



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 03:12 AM EDT

PDB ID : 2HAK
Title : Catalytic and ubiquitin-associated domains of MARK1/PAR-1
Authors : Marx, A.; Nugoor, C.; Mueller, J.; Panneerselvam, S.; Mandelkow, E.-M.;
Mandelkow, E.
Deposited on : 2006-06-13
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

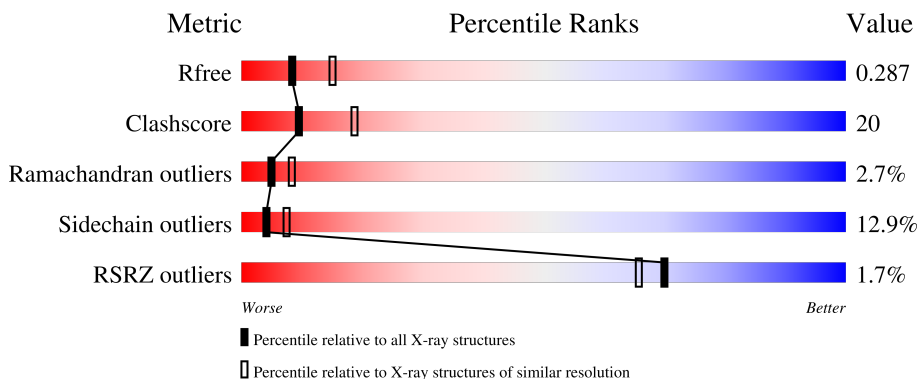
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



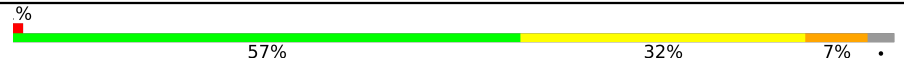


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	328	62% 27% 5% • 6%
1	B	328	2% 41% 31% 10% • 15%
1	C	328	59% 28% 5% • 5%
1	D	328	% 57% 31% 5% • 6%
1	E	328	66% 25% 6% •

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Mol	Chain	Length	Quality of chain
1	F	328	 <p>%</p> <p>57% 32% 7% •</p>
1	G	328	 <p>3%</p> <p>42% 37% 10% • 9%</p>
1	H	328	 <p>5%</p> <p>52% 29% • 16%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19579 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 Serine/threonine-protein kinase MARK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	Total 2490	C 1599	N 426	O 453	S 12	0	0	0
1	B	279	Total 2231	C 1434	N 380	O 405	S 12	0	0	0
1	C	310	Total 2512	C 1612	N 432	O 456	S 12	0	0	0
1	D	309	Total 2503	C 1607	N 432	O 452	S 12	0	0	0
1	E	318	Total 2538	C 1627	N 437	O 461	S 13	0	0	0
1	F	318	Total 2562	C 1641	N 439	O 469	S 13	0	0	0
1	G	297	Total 2349	C 1506	N 402	O 429	S 12	0	0	0
1	H	277	Total 2184	C 1405	N 367	O 400	S 12	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	cloning artifact	UNP Q9P0L2
B	37	GLY	-	cloning artifact	UNP Q9P0L2
C	37	GLY	-	cloning artifact	UNP Q9P0L2
D	37	GLY	-	cloning artifact	UNP Q9P0L2
E	37	GLY	-	cloning artifact	UNP Q9P0L2
F	37	GLY	-	cloning artifact	UNP Q9P0L2
G	37	GLY	-	cloning artifact	UNP Q9P0L2
H	37	GLY	-	cloning artifact	UNP Q9P0L2

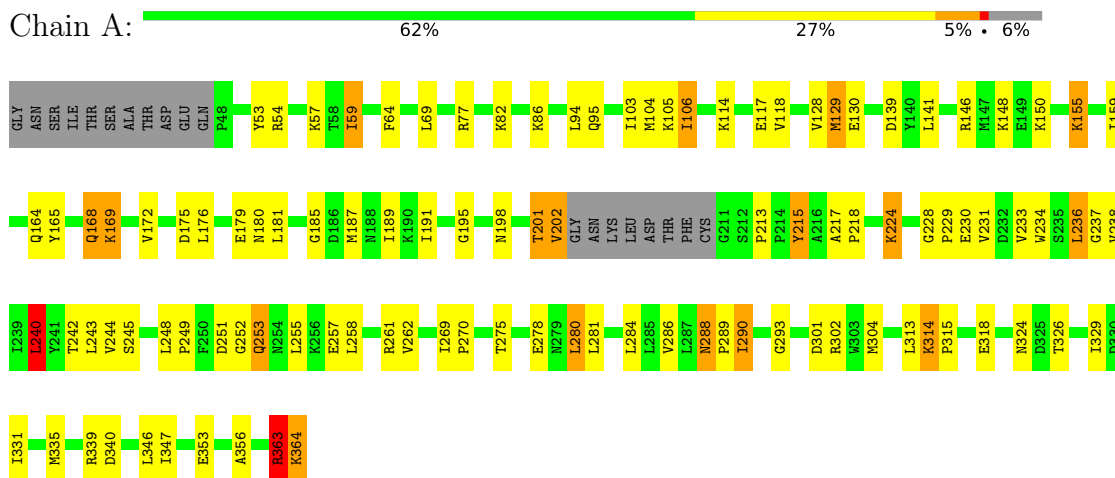
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	17	Total O 17 17	0	0
2	C	47	Total O 47 47	0	0
2	D	24	Total O 24 24	0	0
2	E	35	Total O 35 35	0	0
2	F	37	Total O 37 37	0	0
2	G	14	Total O 14 14	0	0
2	H	9	Total O 9 9	0	0

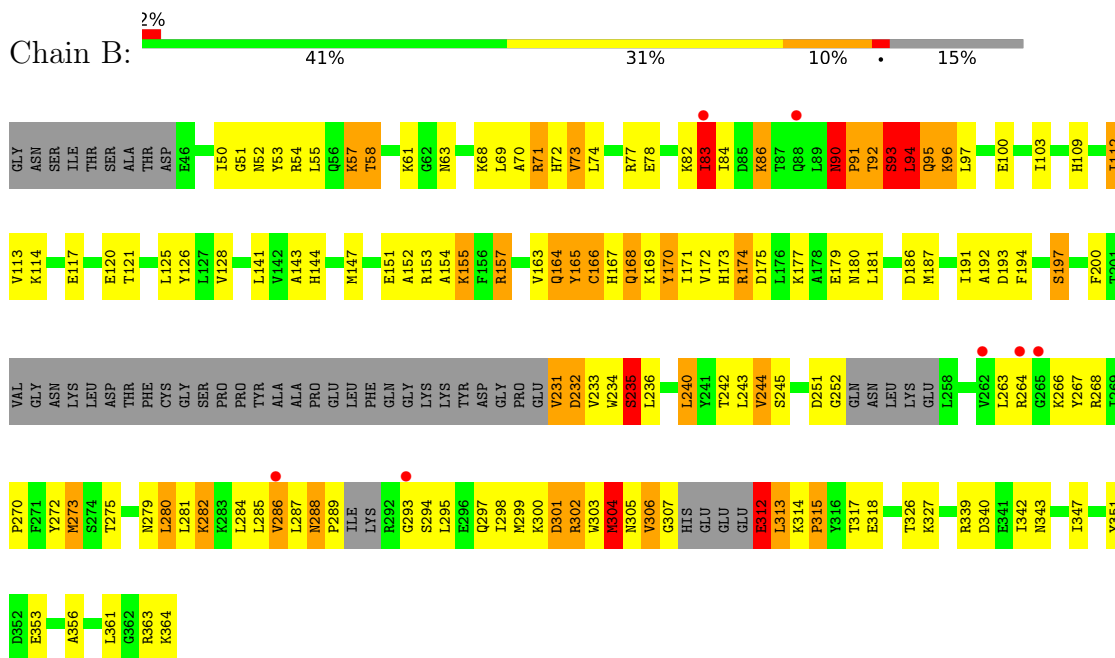
3 Residue-property plots [i](#)

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

- Molecule 1: Serine/threonine-protein kinase MARK1

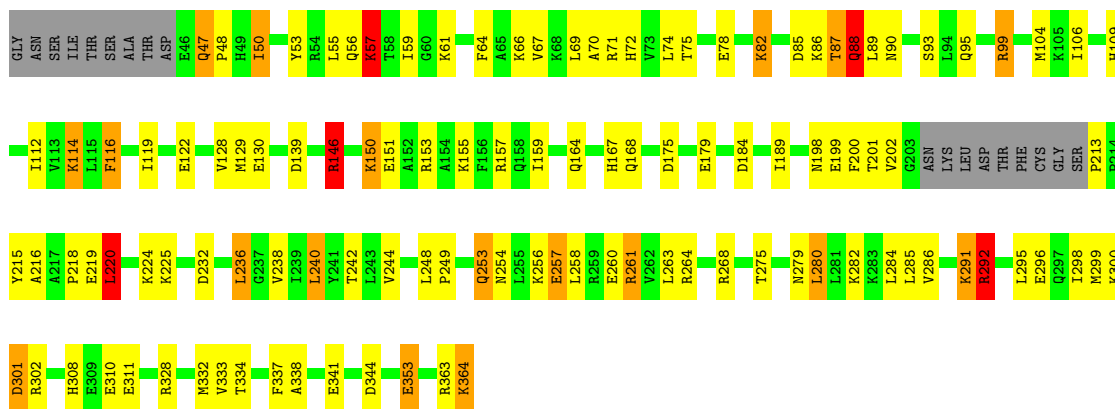


- Molecule 1: Serine/threonine-protein kinase MARK1



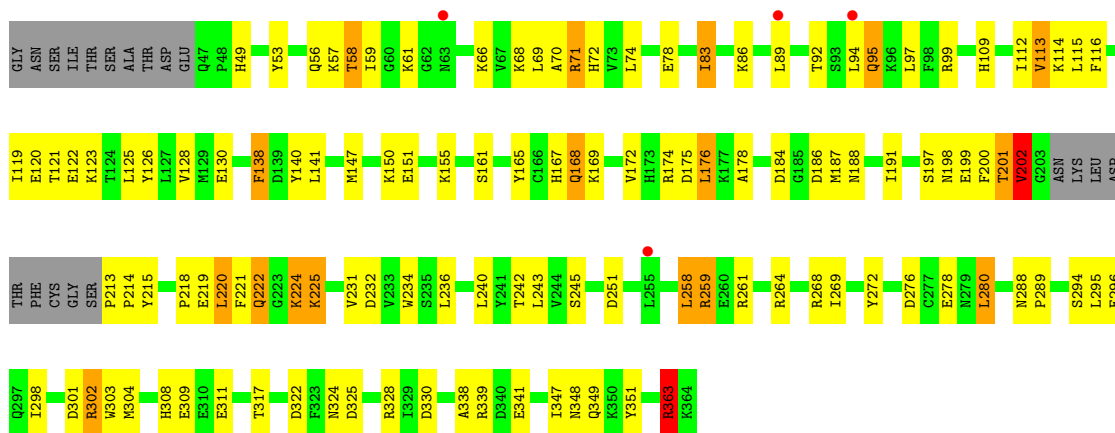
- Molecule 1: Serine/threonine-protein kinase MARK1

