD13	3:L:392:LEU:HD11	2.00	0.43
3:L:418:LEU:HB3	3:L:422:PHE:CE1	2.53	0.43
1:C:179:VAL:CG2	1:C:294:LEU:HD23	2.49	0.43
3:D:345:GLN:N	3:D:345:GLN:CD	2.76	0.43
3:D:374:ALA:C	3:D:376:ILE:H	2.26	0.43
3:D:769:THR:CG2	3:D:778:VAL:HG13	2.49	0.43
2:G:880:LEU:CD2	2:G:920:ILE:HG23	2.49	0.43
2:H:956:ASN:OD1	2:H:966:THR:HA	2.19	0.43
3:J:356:TYR:HB3	3:J:358:PHE:HE1	1.83	0.43
3:K:371:GLU:HG2	3:K:372:LEU:N	2.33	0.43
3:L:457:TYR:HE1	3:L:461:ASN:ND2	2.17	0.43
1:C:346:LEU:HD23	1:C:346:LEU:C	2.43	0.43
1:E:271:ASN:C	1:E:271:ASN:OD1	2.62	0.43
3:J:422:PHE:HA	3:J:424:ASN:H	1.80	0.43
3:L:415:VAL:H	3:L:436:ASN:CB	2.32	0.43
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.82	0.42
3:D:450:SER:OG	3:D:451:VAL:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:766:LEU:HD12	3:D:767:PRO:CD	2.48	0.42
2:I:940:PRO:HA	2:I:942:ASN:N	2.34	0.42
3:J:415:VAL:H	3:J:436:ASN:HB3	1.84	0.42
3:K:522:MET:C	3:K:523:TYR:HD1	2.27	0.42
3:L:374:ALA:C	3:L:376:ILE:N	2.77	0.42
3:L:375:GLU:C	3:L:377:LYS:N	2.76	0.42
1:A:325:ASN:HB2	1:A:326:ASN:HD22	1.84	0.42
3:D:173:GLN:O	3:D:176:ILE:CD1	2.67	0.42
1:F:182:TYR:CE2	1:F:237:PRO:HD3	2.54	0.42
1:F:380:LEU:HD22	1:F:404:GLN:HG2	2.00	0.42
2:G:956:ASN:OD1	2:G:966:THR:HA	2.20	0.42
2:I:921:VAL:O	2:I:924:PHE:HB3	2.19	0.42
2:I:956:ASN:OD1	2:I:966:THR:HA	2.19	0.42
3:J:375:GLU:O	3:J:376:ILE:C	2.61	0.42
3:K:421:GLU:O	3:K:422:PHE:C	2.61	0.42
3:D:150:SER:HA	3:D:152:LEU:CD1	2.50	0.42
3:D:371:GLU:HG2	3:D:372:LEU:N	2.34	0.42
3:D:422:PHE:CA	3:D:424:ASN:N	2.72	0.42
1:F:168:LEU:HD22	1:F:280:ILE:HG23	2.00	0.42
2:G:905:PHE:O	2:G:906:ARG:C	2.59	0.42
2:G:929:LEU:HB3	2:G:972:LEU:HD11	2.00	0.42
2:I:931:ARG:O	2:I:934:GLU:HG3	2.19	0.42
3:K:354:PHE:HE2	3:K:373:PRO:HG2	1.81	0.42
3:K:413:ASN:HB2	3:K:436:ASN:ND2	2.34	0.42
1:A:158:LEU:HD11	1:A:385:PHE:CE2	2.54	0.42
1:A:336:GLN:HB3	2:B:937:ILE:HD11	2.00	0.42
3:D:365:ASN:OD1	3:D:365:ASN:N	2.49	0.42
1:E:387:ILE:O	1:E:390:THR:HG23	2.18	0.42
2:G:764:LEU:HD12	2:G:864:PHE:CD1	2.55	0.42
2:I:979:THR:C	2:I:981:LYS:N	2.77	0.42
3:J:410:PHE:CG	3:J:410:PHE:O	2.69	0.42
3:K:356:TYR:HD2	3:K:358:PHE:HE1	1.66	0.42
3:K:365:ASN:OD1	3:K:365:ASN:N	2.49	0.42
3:K:809:PHE:HB3	3:K:810:PRO:HA	2.01	0.42
2:B:956:ASN:OD1	2:B:966:THR:HA	2.19	0.42
2:H:905:PHE:O	2:H:906:ARG:C	2.62	0.42
3:J:383:ARG:HG2	3:J:406:LYS:HG3	2.01	0.42
1:A:202:PHE:C	1:A:203:ARG:HG3	2.44	0.42
2:B:813:THR:HG22	2:B:814:PRO:CD	2.50	0.42
1:C:265:LEU:O	1:C:268:SER:HB3	2.20	0.42
1:C:271:ASN:OD1	1:C:271:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ASN:HB2	1:C:326:ASN:HD22	1.84	0.42
3:D:445:ILE:HG13	3:D:457:TYR:HD2	1.84	0.42
1:E:202:PHE:HB2	1:E:203:ARG:H	1.44	0.42
1:F:213:MET:O	1:F:217:VAL:HG23	2.19	0.42
1:F:332:TRP:CZ2	1:F:336:GLN:HG3	2.55	0.42