Chain C:  59% 28% 5% • 5%



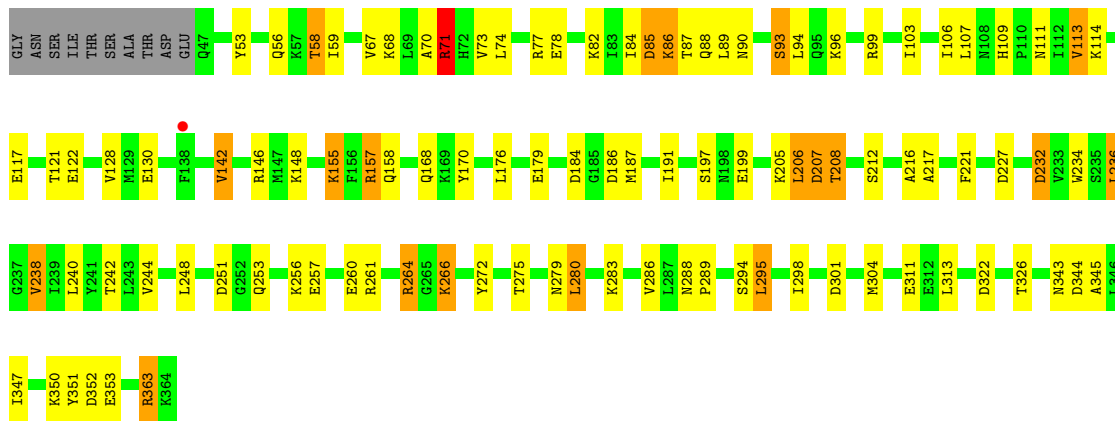
• Molecule 1: Serine/threonine-protein kinase MARK1

Chain D:  57% 31% 5% • 6%

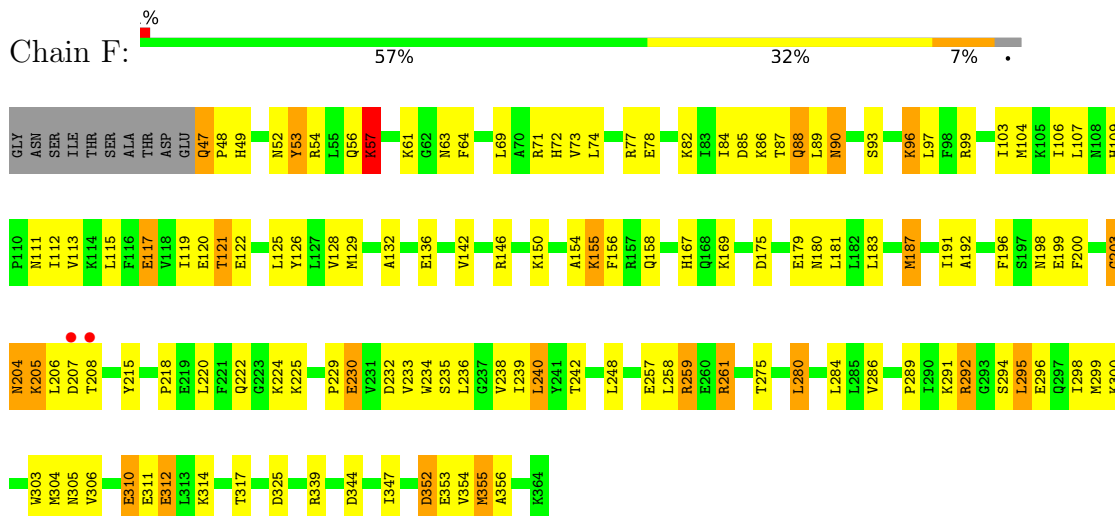


• Molecule 1: Serine/threonine-protein kinase MARK1

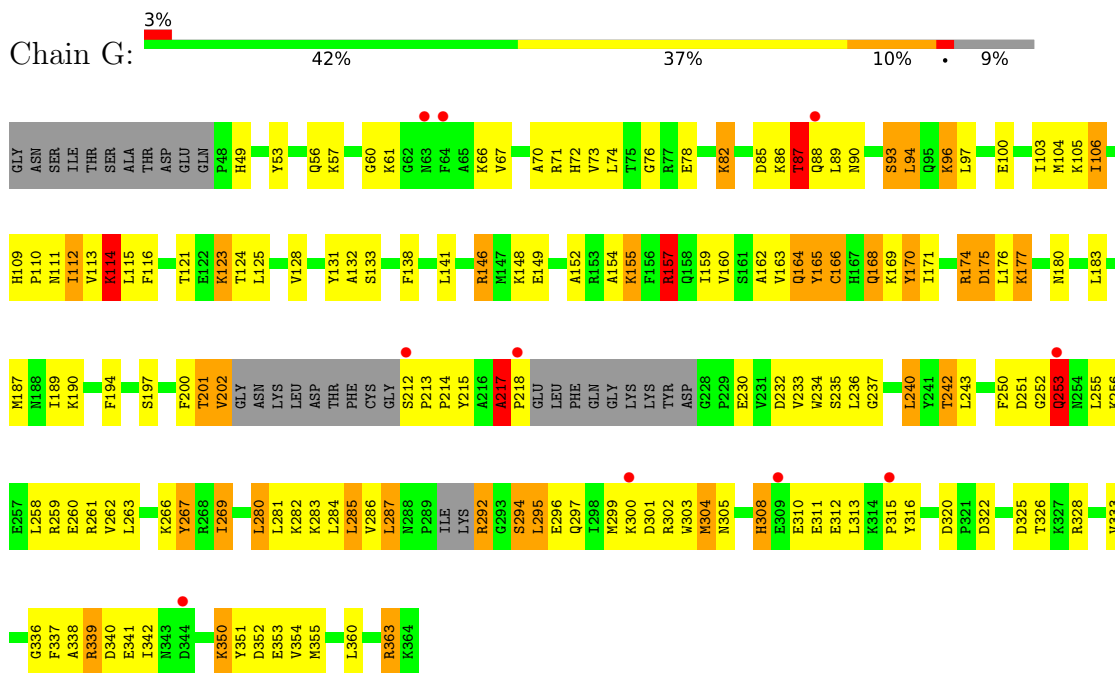
Chain E:  66% 25% 6% •



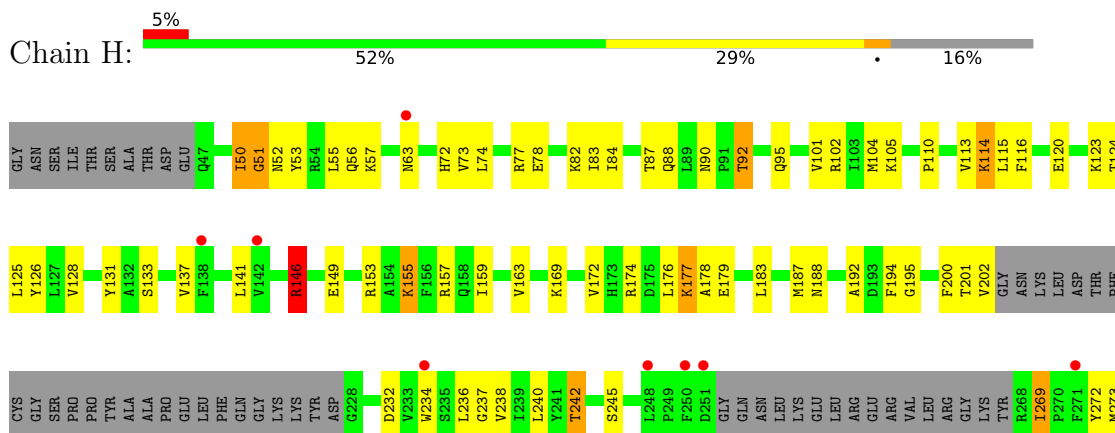
• Molecule 1: Serine/threonine-protein kinase MARK1



• Molecule 1: Serine/threonine-protein kinase MARK1



• Molecule 1: Serine/threonine-protein kinase MARK1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.68Å 116.47Å 285.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 49.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-2.60) 99.3 (49.68-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.212 , 0.290 0.213 , 0.287	Depositor DCC
R_{free} test set	2844 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtrriage
Anisotropy	0.181	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.023 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19579	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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 i

5.1 Standard geometry i

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	1.30	9/2539 (0.4%)	1.17	11/3421 (0.3%)
1	B	1.31	6/2269 (0.3%)	1.27	17/3055 (0.6%)
1	C	1.41	11/2561 (0.4%)	1.25	10/3448 (0.3%)
1	D	1.33	11/2552 (0.4%)	1.16	10/3436 (0.3%)
1	E	1.33	8/2589 (0.3%)	1.22	10/3496 (0.3%)
1	F	1.36	12/2613 (0.5%)	1.20	14/3524 (0.4%)
1	G	1.11	2/2394 (0.1%)	1.06	2/3232 (0.1%)
1	H	1.08	0/2225	1.01	4/3007 (0.1%)
All	All	1.29	59/19742 (0.3%)	1.17	78/26619 (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	1
1	B	0	1
1	E	0	1
1	F	0	1
1	G	0	3
All	All	0	7

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	353	GLU	CG-CD	11.27	1.68	1.51
1	C	353	GLU	CB-CG	9.91	1.71	1.52
1	B	312	GLU	CG-CD	9.07	1.65	1.51
1	B	363	ARG	CG-CD	-8.25	1.31	1.51
1	A	224	LYS	CE-NZ	7.63	1.68	1.49
1	F	296	GLU	CG-CD	7.58	1.63	1.51
1	D	151	GLU	CD-OE1	7.21	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	231	VAL	CB-CG2	-7.01	1.38	1.52
1	C	268	ARG	CG-CD	6.97	1.69	1.51
1	C	116	PHE	CE2-CZ	6.96	1.50	1.37
1	C	168	GLN	CG-CD	6.93	1.67	1.51
1	B	54	ARG	CG-CD	6.60	1.68	1.51
1	F	296	GLU	CD-OE2	6.58	1.32	1.25
1	D	296	GLU	CB-CG	6.30	1.64	1.52
1	E	238	VAL	CB-CG2	6.22	1.66	1.52
1	G	267	TYR	CE2-CZ	-6.16	1.30	1.38
1	A	353	GLU	CB-CG	-6.10	1.40	1.52
1	E	207	ASP	CB-CG	6.09	1.64	1.51
1	F	117	GLU	CD-OE2	6.04	1.32	1.25
1	B	312	GLU	CB-CG	5.96	1.63	1.52
1	D	151	GLU	CG-CD	5.93	1.60	1.51
1	C	300	LYS	CE-NZ	5.89	1.63	1.49
1	A	168	GLN	CG-CD	5.86	1.64	1.51
1	A	179	GLU	CG-CD	5.77	1.60	1.51
1	E	322	ASP	CB-CG	5.76	1.63	1.51
1	C	114	LYS	CD-CE	5.76	1.65	1.51
1	C	151	GLU	CG-CD	5.69	1.60	1.51
1	F	198	ASN	CB-CG	5.69	1.64	1.51
1	C	215	TYR	CD1-CE1	5.66	1.47	1.39
1	E	99	ARG	CG-CD	5.59	1.66	1.51
1	F	136	GLU	CB-CG	5.58	1.62	1.52
1	B	166	CYS	CB-SG	-5.58	1.72	1.81
1	B	312	GLU	CD-OE2	5.57	1.31	1.25
1	G	296	GLU	CG-CD	5.54	1.60	1.51
1	A	54	ARG	CG-CD	5.52	1.65	1.51
1	F	53	TYR	CD2-CE2	5.50	1.47	1.39
1	F	99	ARG	CG-CD	5.49	1.65	1.51
1	F	354	VAL	CB-CG2	-5.46	1.41	1.52
1	F	117	GLU	CD-OE1	5.45	1.31	1.25
1	D	138	PHE	CG-CD2	5.45	1.47	1.38
1	E	179	GLU	CG-CD	5.44	1.60	1.51
1	F	354	VAL	CB-CG1	-5.44	1.41	1.52
1	C	296	GLU	CD-OE2	5.43	1.31	1.25
1	D	168	GLN	CG-CD	5.39	1.63	1.51
1	F	230	GLU	CG-CD	5.37	1.59	1.51
1	F	47	GLN	CA-CB	5.34	1.65	1.53
1	E	179	GLU	CD-OE2	5.30	1.31	1.25
1	A	130	GLU	CD-OE1	5.30	1.31	1.25
1	A	118	VAL	CB-CG1	-5.26	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	130	GLU	CD-OE1	5.21	1.31	1.25
1	D	309	GLU	CB-CG	5.20	1.62	1.52
1	D	325	ASP	CB-CG	-5.15	1.41	1.51
1	A	215	TYR	CE2-CZ	5.15	1.45	1.38
1	A	353	GLU	CD-OE1	5.11	1.31	1.25
1	D	138	PHE	CE1-CZ	5.11	1.47	1.37
1	D	172	VAL	CB-CG2	-5.06	1.42	1.52
1	C	179	GLU	CB-CG	-5.04	1.42	1.52
1	D	309	GLU	CG-CD	5.03	1.59	1.51
1	E	157	ARG	CZ-NH1	5.03	1.39	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	363	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	A	77	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	B	153	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	77	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	B	77	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	292	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	C	292	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	E	264	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	E	71	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	C	139	ASP	CB-CG-OD1	7.13	124.72	118.30
1	B	83	ILE	CB-CA-C	-7.12	97.36	111.60
1	B	231	VAL	CB-CA-C	-7.01	98.08	111.40
1	D	322	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	B	94	LEU	CA-CB-CG	6.90	131.17	115.30
1	C	146	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	F	89	LEU	CA-CB-CG	6.85	131.04	115.30
1	F	344	ASP	CB-CG-OD1	-6.75	112.23	118.30
1	A	340	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	D	322	ASP	CB-CG-OD1	6.68	124.31	118.30
1	E	157	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	H	77	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	D	330	ASP	CB-CG-OD2	6.50	124.15	118.30
1	F	325	ASP	CB-CG-OD1	6.40	124.06	118.30
1	H	77	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	F	325	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	C	89	LEU	CA-CB-CG	6.17	129.50	115.30
1	E	232	ASP	CB-CG-OD2	-6.16	112.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	CA-CB-CG	6.11	126.85	113.40
1	G	355	MET	CG-SD-CE	6.06	109.89	100.20
1	B	273	MET	CG-SD-CE	6.03	109.85	100.20
1	B	361	LEU	CB-CG-CD1	-6.01	100.79	111.00
1	D	147	MET	CG-SD-CE	5.97	109.75	100.20
1	A	339	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	F	352	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	C	157	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	D	259	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	129	MET	CG-SD-CE	-5.88	90.78	100.20
1	F	169	LYS	CD-CE-NZ	-5.82	98.31	111.70
1	C	146	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	99	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	232	ASP	CB-CG-OD1	5.65	123.38	118.30
1	D	328	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	E	176	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	H	269	ILE	N-CA-C	5.60	126.11	111.00
1	E	157	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	184	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	B	157	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	F	295	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	F	220	LEU	CB-CG-CD2	5.47	120.30	111.00
1	B	295	LEU	CA-CB-CG	-5.45	102.76	115.30
1	D	89	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	176	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	B	318	GLU	C-N-CD	5.38	139.70	128.40
1	B	54	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	E	295	LEU	CA-CB-CG	-5.36	102.98	115.30
1	B	112	ILE	CG1-CB-CG2	-5.31	99.71	111.40
1	H	104	MET	CG-SD-CE	5.25	108.60	100.20
1	F	77	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	E	146	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	220	LEU	CB-CG-CD1	5.21	119.86	111.00
1	F	104	MET	CG-SD-CE	5.20	108.53	100.20
1	D	363	ARG	N-CA-CB	-5.20	101.25	110.60
1	A	240	LEU	CA-CB-CG	5.18	127.22	115.30
1	D	276	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	A	104	MET	CG-SD-CE	-5.14	91.97	100.20
1	B	157	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	F	85	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	B	186	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	240	LEU	CA-CB-CG	5.08	126.98	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	339	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	54	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	F	104	MET	CB-CG-SD	-5.03	97.30	112.40
1	F	339	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	139	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	170	TYR	N-CA-C	5.02	124.56	111.00
1	D	328	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	E	212	SER	C-N-CD	5.01	138.91	128.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	ARG	Peptide
1	B	90	ASN	Peptide
1	E	363	ARG	Peptide
1	F	203	GLY	Peptide
1	G	114	LYS	Peptide
1	G	217	ALA	Peptide
1	G	292	ARG	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	2490	0	2520	77	0
1	B	2231	0	2248	142	1
1	C	2512	0	2551	79	1
1	D	2503	0	2547	77	0
1	E	2538	0	2541	74	0
1	F	2562	0	2579	89	0
1	G	2349	0	2332	171	0
1	H	2184	0	2166	64	0
2	A	27	0	0	2	0
2	B	17	0	0	2	0
2	C	47	0	0	8	0
2	D	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	35	0	0	3	0
2	F	37	0	0	3	0
2	G	14	0	0	11	0
2	H	9	0	0	2	0
All	All	19579	0	19484	761	1

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 20.