2:G:979:THR:C	2:G:981:LYS:N	2.76	0.42
2:I:929:LEU:HB3	2:I:972:LEU:HD11	2.00	0.42
3:K:379:LEU:HB3	3:K:382:LEU:HD13	2.01	0.42
3:L:445:ILE:CD1	3:L:457:TYR:CD2	3.02	0.42
1:C:354:PHE:O	1:C:355:LYS:CB	2.67	0.42
1:C:402:PHE:CD1	1:C:402:PHE:C	2.98	0.42
3:D:170:SER:O	3:D:176:ILE:HD12	2.20	0.42
3:D:536:ARG:O	3:D:540:LEU:HG	2.20	0.42
1:E:202:PHE:CZ	1:E:208:TYR:HD1	2.38	0.42
1:E:219:PHE:HZ	3:L:356:TYR:CE2	2.37	0.42
1:F:202:PHE:HB2	1:F:203:ARG:H	1.45	0.42
3:J:464:GLU:HB3	3:J:465:ILE:H	1.57	0.42
3:K:551:LEU:HD21	3:K:601:ILE:CG2	2.50	0.42
2:B:820:PHE:C	2:B:820:PHE:CD1	2.96	0.42
2:G:910:ILE:HG22	2:G:914:LYS:HE2	2.01	0.42
2:G:942:ASN:OD1	2:G:944:TRP:HB3	2.20	0.42
2:I:820:PHE:C	2:I:820:PHE:CD1	2.97	0.42
3:K:163:LEU:HD23	3:K:163:LEU:HA	1.79	0.42
3:K:459:ARG:HD3	3:K:524:ARG:O	2.20	0.42
3:L:423:GLY:H	3:L:458:LEU:HB2	1.85	0.42
1:A:323:MET:HE1	1:A:330:PHE:CE1	2.54	0.42
3:D:353:ILE:O	3:D:356:TYR:HB2	2.19	0.42
1:E:184:HIS:O	1:E:229:LEU:HA	2.20	0.42
1:E:256:ILE:HG23	3:L:346:ILE:HD11	2.01	0.42
1:E:323:MET:HE1	1:E:330:PHE:CE1	2.55	0.42
1:F:154:PRO:HG2	1:F:157:TYR:CG	2.54	0.42
2:H:813:THR:HB	2:H:815:ASN:OD1	2.20	0.42
3:L:418:LEU:CD1	3:L:454:LEU:HD21	2.49	0.42
1:A:307:ALA:O	1:A:308:ALA:C	2.61	0.42
1:C:354:PHE:CZ	1:C:415:ASN:ND2	2.88	0.42
3:D:157:TRP:CZ3	3:D:443:LEU:HD22	2.48	0.42
2:H:837:ASP:O	2:H:840:SER:HB3	2.20	0.42
3:J:369:LEU:N	3:J:390:ASN:OD1	2.52	0.42
3:J:421:GLU:O	3:J:422:PHE:C	2.62	0.42
3:L:349:ILE:HD13	3:L:349:ILE:HA	1.87	0.42
1:C:350:ILE:CD1	1:C:422:TYR:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:PHE:HE2	1:C:415:ASN:HB3	1.85	0.41
3:D:514:CYS:SG	3:D:517:TYR:HD1	2.43	0.41
2:G:940:PRO:HA	2:G:942:ASN:N	2.35	0.41
2:H:792:VAL:HG11	2:H:808:LEU:HB2	2.02	0.41
3:J:141:LEU:HD11	3:J:437:PRO:HD3	2.01	0.41
3:K:170:SER:O	3:K:176:ILE:HD12	2.20	0.41
3:K:405:LEU:HD13	3:K:408:PHE:HB2	2.01	0.41
3:L:176:ILE:H	3:L:176:ILE:HG13	1.39	0.41
3:L:364:LEU:HD23	3:L:364:LEU:HA	1.83	0.41
3:L:420:TRP:CD1	3:L:463:PRO:HD2	2.55	0.41
1:A:422:TYR:CD1	1:A:422:TYR:N	2.88	0.41
2:B:813:THR:HB	2:B:815:ASN:OD1	2.20	0.41
1:C:193:GLY:C	1:C:195:LEU:CD2	2.92	0.41
3:D:166:VAL:HG21	3:D:248:MET:HG3	2.02	0.41
3:D:435:GLY:C	3:D:436:ASN:OD1	2.62	0.41
1:E:165:LYS:NZ	1:E:165:LYS:HB3	2.36	0.41
1:E:199:ILE:HG22	1:E:200:GLY:N	2.34	0.41
1:E:258:SER:C	1:E:260:GLU:N	2.76	0.41
1:F:380:LEU:HD23	1:F:380:LEU:HA	1.71	0.41
3:J:464:GLU:O	3:J:465:ILE:CB	2.67	0.41
3:K:177:TYR:OH	3:K:386:ASP:OD2	2.39	0.41
3:K:513:LEU:HB3	3:K:536:ARG:NH2	2.35	0.41
3:L:245:GLN:NE2	3:L:409:TYR:CE2	2.88	0.41
3:L:343:ASN:OD1	3:L:366:GLY:HA3	2.19	0.41
1:A:219:PHE:CE1	3:D:356:TYR:CE1	3.08	0.41
3:D:244:LYS:CB	3:D:247:LEU:HB2	2.50	0.41
1:E:354:PHE:HE2	1:E:415:ASN:HB3	1.86	0.41
1:F:193:GLY:O	1:F:195:LEU:HG	2.20	0.41