All (761) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:CE	1:A:224:LYS:NZ	1.68	1.55
1:D:347:ILE:CD1	1:D:347:ILE:CG1	1.78	1.54
1:G:164:GLN:NE2	1:G:315:PRO:HB3	1.37	1.37
1:B:125:LEU:HD12	1:B:126:TYR:N	1.56	1.21
1:A:290:ILE:HD12	1:A:290:ILE:O	1.51	1.11
1:G:165:TYR:CG	2:G:375:HOH:O	2.04	1.09
1:G:157:ARG:HH11	1:G:157:ARG:HG2	1.20	1.07
1:B:147:MET:CE	1:B:243:LEU:HD22	1.83	1.07
1:G:299:MET:HG2	1:G:313:LEU:HD23	1.37	1.06
1:F:259:ARG:HD2	2:F:401:HOH:O	1.57	1.04
1:G:217:ALA:HB1	1:G:218:PRO:HD2	1.35	1.04
1:G:164:GLN:HE22	1:G:315:PRO:CB	1.72	1.03
1:B:86:LYS:HB2	1:B:94:LEU:HD13	1.42	1.02
1:G:146:ARG:HG3	1:G:146:ARG:HH11	1.20	1.01
1:F:300:LYS:HE3	1:F:312:GLU:HG2	1.43	0.98
1:B:147:MET:HE1	1:B:243:LEU:HD22	1.39	0.98
1:G:123:LYS:HG3	1:G:124:THR:HG22	1.43	0.98
1:G:282:LYS:HA	2:G:372:HOH:O	1.65	0.97
1:F:82:LYS:HD3	1:F:84:ILE:HD11	1.47	0.97
1:D:363:ARG:CG	1:D:363:ARG:HH11	1.79	0.96
1:G:164:GLN:HE22	1:G:315:PRO:HB3	0.81	0.95
1:B:125:LEU:HD12	1:B:126:TYR:H	1.27	0.95
1:F:121:THR:HG22	1:F:122:GLU:H	1.30	0.93
1:D:363:ARG:HH11	1:D:363:ARG:HG2	1.32	0.93
1:G:155:LYS:O	1:G:159:ILE:HG12	1.70	0.92
1:G:165:TYR:HA	2:G:375:HOH:O	1.69	0.91
1:H:50:ILE:HD12	1:H:50:ILE:H	1.36	0.91
1:B:90:ASN:HB2	1:B:91:PRO:HD3	1.54	0.90
1:B:167:HIS:ND1	1:B:172:VAL:HG21	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:TYR:HD1	2:G:367:HOH:O	1.53	0.90
1:G:146:ARG:HG3	1:G:146:ARG:NH1	1.83	0.89
1:G:164:GLN:NE2	1:G:315:PRO:CB	2.32	0.88
1:G:258:LEU:O	1:G:262:VAL:HG23	1.74	0.88
1:B:171:ILE:HG22	1:B:173:HIS:CE1	2.08	0.87
1:C:146:ARG:HG3	1:C:146:ARG:HH11	1.40	0.86
1:D:167:HIS:HE1	1:D:232:ASP:OD2	1.58	0.86
1:B:304:MET:HE3	1:B:304:MET:HA	1.54	0.86
1:B:90:ASN:CB	1:B:91:PRO:HD3	2.05	0.85
1:G:286:VAL:HG21	1:G:292:ARG:HB2	1.58	0.85
1:G:283:LYS:O	1:G:284:LEU:HD23	1.77	0.85
1:G:157:ARG:HG2	1:G:157:ARG:NH1	1.90	0.85
1:B:299:MET:HG2	1:B:313:LEU:O	1.76	0.84
1:A:331:ILE:O	1:A:335:MET:HG3	1.78	0.83
1:E:71:ARG:HG3	1:E:71:ARG:HH11	1.42	0.83
1:G:157:ARG:HH11	1:G:157:ARG:CG	1.92	0.82
1:D:120:GLU:HG3	1:D:125:LEU:HD12	1.63	0.81
1:B:280:LEU:HD22	1:B:284:LEU:HD12	1.61	0.81
1:B:305:ASN:O	1:B:307:GLY:N	2.11	0.81
2:G:368:HOH:O	1:H:146:ARG:HD2	1.81	0.81
1:B:300:LYS:HD3	1:B:312:GLU:OE1	1.81	0.79
1:B:293:GLY:HA2	1:B:297:GLN:NE2	1.97	0.79
1:G:109:HIS:HB3	1:G:112:ILE:HG13	1.62	0.79
1:G:316:TYR:HA	2:G:373:HOH:O	1.83	0.78
1:B:234:TRP:HZ3	1:B:285:LEU:O	1.66	0.78
1:E:280:LEU:HG	1:E:301:ASP:OD1	1.83	0.77
1:E:155:LYS:HE3	1:E:187:MET:O	1.84	0.77
1:G:233:VAL:HA	1:G:236:LEU:HD23	1.65	0.76
1:E:71:ARG:HH11	1:E:71:ARG:CG	1.98	0.76
1:D:138:PHE:CZ	1:D:215:TYR:CE2	2.73	0.76
1:D:58:THR:OG1	1:D:68:LYS:HD3	1.86	0.76
1:G:217:ALA:HB1	1:G:218:PRO:CD	2.15	0.76
1:H:105:LYS:HG2	1:H:115:LEU:HD23	1.66	0.76
1:E:157:ARG:HG2	1:E:304:MET:CE	2.16	0.76
1:A:217:ALA:CB	1:A:231:VAL:HG13	2.17	0.75
1:A:253:GLN:N	1:A:257:GLU:OE1	2.18	0.75
1:E:142:VAL:HG12	1:E:142:VAL:O	1.85	0.75
1:G:232:ASP:O	1:G:235:SER:HB2	1.86	0.75
1:D:168:GLN:HG2	2:D:370:HOH:O	1.87	0.75
1:B:280:LEU:HD12	1:B:303:TRP:HB3	1.68	0.75
1:G:146:ARG:HH11	1:G:146:ARG:CG	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:HIS:CE1	1:D:232:ASP:OD2	2.41	0.74
1:C:175:ASP:HB2	2:C:373:HOH:O	1.86	0.74
1:B:164:GLN:HE22	1:B:315:PRO:HB3	1.51	0.74
1:H:120:GLU:HG3	1:H:125:LEU:HD13	1.70	0.74
1:C:167:HIS:HE1	1:C:232:ASP:OD2	1.70	0.74
1:D:141:LEU:HD13	1:D:242:THR:HG22	1.70	0.74
1:H:155:LYS:HE2	1:H:187:MET:O	1.87	0.74
1:D:138:PHE:CZ	1:D:215:TYR:HE2	2.06	0.74
1:B:294:SER:O	1:B:297:GLN:HB2	1.87	0.74
1:B:171:ILE:CG2	1:B:173:HIS:CE1	2.72	0.73
1:G:165:TYR:HE1	1:G:316:TYR:HD2	1.37	0.73
1:G:299:MET:HG2	1:G:313:LEU:CD2	2.17	0.73
1:E:82:LYS:HD3	1:E:84:ILE:HD11	1.71	0.73
1:F:121:THR:CG2	1:F:122:GLU:H	1.93	0.72
1:B:282:LYS:O	1:B:286:VAL:HG12	1.89	0.72
1:D:363:ARG:CG	1:D:363:ARG:NH1	2.42	0.72
1:D:298:ILE:HG22	1:D:304:MET:CE	2.20	0.72
1:G:169:LYS:HB2	2:G:367:HOH:O	1.90	0.72
1:D:363:ARG:NH1	1:D:363:ARG:HG3	2.04	0.72
1:F:54:ARG:HG2	1:F:54:ARG:HH11	1.55	0.72
1:G:85:ASP:OD1	1:G:87:THR:OG1	2.08	0.71
1:B:293:GLY:HA2	1:B:297:GLN:HE21	1.54	0.71
1:G:114:LYS:HG3	1:G:363:ARG:NH2	2.05	0.71
1:B:90:ASN:CG	1:B:91:PRO:HD3	2.11	0.71
1:B:50:ILE:HG21	1:B:126:TYR:CZ	2.25	0.70
1:B:95:GLN:HE21	1:B:95:GLN:C	1.95	0.70
1:E:56:GLN:HE21	1:E:70:ALA:CA	2.03	0.70
1:E:157:ARG:HG2	1:E:304:MET:HE3	1.72	0.70
1:H:50:ILE:HD12	1:H:50:ILE:N	2.05	0.70
1:B:163:VAL:HG13	1:B:194:PHE:CE2	2.27	0.70
1:C:104:MET:HE1	2:C:368:HOH:O	1.90	0.70
1:F:90:ASN:H	1:F:90:ASN:ND2	1.88	0.70
1:A:217:ALA:HB2	1:A:231:VAL:HG13	1.74	0.70
1:H:52:ASN:O	1:H:73:VAL:HG12	1.92	0.70
1:A:364:LYS:O	1:A:364:LYS:HG2	1.91	0.70
1:B:299:MET:CG	1:B:313:LEU:HG	2.21	0.70
1:F:121:THR:HG22	1:F:122:GLU:N	2.06	0.70
1:B:95:GLN:HG3	1:G:171:ILE:HG12	1.74	0.70
1:F:311:GLU:O	1:F:311:GLU:HG3	1.92	0.70
1:G:105:LYS:HD3	1:G:351:TYR:CD2	2.26	0.70
1:E:232:ASP:HA	2:E:389:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LEU:HD12	1:D:303:TRP:CE3	2.28	0.69
1:G:169:LYS:O	1:G:170:TYR:HB3	1.92	0.69
1:B:58:THR:HA	1:B:68:LYS:HG3	1.74	0.69
1:G:168:GLN:OE1	1:G:169:LYS:HG3	1.93	0.69
1:F:187:MET:HE2	1:F:187:MET:HA	1.74	0.69
1:A:169:LYS:HE3	1:A:318:GLU:OE2	1.93	0.69
1:B:174:ARG:NH2	1:B:197:SER:OG	2.26	0.69
1:E:71:ARG:NH1	1:E:78:GLU:OE2	2.26	0.69
1:A:213:PRO:HB3	1:A:215:TYR:CZ	2.27	0.68
1:H:177:LYS:HG3	1:H:179:GLU:OE1	1.94	0.68
1:B:167:HIS:ND1	1:B:172:VAL:CG2	2.57	0.68
1:B:82:LYS:HD3	1:B:84:ILE:HD11	1.74	0.68
1:E:56:GLN:HE21	1:E:70:ALA:HA	1.58	0.68
1:C:338:ALA:HB3	1:C:341:GLU:HG2	1.75	0.68
1:F:86:LYS:HE3	1:F:120:GLU:OE1	1.94	0.68
1:D:202:VAL:HG12	1:D:202:VAL:O	1.92	0.68
1:F:294:SER:O	1:F:298:ILE:HG12	1.94	0.67
1:B:86:LYS:HB2	1:B:94:LEU:CD1	2.21	0.67
1:B:125:LEU:HD12	1:B:125:LEU:C	2.15	0.67
1:E:206:LEU:HD13	1:F:142:VAL:HG23	1.75	0.67
1:B:169:LYS:O	1:B:170:TYR:HB3	1.94	0.67
1:B:339:ARG:NH2	2:B:376:HOH:O	2.14	0.67
1:D:56:GLN:HE21	1:D:70:ALA:CA	2.08	0.67
1:A:228:GLY:C	1:A:230:GLU:H	1.97	0.66
1:G:169:LYS:CB	2:G:367:HOH:O	2.42	0.66
1:B:93:SER:O	1:B:95:GLN:N	2.28	0.66
1:G:165:TYR:CE1	1:G:316:TYR:HD2	2.13	0.66
1:F:71:ARG:HB2	1:F:78:GLU:OE2	1.95	0.66
1:C:56:GLN:HE21	1:C:70:ALA:CA	2.07	0.66
1:D:120:GLU:HG3	1:D:125:LEU:CD1	2.26	0.66
1:G:159:ILE:O	1:G:163:VAL:HG23	1.95	0.66
1:G:299:MET:CG	1:G:313:LEU:HD23	2.21	0.66
1:B:234:TRP:CZ3	1:B:285:LEU:O	2.48	0.65
1:C:93:SER:OG	1:C:199:GLU:OE1	2.08	0.65
1:E:71:ARG:HG3	1:E:71:ARG:NH1	2.07	0.65
1:A:64:PHE:CE2	1:B:268:ARG:HD3	2.32	0.65
1:A:363:ARG:HE	1:A:364:LYS:NZ	1.94	0.65
1:G:109:HIS:CE1	1:G:162:ALA:HA	2.32	0.65
1:B:84:ILE:HG22	1:B:84:ILE:O	1.96	0.65
1:C:88:GLN:HE21	1:C:88:GLN:N	1.93	0.65
1:C:47:GLN:CB	1:C:48:PRO:HD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:LYS:HD3	1:G:351:TYR:CE2	2.31	0.65
1:A:218:PRO:HD3	1:A:234:TRP:CE2	2.32	0.64
1:B:147:MET:HE2	1:B:243:LEU:HD22	1.78	0.64
1:B:306:VAL:HG12	1:B:306:VAL:O	1.95	0.64
1:C:64:PHE:HE2	1:D:268:ARG:HD2	1.62	0.64
1:G:165:TYR:CA	2:G:375:HOH:O	2.30	0.64
1:C:71:ARG:HD3	1:C:78:GLU:OE2	1.97	0.64
1:G:109:HIS:CB	1:G:112:ILE:HG13	2.28	0.64
1:H:238:VAL:O	1:H:242:THR:HG23	1.97	0.64
1:B:90:ASN:HB2	1:B:91:PRO:CD	2.27	0.64
1:B:90:ASN:O	1:B:94:LEU:HB3	1.97	0.64
1:B:232:ASP:HA	1:B:235:SER:OG	1.97	0.63
1:A:240:LEU:HD11	1:A:280:LEU:HD13	1.79	0.63
1:D:347:ILE:CD1	1:D:347:ILE:CB	2.75	0.63
1:B:71:ARG:NH2	1:B:78:GLU:OE2	2.31	0.63
1:A:224:LYS:NZ	1:A:224:LYS:CD	2.60	0.63
1:D:138:PHE:CD2	1:D:178:ALA:HB1	2.34	0.63
1:H:304:MET:HE1	1:H:313:LEU:HD22	1.80	0.63
1:A:290:ILE:HD12	1:A:290:ILE:C	2.17	0.63
1:A:82:LYS:HE2	2:A:366:HOH:O	1.98	0.62
1:D:213:PRO:N	1:D:214:PRO:HD3	2.14	0.62
1:H:169:LYS:HE3	1:H:318:GLU:OE2	1.99	0.62
1:F:204:ASN:O	1:F:206:LEU:N	2.31	0.62
1:A:304:MET:HE1	1:A:313:LEU:HD22	1.81	0.62
1:B:280:LEU:HD22	1:B:284:LEU:CD1	2.30	0.62
1:D:71:ARG:CG	1:D:78:GLU:OE2	2.47	0.62
1:B:301:ASP:OD1	1:B:303:TRP:N	2.28	0.62
1:A:64:PHE:HE2	1:B:268:ARG:NH1	1.97	0.62
1:B:147:MET:HE1	1:B:243:LEU:CD2	2.21	0.62
1:A:240:LEU:CD1	1:A:280:LEU:HD13	2.29	0.62
1:C:150:LYS:HD2	2:C:391:HOH:O	1.99	0.62
1:C:167:HIS:CE1	1:C:232:ASP:OD2	2.51	0.62
1:D:221:PHE:HB3	1:D:259:ARG:HD3	1.81	0.62
1:C:220:LEU:HD12	1:C:224:LYS:O	2.00	0.62
1:F:300:LYS:HE3	1:F:312:GLU:CG	2.25	0.62
1:A:253:GLN:HB2	1:A:257:GLU:OE1	1.99	0.61
1:G:157:ARG:NH2	1:G:308:HIS:CD2	2.68	0.61
1:G:236:LEU:H	1:G:236:LEU:HD22	1.66	0.61
1:H:72:HIS:CE1	1:H:74:LEU:HB2	2.34	0.61
1:F:96:LYS:HE3	1:F:199:GLU:OE2	2.01	0.61
1:H:304:MET:HE1	1:H:313:LEU:CD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLU:OE2	1:B:179:GLU:N	2.27	0.61
1:D:109:HIS:HB3	1:D:112:ILE:HD12	1.83	0.61
1:B:52:ASN:O	1:B:73:VAL:HG13	2.00	0.61
1:D:280:LEU:HD12	1:D:303:TRP:HE3	1.65	0.61
1:F:88:GLN:O	1:F:88:GLN:HG2	2.00	0.61
1:G:280:LEU:HD11	1:G:304:MET:HG2	1.83	0.61
1:G:286:VAL:HG21	1:G:292:ARG:CB	2.29	0.61
1:C:47:GLN:CB	1:C:48:PRO:CD	2.79	0.60
1:F:155:LYS:HE3	1:F:187:MET:O	2.00	0.60
1:C:59:ILE:HG12	1:C:67:VAL:HG12	1.83	0.60
1:F:109:HIS:CE1	1:F:111:ASN:HB2	2.36	0.60
1:G:170:TYR:OH	1:G:194:PHE:O	2.12	0.60
1:D:71:ARG:HG2	1:D:78:GLU:OE2	2.01	0.60
1:G:236:LEU:HD22	1:G:236:LEU:N	2.16	0.60
1:B:304:MET:CE	1:B:304:MET:CA	2.78	0.60
1:A:252:GLY:HA3	1:A:257:GLU:HB3	1.83	0.60
1:C:56:GLN:HE21	1:C:70:ALA:HA	1.65	0.60
1:F:175:ASP:HB2	2:F:372:HOH:O	2.01	0.60
1:H:183:LEU:HA	1:H:188:ASN:O	2.01	0.60
1:C:50:ILE:CD1	1:C:119:ILE:HG21	2.31	0.60
1:G:155:LYS:HE3	1:G:187:MET:O	2.01	0.59
1:D:86:LYS:NZ	1:D:121:THR:O	2.36	0.59
1:E:216:ALA:HB3	1:E:221:PHE:CE2	2.37	0.59
1:E:345:ALA:HA	1:E:350:LYS:CD	2.32	0.59
1:B:91:PRO:CG	1:B:92:THR:H	2.15	0.59
1:A:238:VAL:O	1:A:242:THR:HG23	2.02	0.59
1:G:253:GLN:HE21	1:G:253:GLN:HA	1.67	0.59
1:B:299:MET:HG2	1:B:313:LEU:HG	1.84	0.59
1:C:200:PHE:HB2	2:C:379:HOH:O	2.01	0.59
1:E:93:SER:OG	1:E:199:GLU:OE1	2.20	0.59
1:B:301:ASP:OD1	1:B:302:ARG:N	2.36	0.59
1:C:88:GLN:HE21	1:C:88:GLN:CA	2.14	0.59
1:F:179:GLU:OE1	1:F:207:ASP:HB2	2.02	0.59
1:G:342:ILE:HA	1:G:354:VAL:HG11	1.85	0.59
1:H:78:GLU:HB2	1:H:364:LYS:HZ1	1.67	0.59
1:B:266:LYS:HG3	1:B:267:TYR:H	1.68	0.59
1:F:96:LYS:CE	1:F:199:GLU:OE2	2.50	0.59
1:B:164:GLN:NE2	1:B:315:PRO:HB3	2.18	0.59
1:E:242:THR:HG22	1:E:248:LEU:HA	1.85	0.59
1:G:123:LYS:CG	1:G:124:THR:HG22	2.28	0.58
1:A:141:LEU:HD11	1:A:243:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HG23	1:A:202:VAL:N	2.18	0.58
1:B:91:PRO:CD	1:B:92:THR:H	2.15	0.58
1:B:103:ILE:HD13	1:B:170:TYR:CD2	2.38	0.58
1:B:304:MET:HE3	1:B:304:MET:CA	2.23	0.58
1:D:115:LEU:HD23	1:D:351:TYR:CE1	2.38	0.58
1:F:295:LEU:O	1:F:299:MET:HG3	2.03	0.58
1:G:294:SER:HB3	1:G:297:GLN:OE1	2.02	0.58
1:G:164:GLN:HB2	1:G:295:LEU:HD13	1.83	0.58
1:F:242:THR:HG21	1:F:248:LEU:HD23	1.85	0.58
1:G:237:GLY:HA3	1:G:285:LEU:HD23	1.85	0.58
1:A:64:PHE:CE2	1:B:268:ARG:NH1	2.71	0.58
1:A:213:PRO:HB3	1:A:215:TYR:CE1	2.38	0.58
1:E:103:ILE:O	1:E:106:ILE:HG12	2.03	0.58
1:H:295:LEU:O	1:H:299:MET:HG3	2.03	0.58
1:A:233:VAL:HG21	1:A:293:GLY:O	2.04	0.58
1:B:339:ARG:HG3	2:B:377:HOH:O	2.04	0.58
1:C:238:VAL:O	1:C:242:THR:HG23	2.04	0.58
1:B:174:ARG:CZ	1:B:197:SER:HA	2.33	0.57
1:E:264:ARG:HG2	1:E:266:LYS:HG2	1.86	0.57
1:G:72:HIS:CE1	1:G:74:LEU:HB2	2.38	0.57
1:C:308:HIS:HB3	1:C:311:GLU:O	2.05	0.57
1:C:104:MET:CE	2:C:368:HOH:O	2.49	0.57
1:F:156:PHE:CE2	1:F:304:MET:HE1	2.39	0.57
1:A:228:GLY:O	1:A:230:GLU:N	2.37	0.57
1:A:363:ARG:HE	1:A:364:LYS:HZ1	1.51	0.57
1:H:105:LYS:HG2	1:H:115:LEU:CD2	2.35	0.57
1:C:280:LEU:HD22	1:C:284:LEU:HD11	1.86	0.57
1:F:90:ASN:H	1:F:90:ASN:HD22	1.53	0.57
1:C:64:PHE:CE2	1:D:268:ARG:HD2	2.39	0.57
1:F:280:LEU:HD22	1:F:284:LEU:HD11	1.86	0.57
1:B:167:HIS:CE1	1:B:172:VAL:HG21	2.40	0.56
1:G:286:VAL:CG2	1:G:292:ARG:HE	2.18	0.56
1:H:364:LYS:HG3	2:H:369:HOH:O	2.05	0.56
1:H:327:LYS:O	1:H:331:ILE:HG13	2.06	0.56
1:G:322:ASP:OD1	1:G:322:ASP:C	2.43	0.56
1:C:238:VAL:HG13	1:C:249:PRO:HD2	1.87	0.56
1:G:109:HIS:HD2	1:G:110:PRO:CD	2.18	0.56
1:B:240:LEU:HD11	1:B:280:LEU:HD13	1.88	0.56
1:G:149:GLU:O	1:G:152:ALA:HB3	2.05	0.56
1:C:254:ASN:OD1	1:C:256:LYS:N	2.39	0.56
1:H:304:MET:CE	1:H:313:LEU:CD2	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLU:H	1:B:179:GLU:CD	2.07	0.56
1:D:138:PHE:CE1	1:D:242:THR:HG21	2.41	0.56
1:F:187:MET:HA	1:F:187:MET:CE	2.36	0.56
1:H:351:TYR:CE2	1:H:355:MET:HE1	2.41	0.56
1:E:283:LYS:NZ	1:E:301:ASP:OD2	2.39	0.56
1:A:155:LYS:HE3	1:A:187:MET:O	2.06	0.55
1:C:219:GLU:OE2	1:C:292:ARG:NH2	2.40	0.55
1:C:95:GLN:O	1:C:99:ARG:HB2	2.06	0.55
1:H:153:ARG:O	1:H:157:ARG:HG3	2.07	0.55
1:A:364:LYS:O	1:A:364:LYS:CG	2.54	0.55
1:B:164:GLN:OE1	1:B:164:GLN:C	2.45	0.55
1:G:294:SER:O	1:G:297:GLN:HB2	2.07	0.55
1:C:218:PRO:HB3	1:C:263:LEU:HD23	1.88	0.55
1:C:256:LYS:O	1:C:260:GLU:HG2	2.05	0.55
1:F:204:ASN:O	1:F:205:LYS:C	2.44	0.55
1:G:106:ILE:HG22	1:G:169:LYS:HZ3	1.72	0.55
1:C:56:GLN:O	1:C:57:LYS:C	2.45	0.54
1:A:164:GLN:NE2	1:A:315:PRO:HB3	2.21	0.54
1:C:47:GLN:HB3	1:C:48:PRO:CD	2.37	0.54
1:C:159:ILE:HG13	1:C:189:ILE:HG13	1.88	0.54
1:C:198:ASN:O	1:C:199:GLU:C	2.44	0.54
1:H:141:LEU:HD13	1:H:242:THR:O	2.07	0.54
1:F:53:TYR:CZ	1:F:128:VAL:HG11	2.42	0.54
1:C:213:PRO:HG2	1:C:216:ALA:HB2	1.90	0.54
1:E:71:ARG:HH11	1:E:71:ARG:CB	2.21	0.54