1:F:323:MET:HE2	1:F:324:PRO:HD2	2.02	0.41
2:G:977:ASN:O	2:G:978:LEU:HD23	2.20	0.41
3:J:150:SER:CA	3:J:152:LEU:HD12	2.34	0.41
3:L:372:LEU:HA	3:L:373:PRO:HD2	1.82	0.41
3:L:421:GLU:O	3:L:422:PHE:C	2.62	0.41
1:A:256:ILE:HG13	3:D:350:SER:H	1.85	0.41
1:A:354:PHE:CE2	1:A:415:ASN:ND2	2.89	0.41
2:B:827:GLN:HA	2:B:827:GLN:OE1	2.21	0.41
3:D:346:ILE:HD12	3:D:367:ASN:ND2	2.35	0.41
3:D:379:LEU:HD23	3:D:379:LEU:HA	1.82	0.41
1:E:325:ASN:HB2	1:E:326:ASN:HD22	1.85	0.41
2:G:803:ASN:O	2:G:806:ASP:N	2.53	0.41
2:H:909:LEU:HD21	2:H:925:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:909:LEU:HD12	2:I:951:LEU:HD23	2.03	0.41
3:J:420:TRP:O	3:J:422:PHE:O	2.38	0.41
3:J:422:PHE:CA	3:J:424:ASN:H	2.33	0.41
3:J:444:LYS:O	3:J:447:THR:O	2.38	0.41
3:K:353:ILE:O	3:K:356:TYR:HB2	2.20	0.41
3:K:456:PHE:O	3:K:457:TYR:C	2.61	0.41
3:K:514:CYS:SG	3:K:517:TYR:HD1	2.43	0.41
3:K:810:PRO:HB3	3:K:816:SER:N	2.35	0.41
3:L:180:GLN:OE1	3:L:244:LYS:N	2.54	0.41
3:L:379:LEU:HB3	3:L:382:LEU:HD13	2.03	0.41
3:L:392:LEU:O	3:L:413:ASN:HB3	2.21	0.41
1:A:256:ILE:CG1	3:D:350:SER:H	2.34	0.41
1:C:289:LEU:HD23	1:C:318:LEU:HD21	2.01	0.41
1:C:387:ILE:O	1:C:390:THR:HG23	2.20	0.41
3:D:400:GLY:O	3:D:424:ASN:ND2	2.52	0.41
1:E:343:ASP:OD1	1:E:345:ASN:HB3	2.21	0.41
1:E:380:LEU:HA	1:E:380:LEU:HD23	1.71	0.41
2:G:956:ASN:ND2	2:G:966:THR:HG23	2.33	0.41
2:I:979:THR:C	2:I:981:LYS:H	2.28	0.41
3:J:349:ILE:HD13	3:J:349:ILE:HA	1.90	0.41
3:K:398:GLU:C	3:K:400:GLY:N	2.75	0.41
3:K:768:PHE:HA	3:K:778:VAL:HG22	2.03	0.41
3:L:419:PRO:HG2	3:L:422:PHE:CE1	2.55	0.41
1:A:199:ILE:HG22	1:A:200:GLY:N	2.35	0.41
1:A:426:ILE:HG22	1:A:427:TYR:N	2.23	0.41
1:C:332:TRP:CZ2	1:C:336:GLN:HG3	2.56	0.41
3:D:768:PHE:CD1	3:D:768:PHE:N	2.89	0.41
1:F:263:GLU:OE1	1:F:263:GLU:HA	2.19	0.41
1:F:314:LEU:HA	1:F:314:LEU:HD12	1.78	0.41
2:H:791:PHE:CE1	2:H:795:ASN:ND2	2.89	0.41
2:H:929:LEU:HB3	2:H:972:LEU:HD11	2.02	0.41
2:I:910:ILE:HG22	2:I:914:LYS:HE2	2.02	0.41
3:J:407:TYR:N	3:J:407:TYR:HD1	2.18	0.41
3:L:419:PRO:CD	3:L:422:PHE:HE1	2.33	0.41
1:C:287:GLN:HG2	2:H:944:TRP:HA	2.02	0.41
3:D:163:LEU:HD11	3:D:249:GLU:CA	2.41	0.41
2:G:936:LYS:HA	2:G:939:LYS:HE2	2.03	0.41
2:I:909:LEU:HD21	2:I:925:VAL:HG21	2.02	0.41
3:K:345:GLN:N	3:K:345:GLN:CD	2.78	0.41
3:K:369:LEU:HD12	3:K:369:LEU:N	2.36	0.41
3:K:440:LYS:HA	3:K:443:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:HIS:O	1:A:229:LEU:HA	2.21	0.41
1:A:301:THR:HG23	1:A:340:ASN:OD1	2.21	0.41
2:B:803:ASN:O	2:B:804:LYS:C	2.64	0.41
1:C:307:ALA:O	1:C:308:ALA:C	2.62	0.41
1:C:323:MET:HA	1:C:324:PRO:HD3	1.85	0.41
3:D:254:LEU:HD23	3:D:254:LEU:HA	1.74	0.41
1:E:182:TYR:CE2	1:E:237:PRO:HD3	2.56	0.41
1:E:314:LEU:HD12	1:E:314:LEU:HA	1.78	0.41
1:F:346:LEU:HD23	1:F:350:ILE:HG13	2.03	0.41