1:E:253:GLN:OE1	1:E:253:GLN:HA	2.07	0.54
1:H:345:ALA:HA	1:H:350:LYS:HD2	1.89	0.54
1:A:215:TYR:CD2	1:A:215:TYR:O	2.61	0.54
1:C:47:GLN:HB3	1:C:48:PRO:HD2	1.90	0.54
1:E:157:ARG:HG2	1:E:304:MET:HE1	1.89	0.54
1:E:184:ASP:OD1	1:E:184:ASP:C	2.45	0.54
1:G:67:VAL:HG23	1:G:202:VAL:HG21	1.90	0.54
1:G:280:LEU:C	1:G:282:LYS:H	2.11	0.53
1:B:109:HIS:HB3	1:B:112:ILE:HD12	1.89	0.53
1:B:155:LYS:HE3	1:B:187:MET:O	2.08	0.53
1:C:333:VAL:HA	1:C:337:PHE:O	2.08	0.53
1:B:117:GLU:HB2	1:B:356:ALA:HB2	1.89	0.53
1:D:57:LYS:HE2	1:D:59:ILE:HG22	1.90	0.53
1:F:179:GLU:HG2	1:F:204:ASN:HB3	1.90	0.53
1:F:280:LEU:HD12	1:F:303:TRP:CE3	2.44	0.53
1:F:56:GLN:O	1:F:57:LYS:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:LEU:HD22	1:F:215:TYR:HE2	1.72	0.53
1:B:53:TYR:CE2	1:B:128:VAL:HG11	2.43	0.53
1:C:74:LEU:HD23	1:C:74:LEU:N	2.23	0.53
1:E:56:GLN:NE2	1:E:78:GLU:OE1	2.27	0.53
1:G:240:LEU:HB3	1:G:281:LEU:HD21	1.90	0.53
1:B:95:GLN:O	1:B:95:GLN:NE2	2.37	0.53
1:E:77:ARG:NH2	1:E:363:ARG:O	2.40	0.53
1:E:205:LYS:O	1:E:208:THR:HB	2.08	0.53
1:A:53:TYR:CZ	1:A:128:VAL:HG11	2.44	0.53
1:G:97:LEU:HD21	1:G:125:LEU:HD22	1.91	0.53
1:A:238:VAL:HG13	1:A:249:PRO:HD2	1.91	0.53
1:D:83:ILE:HG23	1:D:126:TYR:CE2	2.43	0.53
1:E:238:VAL:O	1:E:242:THR:HG23	2.08	0.53
1:G:297:GLN:O	1:G:300:LYS:N	2.41	0.53
1:B:171:ILE:CG2	1:B:173:HIS:HE1	2.22	0.52
1:B:280:LEU:HD11	1:B:304:MET:HG2	1.90	0.52
1:D:138:PHE:CE1	1:D:215:TYR:HE2	2.28	0.52
1:G:109:HIS:CE1	1:G:162:ALA:CA	2.91	0.52
1:D:56:GLN:HE21	1:D:70:ALA:HA	1.74	0.52
1:H:53:TYR:CE2	1:H:72:HIS:CD2	2.97	0.52
1:E:71:ARG:CG	1:E:71:ARG:NH1	2.65	0.52
1:B:312:GLU:O	1:B:313:LEU:C	2.48	0.52
1:D:141:LEU:HD11	1:D:243:LEU:HD23	1.91	0.52
1:G:325:ASP:OD2	1:G:328:ARG:HG3	2.08	0.52
1:E:142:VAL:O	1:E:142:VAL:CG1	2.52	0.52
1:G:232:ASP:O	1:G:235:SER:CB	2.56	0.52
1:C:150:LYS:NZ	2:C:387:HOH:O	2.43	0.52
1:G:109:HIS:HB3	1:G:112:ILE:CG1	2.34	0.52
1:A:198:ASN:HB2	1:A:201:THR:HB	1.91	0.52
1:A:245:SER:HB2	1:A:270:PRO:HG2	1.91	0.52
1:C:47:GLN:HB2	1:C:48:PRO:HD2	1.90	0.52
1:G:113:VAL:HG23	1:G:113:VAL:O	2.10	0.52
1:G:114:LYS:HG3	1:G:363:ARG:HH21	1.73	0.52
1:B:177:LYS:O	1:B:180:ASN:HB2	2.10	0.51
1:E:59:ILE:CG1	1:E:67:VAL:HG12	2.40	0.51
1:A:242:THR:HG21	1:A:248:LEU:HD23	1.92	0.51
1:B:339:ARG:HA	1:B:342:ILE:HD12	1.91	0.51
1:C:116:PHE:CE2	1:C:130:GLU:HA	2.46	0.51
1:G:165:TYR:CD2	2:G:375:HOH:O	2.44	0.51
1:G:253:GLN:HA	1:G:253:GLN:NE2	2.24	0.51
1:A:304:MET:HE1	1:A:313:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:GLU:HB2	1:H:364:LYS:NZ	2.25	0.51
1:C:109:HIS:HB3	1:C:112:ILE:HD12	1.91	0.51
1:C:219:GLU:CD	1:C:292:ARG:HH22	2.12	0.51
1:E:157:ARG:HA	1:E:304:MET:HE1	1.92	0.51
1:G:53:TYR:HB3	1:G:70:ALA:HB1	1.93	0.51
1:G:138:PHE:CE1	1:G:242:THR:HG21	2.46	0.51
1:A:237:GLY:HA2	1:A:284:LEU:CD1	2.41	0.51
1:A:238:VAL:HG13	1:A:249:PRO:CD	2.40	0.51
1:G:109:HIS:CE1	1:G:162:ALA:HB2	2.46	0.51
1:H:53:TYR:CE2	1:H:72:HIS:HD2	2.29	0.51
1:A:181:LEU:HD23	1:A:191:ILE:HD12	1.93	0.51
1:G:342:ILE:HA	1:G:354:VAL:CG1	2.40	0.51
1:C:279:ASN:HD22	1:C:282:LYS:HE2	1.76	0.51
1:G:71:ARG:HD2	1:G:76:GLY:HA2	1.93	0.51
1:A:172:VAL:HG13	1:A:195:GLY:HA3	1.92	0.51
1:C:72:HIS:CE1	1:C:75:THR:HG23	2.46	0.51
1:G:157:ARG:NH2	1:G:308:HIS:HD2	2.07	0.51
1:G:286:VAL:HG23	1:G:292:ARG:HE	1.75	0.51
1:D:288:ASN:O	1:D:289:PRO:C	2.45	0.50
1:F:154:ALA:O	1:F:158:GLN:HG3	2.10	0.50
1:G:333:VAL:O	1:G:336:GLY:N	2.28	0.50
1:H:304:MET:CE	1:H:313:LEU:HD22	2.41	0.50
1:A:218:PRO:HD3	1:A:234:TRP:CD2	2.46	0.50
1:B:251:ASP:OD1	1:B:252:GLY:N	2.42	0.50
1:C:61:LYS:HD2	1:D:272:TYR:CD2	2.46	0.50
1:C:82:LYS:HE2	2:C:368:HOH:O	2.12	0.50
1:G:106:ILE:CG2	1:G:169:LYS:NZ	2.74	0.50
1:B:91:PRO:HD2	1:B:92:THR:H	1.76	0.50
1:A:103:ILE:O	1:A:106:ILE:HG12	2.11	0.50
1:C:88:GLN:CA	1:C:88:GLN:NE2	2.75	0.50
1:E:294:SER:O	1:E:298:ILE:HG12	2.11	0.50
1:F:53:TYR:CE1	1:F:117:GLU:OE1	2.65	0.50
1:A:258:LEU:O	1:A:262:VAL:HG23	2.12	0.50
1:H:277:CYS:O	1:H:281:LEU:HD12	2.12	0.50
1:D:184:ASP:OD1	1:D:188:ASN:HB2	2.12	0.50
1:E:58:THR:HB	1:E:68:LYS:HG3	1.93	0.50
1:G:159:ILE:HD11	1:G:189:ILE:HD12	1.92	0.50
1:G:174:ARG:HH21	1:G:197:SER:HA	1.76	0.50
1:B:50:ILE:HG21	1:B:126:TYR:CE2	2.47	0.50
1:D:119:ILE:HB	1:D:126:TYR:HB2	1.93	0.50
1:E:71:ARG:HH11	1:E:71:ARG:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:MET:HG3	1:B:313:LEU:HG	1.93	0.49
1:A:59:ILE:HD13	1:A:69:LEU:HB2	1.93	0.49
1:A:228:GLY:C	1:A:230:GLU:N	2.66	0.49
1:H:149:GLU:OE1	1:H:303:TRP:NE1	2.40	0.49
1:B:304:MET:HA	1:B:304:MET:CE	2.34	0.49
1:F:52:ASN:O	1:F:73:VAL:HG22	2.12	0.49
1:F:119:ILE:HB	1:F:126:TYR:HB2	1.93	0.49
1:F:181:LEU:HD11	1:F:239:ILE:HD13	1.93	0.49
1:F:310:GLU:H	1:F:310:GLU:CD	2.16	0.49
1:D:109:HIS:CB	1:D:112:ILE:HD12	2.43	0.49
1:G:350:LYS:HG2	1:G:352:ASP:OD2	2.13	0.49
1:H:50:ILE:HD11	1:H:55:LEU:HD21	1.94	0.49
1:H:113:VAL:CG1	1:H:192:ALA:HB2	2.41	0.49
1:H:304:MET:HE2	1:H:313:LEU:HD23	1.93	0.49
1:B:100:GLU:O	1:B:103:ILE:N	2.45	0.49
1:D:95:GLN:HB3	1:D:99:ARG:NH2	2.27	0.49
1:F:54:ARG:HH11	1:F:54:ARG:CG	2.25	0.49
1:G:236:LEU:H	1:G:236:LEU:CD2	2.26	0.49
1:H:146:ARG:NH2	1:H:272:TYR:OH	2.45	0.49
1:G:103:ILE:O	1:G:104:MET:C	2.51	0.49
1:G:159:ILE:CD1	1:G:189:ILE:HD12	2.43	0.49
1:G:232:ASP:O	1:G:235:SER:N	2.46	0.49
1:A:269:ILE:HD13	1:A:278:GLU:HG3	1.95	0.49
1:A:314:LYS:HE2	1:A:315:PRO:HD2	1.94	0.49
1:B:301:ASP:O	1:B:305:ASN:HB2	2.13	0.49
1:G:141:LEU:HD11	1:G:243:LEU:HD23	1.94	0.49
1:A:240:LEU:HD22	1:A:244:VAL:CG1	2.43	0.48
1:D:218:PRO:HD3	1:D:234:TRP:CE2	2.48	0.48
1:F:47:GLN:N	1:F:48:PRO:CD	2.76	0.48
1:F:109:HIS:HB3	1:F:112:ILE:HD12	1.95	0.48
1:G:106:ILE:CG2	1:G:169:LYS:HZ3	2.26	0.48
1:B:91:PRO:CD	1:B:92:THR:N	2.76	0.48
1:B:192:ALA:O	1:B:193:ASP:HB2	2.13	0.48
1:F:97:LEU:HB2	1:F:200:PHE:CE1	2.48	0.48
1:G:60:GLY:O	1:G:66:LYS:HG2	2.12	0.48
1:G:165:TYR:HD1	1:G:316:TYR:HB3	1.77	0.48
1:A:155:LYS:O	1:A:159:ILE:HG13	2.13	0.48
1:F:72:HIS:CE1	1:F:74:LEU:HB2	2.48	0.48
1:E:85:ASP:OD1	1:E:85:ASP:C	2.52	0.48
1:G:237:GLY:HA3	1:G:285:LEU:CD2	2.42	0.48
1:B:90:ASN:CB	1:B:91:PRO:CD	2.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:HIS:HD2	1:G:110:PRO:HD2	1.79	0.48
1:G:217:ALA:CB	1:G:218:PRO:HD2	2.23	0.48
1:D:140:TYR:CD1	1:D:140:TYR:C	2.87	0.48
1:D:201:THR:O	1:D:202:VAL:HG23	2.13	0.48
1:D:218:PRO:O	1:D:221:PHE:N	2.45	0.48
1:D:225:LYS:CE	1:D:225:LYS:H	2.25	0.48
1:E:353:GLU:HG2	2:E:388:HOH:O	2.13	0.48
1:F:47:GLN:N	1:F:48:PRO:HD2	2.29	0.48
1:H:50:ILE:HG21	1:H:126:TYR:CE1	2.47	0.48
1:B:167:HIS:C	1:B:169:LYS:H	2.16	0.48
1:G:363:ARG:HG3	1:G:363:ARG:HH11	1.79	0.48
1:B:270:PRO:HD2	1:B:273:MET:CE	2.43	0.48
1:D:53:TYR:CE2	1:D:128:VAL:HG11	2.49	0.48
1:D:339:ARG:HG2	2:D:382:HOH:O	2.12	0.48
1:D:66:LYS:NZ	1:D:68:LYS:NZ	2.61	0.48
1:F:208:THR:HG22	2:F:384:HOH:O	2.13	0.48
1:G:263:LEU:O	1:G:287:LEU:HD21	2.13	0.48
1:B:93:SER:HB3	1:B:94:LEU:H	1.45	0.47
1:E:58:THR:HA	1:E:68:LYS:HA	1.96	0.47
1:B:53:TYR:N	1:B:53:TYR:CD1	2.82	0.47
1:G:280:LEU:HD22	1:G:284:LEU:HD11	1.95	0.47
1:E:56:GLN:NE2	1:E:70:ALA:CA	2.76	0.47
1:F:56:GLN:O	1:F:57:LYS:C	2.53	0.47
1:F:206:LEU:HD22	1:F:215:TYR:CE2	2.49	0.47
1:D:219:GLU:O	1:D:222:GLN:HB2	2.15	0.47
1:H:120:GLU:HG3	1:H:125:LEU:CD1	2.42	0.47
1:D:57:LYS:HE2	1:D:59:ILE:CG2	2.43	0.47
1:G:159:ILE:HD11	1:G:189:ILE:CD1	2.45	0.47
1:G:286:VAL:HG22	1:G:292:ARG:HG3	1.97	0.47
1:A:304:MET:CE	1:A:313:LEU:HD22	2.45	0.47
1:B:55:LEU:HD23	1:B:70:ALA:HB2	1.96	0.47
1:C:55:LEU:HD23	1:C:70:ALA:HB2	1.97	0.47
1:D:97:LEU:HB2	1:D:200:PHE:CZ	2.49	0.47
1:D:116:PHE:CE2	1:D:130:GLU:HA	2.50	0.47
1:D:186:ASP:O	1:D:187:MET:HB2	2.13	0.47
1:F:69:LEU:HD12	1:F:69:LEU:HA	1.64	0.47
1:G:165:TYR:O	1:G:168:GLN:HG3	2.14	0.47
1:G:255:LEU:O	1:G:259:ARG:CB	2.63	0.47
1:B:281:LEU:HA	1:B:284:LEU:HB2	1.96	0.47
1:D:202:VAL:O	1:D:202:VAL:CG1	2.60	0.47
1:E:85:ASP:OD1	1:E:87:THR:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:LYS:O	1:H:159:ILE:HG13	2.15	0.47
1:B:97:LEU:N	1:B:200:PHE:CE1	2.83	0.47
1:C:257:GLU:OE2	1:C:261:ARG:NH1	2.48	0.47
1:G:53:TYR:CZ	1:G:128:VAL:HG11	2.49	0.47
1:G:301:ASP:CG	1:G:302:ARG:N	2.67	0.47
1:E:90:ASN:ND2	1:E:90:ASN:H	2.13	0.47
1:F:115:LEU:HD12	1:F:128:VAL:O	2.14	0.47
1:A:240:LEU:HD13	1:A:281:LEU:HG	1.96	0.46
1:A:288:ASN:HA	1:A:289:PRO:HD3	1.83	0.46
1:F:117:GLU:OE2	1:F:353:GLU:HA	2.15	0.46
1:H:114:LYS:HG2	2:H:370:HOH:O	2.15	0.46
1:B:125:LEU:CD1	1:B:126:TYR:N	2.51	0.46
1:C:53:TYR:CZ	1:C:128:VAL:HG11	2.51	0.46
1:G:96:LYS:HZ3	1:G:197:SER:H	1.63	0.46
1:D:347:ILE:CD1	1:D:347:ILE:HG21	2.45	0.46
1:E:352:ASP:HB2	2:E:388:HOH:O	2.15	0.46
1:F:167:HIS:NE2	1:F:232:ASP:OD2	2.35	0.46
1:G:132:ALA:HB1	1:G:183:LEU:O	2.14	0.46
1:B:231:VAL:C	1:B:233:VAL:N	2.69	0.46
1:D:258:LEU:HD23	1:D:258:LEU:HA	1.70	0.46
1:F:181:LEU:HD11	1:F:239:ILE:CD1	2.46	0.46
1:F:355:MET:O	1:F:356:ALA:C	2.53	0.46
1:G:109:HIS:HD2	1:G:110:PRO:N	2.13	0.46
1:G:213:PRO:O	1:G:215:TYR:N	2.46	0.46
1:G:294:SER:OG	1:G:297:GLN:N	2.48	0.46
1:B:240:LEU:O	1:B:244:VAL:HG13	2.16	0.46
1:E:345:ALA:HA	1:E:350:LYS:HD3	1.97	0.46
1:G:105:LYS:HG2	1:G:115:LEU:HD23	1.98	0.46
1:G:157:ARG:HH12	1:G:313:LEU:HB2	1.80	0.46
1:B:303:TRP:C	1:B:305:ASN:H	2.19	0.46
1:F:238:VAL:O	1:F:242:THR:HG23	2.15	0.46
1:G:109:HIS:CD2	1:G:111:ASN:H	2.33	0.46
1:B:312:GLU:O	1:B:314:LYS:N	2.49	0.46
1:G:233:VAL:O	1:G:234:TRP:C	2.54	0.46
1:H:163:VAL:HG13	1:H:194:PHE:HE2	1.81	0.46
1:F:53:TYR:CE2	1:F:128:VAL:HG11	2.51	0.46
1:G:109:HIS:HE1	1:G:162:ALA:CA	2.28	0.46
1:B:90:ASN:OD1	1:B:91:PRO:CD	2.63	0.46
1:B:181:LEU:HD23	1:B:191:ILE:HG12	1.98	0.46
1:C:164:GLN:HG3	1:C:299:MET:CE	2.46	0.46
1:F:53:TYR:HE1	1:F:117:GLU:OE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:SER:HB3	1:F:199:GLU:OE1	2.16	0.46
1:G:109:HIS:CD2	1:G:110:PRO:HD2	2.50	0.46
1:B:168:GLN:O	1:B:168:GLN:HG2	2.17	0.45
1:B:304:MET:HB3	1:B:304:MET:HE2	1.60	0.45
1:D:221:PHE:CD1	1:D:259:ARG:HB2	2.51	0.45
1:G:157:ARG:HH21	1:G:308:HIS:CD2	2.34	0.45
1:H:56:GLN:NE2	1:H:78:GLU:OE1	2.40	0.45
1:H:82:LYS:HE2	1:H:200:PHE:O	2.16	0.45
1:H:179:GLU:H	1:H:179:GLU:CD	2.19	0.45
1:H:50:ILE:O	1:H:51:GLY:C	2.54	0.45
1:C:328:ARG:O	1:C:332:MET:HG3	2.16	0.45
1:F:103:ILE:O	1:F:106:ILE:HG12	2.16	0.45
1:F:156:PHE:CD2	1:F:304:MET:HE1	2.51	0.45
1:A:242:THR:HG22	1:A:248:LEU:HA	1.98	0.45
1:B:143:ALA:HB3	1:B:144:HIS:HD2	1.82	0.45
1:B:245:SER:HA	1:B:272:TYR:OH	2.16	0.45
1:C:53:TYR:CE2	1:C:128:VAL:HG11	2.52	0.45
1:E:86:LYS:HA	1:E:89:LEU:HD12	1.97	0.45
1:D:269:ILE:HG12	1:D:278:GLU:HG3	1.98	0.45
1:E:109:HIS:CE1	1:E:111:ASN:HB2	2.52	0.45
1:F:233:VAL:HG13	1:F:284:LEU:CD2	2.47	0.45
1:G:280:LEU:C	1:G:282:LYS:N	2.70	0.45
1:A:64:PHE:CZ	1:B:268:ARG:HD3	2.52	0.45
1:A:164:GLN:HE22	1:A:315:PRO:HB3	1.80	0.45
1:C:159:ILE:HG22	1:C:236:LEU:HD11	1.98	0.45
1:G:267:TYR:N	1:G:267:TYR:CD2	2.84	0.45
1:G:333:VAL:HA	1:G:337:PHE:O	2.17	0.45
1:A:180:ASN:O	1:A:191:ILE:HA	2.17	0.45
1:F:257:GLU:OE2	1:F:261:ARG:NH1	2.41	0.45
1:G:160:VAL:O	1:G:162:ALA:N	2.50	0.45
1:F:86:LYS:O	1:F:87:THR:C	2.54	0.45
1:F:218:PRO:HD3	1:F:234:TRP:CE2	2.52	0.45
1:E:217:ALA:HA	1:E:234:TRP:CD1	2.51	0.44
1:H:237:GLY:HA2	1:H:284:LEU:CD1	2.47	0.44
1:C:286:VAL:HG21	1:C:291:LYS:HB2	2.00	0.44
1:D:72:HIS:CE1	1:D:74:LEU:HB2	2.52	0.44
1:D:224:LYS:HD3	1:D:224:LYS:N	2.32	0.44
1:F:289:PRO:O	1:F:292:ARG:HG3	2.17	0.44
1:B:92:THR:O	1:B:93:SER:O	2.36	0.44
1:D:57:LYS:CE	1:D:59:ILE:HG22	2.47	0.44
1:D:69:LEU:HD12	1:D:69:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:ILE:HD13	1:G:170:TYR:CD2	2.52	0.44
1:G:131:TYR:CE2	1:G:133:SER:HB3	2.52	0.44
1:B:90:ASN:O	1:B:94:LEU:CB	2.64	0.44
1:C:146:ARG:HG3	1:C:146:ARG:NH1	2.17	0.44
1:C:240:LEU:O	1:C:244:VAL:HG13	2.16	0.44
1:C:280:LEU:HG	1:C:301:ASP:OD1	2.16	0.44
1:D:218:PRO:O	1:D:220:LEU:N	2.50	0.44
1:F:120:GLU:HB2	1:F:125:LEU:CD1	2.47	0.44
1:G:90:ASN:ND2	1:G:93:SER:HB2	2.32	0.44
1:H:131:TYR:CZ	1:H:133:SER:HA	2.52	0.44
1:E:304:MET:CE	1:E:313:LEU:HD22	2.48	0.44
1:H:83:ILE:C	1:H:84:ILE:HG13	2.38	0.44
1:C:71:ARG:HG2	2:C:400:HOH:O	2.17	0.44
1:C:90:ASN:OD1	1:C:90:ASN:N	2.47	0.44
1:G:71:ARG:CZ	1:G:78:GLU:OE2	2.65	0.44
1:H:53:TYR:CZ	1:H:128:VAL:HG11	2.51	0.44
1:A:217:ALA:HB2	1:A:231:VAL:CG1	2.46	0.44
1:D:218:PRO:O	1:D:219:GLU:C	2.53	0.44
1:B:154:ALA:O	1:B:155:LYS:C	2.53	0.44
1:C:50:ILE:HD11	1:C:119:ILE:HG21	1.98	0.44
1:G:154:ALA:O	1:G:155:LYS:C	2.56	0.44
1:G:180:ASN:N	1:G:180:ASN:HD22	2.14	0.44
1:G:256:LYS:O	1:G:260:GLU:CB	2.66	0.44
1:C:159:ILE:CG2	1:C:236:LEU:HD11	2.48	0.44
1:F:54:ARG:HG2	1:F:54:ARG:NH1	2.30	0.44
1:G:103:ILE:C	1:G:105:LYS:N	2.70	0.44
1:H:304:MET:CE	1:H:313:LEU:HD23	2.47	0.44
1:F:180:ASN:O	1:F:191:ILE:HA	2.18	0.43
1:G:74:LEU:N	1:G:74:LEU:HD23	2.33	0.43
1:G:100:GLU:OE2	1:G:200:PHE:HD1	2.01	0.43
1:G:141:LEU:HD13	1:G:242:THR:HG23	2.00	0.43
1:H:286:VAL:HB	1:H:292:ARG:HG2	1.99	0.43
1:C:280:LEU:HG	1:C:301:ASP:CG	2.37	0.43
1:G:286:VAL:CG2	1:G:292:ARG:HG3	2.47	0.43
1:G:338:ALA:HB3	1:G:341:GLU:HG2	2.01	0.43
1:B:171:ILE:HG22	1:B:173:HIS:ND1	2.31	0.43
1:C:240:LEU:HD11	1:C:280:LEU:HD13	2.00	0.43
1:D:347:ILE:HG21	1:D:347:ILE:HD13	2.00	0.43
1:G:312:GLU:O	1:G:313:LEU:C	2.56	0.43
1:E:207:ASP:HB3	1:F:142:VAL:HG13	2.00	0.43
1:G:113:VAL:HG12	1:G:190:LYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:TYR:CE2	1:G:169:LYS:HD3	2.52	0.43