2:G:979:THR:C	2:G:981:LYS:H	2.28	0.41
3:J:388:SER:CB	3:J:389:HIS:CD2	3.04	0.41
3:J:462:ARG:HA	3:J:463:PRO:HD3	1.70	0.41
3:K:425:LEU:O	3:K:425:LEU:HD12	2.21	0.41
3:K:441:GLN:O	3:K:444:LYS:HB2	2.21	0.41
3:L:163:LEU:HD23	3:L:163:LEU:HA	1.86	0.41
3:L:420:TRP:CZ2	3:L:463:PRO:HD3	2.54	0.41
1:A:182:TYR:CE2	1:A:237:PRO:HD3	2.56	0.41
2:B:911:GLU:O	2:B:915:GLU:HG2	2.20	0.41
1:C:320:ASN:HB3	2:H:941:PRO:O	2.21	0.41
3:D:177:TYR:HE1	3:D:365:ASN:HD21	1.68	0.41
3:D:336:TRP:O	3:D:336:TRP:CG	2.72	0.41
3:D:513:LEU:HB3	3:D:536:ARG:NH2	2.36	0.41
1:F:163:VAL:HG12	1:F:280:ILE:HD11	2.02	0.41
1:F:271:ASN:OD1	1:F:271:ASN:C	2.64	0.41
2:G:762:ILE:HB	2:G:763:PRO:HD2	2.03	0.41
3:J:346:ILE:HD13	3:J:346:ILE:HG21	1.58	0.41
3:L:408:PHE:CD1	3:L:409:TYR:N	2.89	0.41
1:A:179:VAL:CG2	1:A:294:LEU:HD23	2.51	0.41
1:A:193:GLY:C	1:A:195:LEU:CD2	2.94	0.41
1:A:214:ARG:HG2	1:A:215:ALA:N	2.34	0.41
1:A:271:ASN:OD1	1:A:271:ASN:C	2.64	0.41
3:D:400:GLY:C	3:D:402:CYS:H	2.28	0.41
1:F:258:SER:O	1:F:260:GLU:N	2.54	0.41
2:I:803:ASN:O	2:I:804:LYS:C	2.64	0.41
3:L:423:GLY:CA	3:L:455:ILE:HD12	2.51	0.41
1:A:202:PHE:O	1:A:203:ARG:HG3	2.21	0.40
1:A:258:SER:O	1:A:260:GLU:N	2.54	0.40
2:B:836:HIS:O	2:B:837:ASP:C	2.64	0.40
1:C:323:MET:HE1	1:C:330:PHE:CD1	2.55	0.40
3:D:176:ILE:H	3:D:176:ILE:HG12	1.49	0.40
1:E:350:ILE:CD1	1:E:422:TYR:CZ	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:356:TYR:HB3	3:J:358:PHE:CE1	2.56	0.40
3:J:418:LEU:HB3	3:J:422:PHE:CE1	2.55	0.40
3:K:563:GLU:HG2	3:K:563:GLU:H	1.77	0.40
3:K:768:PHE:HA	3:K:777:ASP:O	2.21	0.40
1:A:168:LEU:HD22	1:A:280:ILE:HG23	2.03	0.40
2:B:905:PHE:O	2:B:906:ARG:C	2.64	0.40
3:D:135:ASN:HA	3:D:138:ASN:HB2	2.04	0.40
3:D:177:TYR:OH	3:D:386:ASP:OD2	2.40	0.40
2:G:791:PHE:CE1	2:G:795:ASN:ND2	2.90	0.40
2:I:812:LEU:HD23	2:I:846:MET:CE	2.48	0.40
3:J:411:PHE:O	3:J:412:ASP:HB3	2.21	0.40
3:K:379:LEU:HD23	3:K:379:LEU:HA	1.78	0.40
1:A:350:ILE:CD1	1:A:422:TYR:CZ	3.04	0.40
1:C:257:MET:O	3:K:347:PHE:CD1	2.74	0.40
3:D:420:TRP:O	3:D:421:GLU:C	2.65	0.40
3:D:465:ILE:HD13	3:D:465:ILE:HA	1.85	0.40
3:D:521:LYS:HA	3:D:524:ARG:NH1	2.37	0.40
1:E:305:TYR:O	1:E:306:HIS:HB3	2.20	0.40
1:F:307:ALA:O	1:F:308:ALA:C	2.64	0.40
2:H:942:ASN:OD1	2:H:944:TRP:HB3	2.21	0.40
3:J:177:TYR:CE2	3:J:363:TYR:CE1	3.10	0.40
3:J:410:PHE:O	3:J:410:PHE:CD2	2.75	0.40
3:L:408:PHE:HD1	3:L:409:TYR:N	2.20	0.40
3:L:414:MET:HA	3:L:437:PRO:HD2	2.03	0.40
3:L:420:TRP:O	3:L:422:PHE:O	2.39	0.40
3:D:398:GLU:C	3:D:400:GLY:N	2.77	0.40
1:E:346:LEU:HD23	1:E:350:ILE:HG13	2.04	0.40
1:E:354:PHE:CE2	1:E:415:ASN:ND2	2.90	0.40
1:E:405:LEU:HD12	1:E:405:LEU:O	2.21	0.40
1:F:346:LEU:O	1:F:350:ILE:HG13	2.22	0.40
2:I:836:HIS:O	2:I:837:ASP:C	2.64	0.40
3:K:173:GLN:O	3:K:176:ILE:CD1	2.70	0.40
3:L:341:LEU:O	3:L:344:LEU:HD11	2.21	0.40
3:L:375:GLU:O	3:L:376:ILE:C	2.63	0.40
1:A:305:TYR:CD1	1:A:344:LEU:HD23	2.57	0.40
3:D:809:PHE:HB3	3:D:810:PRO:HA	2.03	0.40
1:E:202:PHE:CE1	3:L:336:TRP:CB	3.04	0.40
1:F:185:VAL:HG23	1:F:229:LEU:CD1	2.51	0.40
2:H:861:ARG:O	2:H:864:PHE:HB3	2.21	0.40
3:J:457:TYR:HE1	3:J:461:ASN:ND2	2.19	0.40
3:K:420:TRP:O	3:K:422:PHE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:768:PHE:CD1	3:K:768:PHE:N	2.90	0.40
3:L:374:ALA:C	3:L:376:ILE:H	2.30	0.40
3:L:417:THR:HG22	3:L:418:LEU:N	2.37	0.40
3:L:419:PRO:HB2	3:L:421:GLU:HG2	2.03	0.40
3:L:422:PHE:HD2	3:L:425:LEU:HD21	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:SER:OG	3:L:146:LEU:O[1_554]	2.08	0.12
2:G:835:TYR:OH	2:I:800:ASN:CA[1_465]	2.10	0.10
1:E:166:SER:OG	3:J:146:LEU:O[1_455]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	30	59
1	C	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	30	59
1	E	263/288 (91%)	249 (95%)	13 (5%)	1 (0%)	30	59
1	F	263/288 (91%)	250 (95%)	13 (5%)	0	100	100
2	B	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
2	G	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
2	H	231/249 (93%)	221 (96%)	10 (4%)	0	100	100
2	I	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
3	D	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	36	65
3	J	204/727 (28%)	168 (82%)	34 (17%)	2 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	K	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	36 65
3	L	204/727 (28%)	171 (84%)	31 (15%)	2 (1%)	12 39
All	All	2984/5056 (59%)	2731 (92%)	244 (8%)	9 (0%)	36 65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	380	SER
3	K	380	SER
3	J	464	GLU
3	J	465	ILE
3	L	465	ILE
1	A	260	GLU
1	C	260	GLU
3	L	464	GLU
1	E	426	ILE

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	241/264 (91%)	215 (89%)	26 (11%)	6 22
1	C	242/264 (92%)	214 (88%)	28 (12%)	5 20
1	E	242/264 (92%)	215 (89%)	27 (11%)	6 21
1	F	241/264 (91%)	213 (88%)	28 (12%)	5 20
2	B	211/231 (91%)	200 (95%)	11 (5%)	21 47
2	G	211/231 (91%)	198 (94%)	13 (6%)	16 42
2	H	211/231 (91%)	198 (94%)	13 (6%)	16 42
2	I	211/231 (91%)	197 (93%)	14 (7%)	15 40
3	D	258/648 (40%)	206 (80%)	52 (20%)	1 4
3	J	165/648 (26%)	126 (76%)	39 (24%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	261/648 (40%)	207 (79%)	54 (21%)	1	4
3	L	165/648 (26%)	128 (78%)	37 (22%)	1	3
All	All	2659/4572 (58%)	2317 (87%)	342 (13%)	4	16

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	PHE
1	A	152	LEU
1	A	165	LYS
1	A	166	SER
1	A	172	PHE
1	A	180	SER
1	A	191	PHE
1	A	192	VAL
1	A	199	ILE
1	A	202	PHE
1	A	223	ILE
1	A	229	LEU
1	A	255	GLU
1	A	257	MET
1	A	259	THR
1	A	266	ARG
1	A	280	ILE
1	A	298	ASP
1	A	323	MET
1	A	327	LYS
1	A	338	MET
1	A	354	PHE
1	A	356	ASN
1	A	374	THR
1	A	386	SER
1	A	426	ILE
2	B	761	MET
2	B	774	CYS
2	B	813	THR
2	B	822	THR
2	B	844	VAL
2	B	857	ASN
2	B	901	LYS
2	B	934	GLU

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Mol	Chain	Res	Type
2	B	968	GLU
2	B	978	LEU
2	B	983	LEU
1	C	152	LEU
1	C	165	LYS
1	C	166	SER
1	C	170	SER
1	C	172	PHE
1	C	180	SER
1	C	191	PHE
1	C	192	VAL
1	C	199	ILE
1	C	202	PHE
1	C	223	ILE
1	C	229	LEU
1	C	239	ASN
1	C	255	GLU
1	C	257	MET
1	C	259	THR
1	C	266	ARG
1	C	280	ILE
1	C	298	ASP
1	C	323	MET
1	C	327	LYS
1	C	338	MET
1	C	354	PHE
1	C	355	LYS
1	C	356	ASN
1	C	374	THR
1	C	386	SER
1	C	426	ILE
3	D	141	LEU
3	D	142	HIS
3	D	145	HIS
3	D	156	ILE
3	D	159	LEU
3	D	176	ILE
3	D	254	LEU
3	D	255	THR
3	D	256	ASP
3	D	341	LEU
3	D	344	LEU

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Mol	Chain	Res	Type
3	D	347	PHE
3	D	348	ASN
3	D	358	PHE
3	D	359	LEU
3	D	370	THR
3	D	372	LEU
3	D	376	ILE
3	D	377	LYS
3	D	382	LEU
3	D	384	VAL
3	D	398	GLU
3	D	399	LEU
3	D	401	SER
3	D	404	GLN
3	D	416	THR
3	D	425	LEU
3	D	426	CYS
3	D	431	LEU
3	D	436	ASN
3	D	448	GLU
3	D	451	VAL
3	D	455	ILE
3	D	461	ASN
3	D	467	LEU
3	D	512	THR
3	D	514	CYS
3	D	519	THR
3	D	526	THR
3	D	554	LEU
3	D	557	VAL
3	D	564	GLU
3	D	565	TYR
3	D	599	CYS
3	D	600	CYS
3	D	777	ASP
3	D	779	ILE
3	D	798	VAL
3	D	803	VAL
3	D	814	PHE
3	D	817	ASP
3	D	819	ILE
1	E	152	LEU

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Mol	Chain	Res	Type
1	E	165	LYS
1	E	166	SER
1	E	172	PHE
1	E	180	SER
1	E	191	PHE
1	E	192	VAL
1	E	199	ILE
1	E	201	THR
1	E	202	PHE
1	E	229	LEU
1	E	239	ASN
1	E	255	GLU
1	E	257	MET
1	E	259	THR
1	E	266	ARG
1	E	280	ILE
1	E	298	ASP
1	E	323	MET
1	E	327	LYS
1	E	338	MET
1	E	354	PHE
1	E	356	ASN
1	E	374	THR
1	E	386	SER
1	E	405	LEU
1	E	426	ILE
1	F	152	LEU
1	F	165	LYS
1	F	166	SER
1	F	172	PHE
1	F	180	SER
1	F	191	PHE
1	F	192	VAL
1	F	199	ILE
1	F	201	THR
1	F	202	PHE
1	F	223	ILE
1	F	229	LEU
1	F	239	ASN
1	F	255	GLU
1	F	257	MET
1	F	259	THR

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Mol	Chain	Res	Type
1	F	266	ARG
1	F	280	ILE
1	F	298	ASP
1	F	323	MET
1	F	327	LYS
1	F	338	MET
1	F	354	PHE
1	F	356	ASN
1	F	374	THR
1	F	386	SER
1	F	390	THR
1	F	426	ILE
2	G	761	MET
2	G	774	CYS
2	G	790	LEU
2	G	813	THR
2	G	822	THR
2	G	844	VAL
2	G	857	ASN
2	G	901	LYS
2	G	934	GLU
2	G	967	PHE
2	G	968	GLU
2	G	978	LEU
2	G	983	LEU
2	H	761	MET
2	H	774	CYS
2	H	790	LEU
2	H	804	LYS
2	H	813	THR
2	H	822	THR
2	H	844	VAL
2	H	857	ASN
2	H	901	LYS
2	H	934	GLU
2	H	968	GLU
2	H	978	LEU
2	H	983	LEU
2	I	761	MET
2	I	774	CYS
2	I	790	LEU
2	I	804	LYS

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Mol	Chain	Res	Type
2	I	813	THR
2	I	822	THR
2	I	844	VAL
2	I	857	ASN
2	I	901	LYS
2	I	934	GLU
2	I	967	PHE
2	I	968	GLU
2	I	978	LEU
2	I	983	LEU
3	J	139	PRO
3	J	146	LEU
3	J	147	ASP
3	J	151	LEU
3	J	152	LEU
3	J	175	ASN
3	J	176	ILE
3	J	183	MET
3	J	245	GLN
3	J	256	ASP
3	J	341	LEU
3	J	344	LEU
3	J	345	GLN
3	J	346	ILE
3	J	348	ASN
3	J	349	ILE
3	J	358	PHE
3	J	370	THR
3	J	375	GLU
3	J	378	ASN
3	J	381	ASN
3	J	382	LEU
3	J	383	ARG
3	J	384	VAL
3	J	393	THR
3	J	394	SER
3	J	398	GLU
3	J	399	LEU
3	J	401	SER
3	J	404	GLN
3	J	407	TYR
3	J	422	PHE

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Mol	Chain	Res	Type
3	J	425	LEU
3	J	426	CYS
3	J	436	ASN
3	J	443	LEU
3	J	452	THR
3	J	456	PHE
3	J	461	ASN
3	K	141	LEU
3	K	142	HIS
3	K	145	HIS
3	K	156	ILE
3	K	159	LEU
3	K	176	ILE
3	K	254	LEU
3	K	255	THR
3	K	256	ASP
3	K	341	LEU
3	K	344	LEU
3	K	347	PHE
3	K	348	ASN
3	K	358	PHE
3	K	359	LEU
3	K	370	THR
3	K	372	LEU
3	K	376	ILE
3	K	377	LYS
3	K	382	LEU
3	K	384	VAL
3	K	398	GLU
3	K	399	LEU
3	K	401	SER
3	K	404	GLN
3	K	416	THR
3	K	425	LEU
3	K	426	CYS
3	K	431	LEU
3	K	436	ASN
3	K	448	GLU
3	K	451	VAL
3	K	455	ILE
3	K	461	ASN
3	K	467	LEU

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Mol	Chain	Res	Type
3	K	512	THR
3	K	514	CYS
3	K	516	HIS
3	K	519	THR
3	K	526	THR
3	K	552	LEU
3	K	554	LEU
3	K	557	VAL
3	K	564	GLU
3	K	565	TYR
3	K	576	THR
3	K	578	ILE
3	K	597	ASP
3	K	777	ASP
3	K	779	ILE
3	K	798	VAL
3	K	814	PHE
3	K	817	ASP
3	K	819	ILE
3	L	139	PRO
3	L	147	ASP
3	L	151	LEU
3	L	152	LEU
3	L	175	ASN
3	L	176	ILE
3	L	183	MET
3	L	245	GLN
3	L	256	ASP
3	L	341	LEU
3	L	344	LEU
3	L	345	GLN
3	L	346	ILE
3	L	348	ASN
3	L	349	ILE
3	L	358	PHE
3	L	370	THR
3	L	375	GLU
3	L	378	ASN
3	L	381	ASN
3	L	383	ARG
3	L	384	VAL
3	L	393	THR

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Mol	Chain	Res	Type
3	L	394	SER
3	L	398	GLU
3	L	399	LEU
3	L	401	SER
3	L	404	GLN
3	L	407	TYR
3	L	422	PHE
3	L	425	LEU
3	L	426	CYS
3	L	436	ASN
3	L	443	LEU
3	L	452	THR
3	L	456	PHE
3	L	461	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	336	GLN
1	A	352	GLN
1	A	411	HIS
2	B	857	ASN
2	B	882	ASN
2	B	895	ASN
1	C	287	GLN
1	C	320	ASN
1	C	335	HIS
1	C	336	GLN
1	C	352	GLN
3	D	413	ASN
3	D	424	ASN
3	D	818	HIS
1	E	287	GLN
1	E	316	ASN
1	E	335	HIS
1	E	352	GLN
1	F	287	GLN
1	F	352	GLN
2	G	882	ASN
2	G	895	ASN
2	H	895	ASN

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Mol	Chain	Res	Type
2	I	857	ASN
2	I	882	ASN
2	I	895	ASN
3	J	389	HIS
3	J	427	ASN
3	K	142	HIS
3	K	352	ASN
3	K	413	ASN
3	K	424	ASN
3	K	818	HIS
3	L	145	HIS
3	L	175	ASN
3	L	181	ASN
3	L	389	HIS
3	L	427	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/288 (92%)	0.03	4 (1%) 72 58	36, 58, 98, 121	0
1	C	267/288 (92%)	-0.02	6 (2%) 62 47	36, 58, 99, 121	0
1	E	267/288 (92%)	0.09	9 (3%) 48 35	35, 58, 100, 121	0
1	F	267/288 (92%)	0.13	7 (2%) 57 42	36, 59, 98, 124	0
2	B	233/249 (93%)	0.19	4 (1%) 69 54	48, 79, 115, 146	0
2	G	233/249 (93%)	0.28	12 (5%) 33 24	49, 81, 112, 146	0
2	H	233/249 (93%)	0.28	10 (4%) 40 29	48, 80, 115, 145	0
2	I	233/249 (93%)	0.28	11 (4%) 36 27	50, 81, 114, 145	0
3	D	318/727 (43%)	0.42	11 (3%) 47 34	50, 87, 136, 160	0
3	J	210/727 (28%)	0.17	14 (6%) 24 19	35, 61, 101, 127	0
3	K	318/727 (43%)	0.44	18 (5%) 29 22	50, 87, 136, 160	0
3	L	210/727 (28%)	0.17	14 (6%) 24 19	35, 62, 102, 131	0
All	All	3056/5056 (60%)	0.21	120 (3%) 43 30	35, 72, 115, 160	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	991	THR	9.3
2	H	991	THR	8.4
3	J	252	ASP	4.8
2	I	773	SER	4.4
3	L	468	PRO	4.3
3	J	468	PRO	4.2
3	L	466	PRO	4.2
3	D	576	THR	4.0
1	E	428	GLY	4.0
2	H	990	ASN	3.7
3	L	467	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	L	423	GLY	3.6
3	D	568	PRO	3.6
3	L	332	ASP	3.6
3	K	597	ASP	3.6
3	L	424	ASN	3.5
2	H	967	PHE	3.5
3	J	261	LYS	3.4
3	J	184	LYS	3.4
3	L	261	LYS	3.4
3	K	332	ASP	3.4
1	F	194	THR	3.4
1	C	355	LYS	3.4
3	J	333	ASP	3.4
3	J	136	ALA	3.4
2	H	964	SER	3.3
3	L	334	GLN	3.3
3	K	149	PRO	3.2
3	J	332	ASP	3.2
2	B	990	ASN	3.2
1	F	427	TYR	3.2
1	C	149	PRO	3.2
3	J	334	GLN	3.2
3	K	576	THR	3.2
2	G	770	ASP	3.0
1	F	149	PRO	3.0
2	G	781	ALA	3.0
3	K	136	ALA	2.9
3	J	466	PRO	2.9
2	I	771	GLU	2.9
3	J	426	CYS	2.9
2	B	967	PHE	2.8
1	E	427	TYR	2.8
2	H	801	LEU	2.8
3	K	333	ASP	2.8
3	K	406	LYS	2.8
2	G	835	TYR	2.8
2	G	991	THR	2.7
3	D	243	THR	2.7
3	J	242	CYS	2.7
1	A	149	PRO	2.7
1	E	202	PHE	2.7
3	L	333	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	K	568	PRO	2.7
3	K	779	ILE	2.7
1	F	370	GLN	2.6
1	F	150	ILE	2.6
1	E	371	TYR	2.6
3	D	136	ALA	2.6
1	E	406	SER	2.6
3	K	463	PRO	2.6
2	H	805	VAL	2.6
1	E	204	SER	2.5
3	K	438	LEU	2.5
1	C	427	TYR	2.5
1	A	370	GLN	2.5
3	J	254	LEU	2.5
3	L	134	VAL	2.5
2	I	967	PHE	2.4
3	K	135	ASN	2.4
2	I	960	ASN	2.4
3	D	180	GLN	2.4
1	F	202	PHE	2.4
2	I	791	PHE	2.4
2	H	962	LYS	2.3
3	D	512	THR	2.3
3	D	811	ASN	2.3
3	K	811	ASN	2.3
2	I	991	THR	2.3
3	L	254	LEU	2.3
2	G	798	LEU	2.3
1	C	356	ASN	2.3
3	J	256	ASP	2.3
3	K	551	LEU	2.2
2	G	777	ASN	2.2
3	J	467	LEU	2.2
1	E	277	ASN	2.2
3	D	779	ILE	2.2
2	G	773	SER	2.2
1	A	421	LYS	2.2
3	L	253	THR	2.2
3	D	170	SER	2.2
3	K	820	PRO	2.2
2	G	776	ILE	2.1
2	G	872	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	967	PHE	2.1
2	B	770	ASP	2.1
3	K	429	GLN	2.1
1	E	193	GLY	2.1
3	K	154	ASN	2.1
2	H	963	LEU	2.1
2	I	835	TYR	2.1
2	H	809	LYS	2.1
2	I	777	ASN	2.1
2	H	798	LEU	2.1
3	D	332	ASP	2.1
1	E	194	THR	2.1
2	I	872	GLU	2.1
3	D	143	PRO	2.1
1	C	150	ILE	2.0
1	C	259	THR	2.0
2	G	832	GLU	2.0
1	F	345	ASN	2.0
3	L	260	ALA	2.0
1	A	371	TYR	2.0
2	I	775	GLN	2.0
3	K	134	VAL	2.0
2	G	963	LEU	2.0
2	I	989	ILE	2.0
3	L	465	ILE	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.