1:H:87:THR:HG21	1:H:123:LYS:HG2	1.99	0.43
1:A:57:LYS:HE3	1:A:59:ILE:HG22	1.99	0.43
1:E:216:ALA:O	1:E:221:PHE:HE2	2.02	0.43
1:F:97:LEU:HB2	1:F:200:PHE:CZ	2.53	0.43
1:B:231:VAL:HB	1:B:232:ASP:H	1.33	0.43
1:B:303:TRP:C	1:B:305:ASN:N	2.70	0.43
1:C:285:LEU:HD23	1:C:285:LEU:HA	1.66	0.43
1:E:288:ASN:HA	1:E:289:PRO:HD3	1.80	0.43
1:G:86:LYS:NZ	1:G:121:THR:O	2.43	0.43
1:G:171:ILE:HG22	1:G:171:ILE:O	2.18	0.43
1:G:174:ARG:HB2	1:G:175:ASP:H	1.74	0.43
1:A:165:TYR:O	1:A:168:GLN:HB2	2.18	0.43
1:A:237:GLY:HA2	1:A:284:LEU:HD13	2.01	0.43
1:B:164:GLN:O	1:B:165:TYR:C	2.57	0.43
1:G:155:LYS:O	1:G:159:ILE:CG1	2.55	0.43
1:H:177:LYS:O	1:H:178:ALA:C	2.57	0.43
1:B:157:ARG:NH1	1:B:313:LEU:HB2	2.33	0.43
1:D:294:SER:O	1:D:295:LEU:C	2.56	0.43
1:D:347:ILE:CD1	1:D:347:ILE:CG2	2.96	0.43
1:G:90:ASN:CG	1:G:93:SER:HB2	2.38	0.43
1:G:337:PHE:CD2	1:G:354:VAL:HG22	2.54	0.43
1:B:53:TYR:HA	1:B:71:ARG:O	2.19	0.43
1:C:242:THR:HG22	1:C:248:LEU:HA	2.01	0.43
1:G:106:ILE:HG21	1:G:169:LYS:NZ	2.32	0.43
1:B:57:LYS:H	1:B:57:LYS:HG3	1.45	0.43
1:B:279:ASN:O	1:B:282:LYS:N	2.49	0.43
1:E:73:VAL:HG23	1:E:74:LEU:HD23	2.00	0.43
1:E:232:ASP:O	1:E:236:LEU:HD22	2.19	0.43
1:G:82:LYS:HE2	1:G:200:PHE:O	2.18	0.43
1:G:160:VAL:C	1:G:162:ALA:H	2.21	0.43
1:G:176:LEU:HD12	1:G:176:LEU:HA	1.80	0.43
1:G:217:ALA:CB	1:G:218:PRO:CD	2.90	0.43
1:B:83:ILE:H	1:B:83:ILE:HG12	1.43	0.42
1:B:175:ASP:O	1:B:177:LYS:NZ	2.51	0.42
1:B:288:ASN:HA	1:B:289:PRO:HD3	1.81	0.42
1:C:253:GLN:H	1:C:253:GLN:HE21	1.67	0.42
1:G:177:LYS:HZ2	1:G:177:LYS:HG3	1.60	0.42
1:G:252:GLY:HA3	1:G:261:ARG:HH21	1.84	0.42
1:G:303:TRP:C	1:G:305:ASN:N	2.72	0.42
1:D:280:LEU:HG	1:D:301:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:LEU:HB3	1:F:142:VAL:HG22	2.01	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.89	0.42
1:B:171:ILE:HG21	1:B:173:HIS:HE1	1.83	0.42
1:E:113:VAL:O	1:E:113:VAL:CG2	2.65	0.42
1:F:304:MET:HE3	1:F:304:MET:HB2	1.80	0.42
1:H:101:VAL:O	1:H:105:LYS:HG3	2.19	0.42
1:H:172:VAL:HG13	1:H:195:GLY:HA3	2.01	0.42
1:A:258:LEU:HD23	1:A:262:VAL:HG23	2.02	0.42
1:A:269:ILE:HD13	1:A:278:GLU:CG	2.48	0.42
1:B:166:CYS:O	1:B:170:TYR:CD1	2.72	0.42
1:E:345:ALA:HA	1:E:350:LYS:HD2	2.01	0.42
1:F:156:PHE:HE2	1:F:304:MET:HE1	1.82	0.42
1:G:89:LEU:HB3	1:G:94:LEU:HD12	2.00	0.42
1:G:106:ILE:HG21	1:G:169:LYS:HZ1	1.85	0.42
1:A:364:LYS:HB3	1:A:364:LYS:HE3	1.91	0.42
1:B:151:GLU:O	1:B:152:ALA:C	2.58	0.42
1:C:59:ILE:CG1	1:C:67:VAL:HG12	2.49	0.42
1:E:53:TYR:CE2	1:E:128:VAL:HG11	2.54	0.42
1:E:186:ASP:O	1:E:187:MET:HB2	2.19	0.42
1:B:113:VAL:HG11	1:B:192:ALA:HB2	2.01	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.70	0.42
1:D:302:ARG:NH1	1:D:302:ARG:HG2	2.35	0.42
1:E:85:ASP:OD1	1:E:86:LYS:N	2.53	0.42
1:F:53:TYR:OH	1:F:117:GLU:OE1	2.26	0.42
1:B:264:ARG:NH1	1:B:264:ARG:HB2	2.35	0.42
1:E:272:TYR:HA	1:H:336:GLY:O	2.19	0.42
1:F:305:ASN:O	1:F:306:VAL:C	2.57	0.42
1:F:352:ASP:C	1:F:352:ASP:OD1	2.57	0.42
1:G:56:GLN:NE2	1:G:70:ALA:C	2.73	0.42
1:G:269:ILE:HD12	1:G:269:ILE:HA	1.68	0.42
1:H:115:LEU:HD12	1:H:128:VAL:O	2.20	0.42
1:A:304:MET:HE3	1:A:304:MET:HB3	1.61	0.42
1:C:201:THR:HB	1:C:202:VAL:H	1.64	0.42
1:E:96:LYS:HD3	1:E:197:SER:OG	2.20	0.42
1:E:113:VAL:HG13	1:E:191:ILE:O	2.20	0.42
1:E:121:THR:O	1:E:122:GLU:C	2.58	0.42
1:F:129:MET:HE3	1:F:129:MET:HB3	1.84	0.42
1:A:57:LYS:HE3	1:A:59:ILE:CG2	2.50	0.42
1:B:69:LEU:HD12	1:B:69:LEU:HA	1.93	0.42
1:G:316:TYR:CD1	2:G:373:HOH:O	2.57	0.42
1:H:116:PHE:CD2	1:H:360:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.82	0.41
1:E:205:LYS:O	1:E:206:LEU:C	2.57	0.41
1:F:117:GLU:HB3	1:F:128:VAL:HB	2.02	0.41
1:F:132:ALA:HB1	1:F:183:LEU:O	2.20	0.41
1:H:92:THR:HA	1:H:95:GLN:HB2	2.01	0.41
1:H:361:LEU:HD23	1:H:361:LEU:HA	1.90	0.41
1:A:248:LEU:HG	2:A:387:HOH:O	2.19	0.41
1:B:91:PRO:HG2	1:B:92:THR:H	1.85	0.41
1:B:95:GLN:HE21	1:B:96:LYS:HA	1.85	0.41
1:B:174:ARG:HB3	1:B:177:LYS:HZ1	1.84	0.41
1:B:306:VAL:O	1:B:306:VAL:CG1	2.67	0.41
1:C:82:LYS:HZ3	1:C:82:LYS:HG3	1.75	0.41
1:F:113:VAL:CG1	1:F:192:ALA:HB2	2.50	0.41
1:G:116:PHE:CD2	1:G:360:LEU:HD21	2.55	0.41
1:H:281:LEU:C	1:H:283:LYS:N	2.74	0.41
1:B:83:ILE:HG23	1:B:126:TYR:CE2	2.55	0.41
1:C:280:LEU:HD22	1:C:284:LEU:CD1	2.50	0.41
1:E:71:ARG:NH1	1:E:71:ARG:HB2	2.35	0.41
1:B:91:PRO:CG	1:B:92:THR:N	2.82	0.41
1:B:141:LEU:HD13	1:B:242:THR:O	2.20	0.41
1:F:179:GLU:CG	1:F:204:ASN:HB3	2.51	0.41
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.93	0.41
1:B:95:GLN:C	1:B:95:GLN:NE2	2.70	0.41
1:D:97:LEU:HD21	1:D:125:LEU:HD22	2.02	0.41
1:D:348:ASN:O	1:D:349:GLN:C	2.59	0.41
1:F:233:VAL:HG13	1:F:284:LEU:HD23	2.02	0.41
1:H:351:TYR:CE2	1:H:355:MET:CE	3.03	0.41
1:B:72:HIS:CE1	1:B:74:LEU:HB2	2.55	0.41
1:E:107:LEU:HD21	1:E:170:TYR:CE1	2.56	0.41
1:E:295:LEU:HD23	1:E:295:LEU:HA	1.87	0.41
1:E:313:LEU:HD12	1:E:313:LEU:HA	1.81	0.41
1:G:159:ILE:HD13	1:G:189:ILE:HG21	2.01	0.41
1:H:325:ASP:C	1:H:325:ASP:OD1	2.55	0.41
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.77	0.41
1:B:266:LYS:HG3	1:B:267:TYR:N	2.35	0.41
1:E:53:TYR:OH	1:E:117:GLU:OE1	2.19	0.41
1:E:111:ASN:CG	1:E:158:GLN:HB3	2.41	0.41
1:G:49:HIS:HE1	1:G:73:VAL:HG11	1.86	0.41
1:H:50:ILE:HG12	1:H:126:TYR:CE2	2.54	0.41
1:A:217:ALA:HA	1:A:234:TRP:CD1	2.55	0.41
1:C:298:ILE:N	1:C:298:ILE:HD13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:GLN:HE21	1:E:70:ALA:N	2.18	0.41
1:F:242:THR:CG2	1:F:248:LEU:HD23	2.50	0.41
1:G:176:LEU:HD13	1:G:194:PHE:CD1	2.56	0.41
1:C:198:ASN:O	1:C:200:PHE:N	2.54	0.41
1:G:90:ASN:O	1:G:94:LEU:HB2	2.21	0.41
1:G:109:HIS:CE1	1:G:162:ALA:CB	3.03	0.41
1:H:234:TRP:CZ3	1:H:285:LEU:O	2.74	0.41
1:B:84:ILE:HG21	1:B:97:LEU:HD21	2.03	0.41
1:B:147:MET:CE	1:B:243:LEU:CD2	2.75	0.41
1:D:112:ILE:O	1:D:113:VAL:C	2.58	0.41
1:E:227:ASP:C	1:E:227:ASP:OD2	2.59	0.41
1:F:229:PRO:O	1:F:230:GLU:C	2.56	0.41
1:G:250:PHE:HE2	1:G:285:LEU:CD1	2.34	0.41
1:D:214:PRO:HD2	1:D:215:TYR:CE1	2.57	0.40
1:D:338:ALA:HB3	1:D:341:GLU:HG2	2.02	0.40
1:F:49:HIS:CD2	1:F:49:HIS:N	2.89	0.40
1:G:165:TYR:O	1:G:166:CYS:C	2.59	0.40
1:G:175:ASP:O	1:G:176:LEU:C	2.60	0.40
1:C:333:VAL:O	1:C:334:THR:C	2.57	0.40
1:F:107:LEU:HD13	1:F:112:ILE:HG21	2.02	0.40
1:B:93:SER:O	1:B:96:LYS:N	2.53	0.40
1:C:295:LEU:O	1:C:299:MET:HG3	2.22	0.40
1:G:97:LEU:O	1:G:97:LEU:HG	2.20	0.40
1:G:236:LEU:N	1:G:236:LEU:CD2	2.84	0.40
1:B:180:ASN:O	1:B:191:ILE:HA	2.21	0.40
1:C:69:LEU:HD12	1:C:69:LEU:HA	1.94	0.40
1:E:257:GLU:OE2	1:E:261:ARG:NH2	2.54	0.40
1:E:279:ASN:HD22	1:E:279:ASN:HA	1.77	0.40
1:H:176:LEU:HD12	1:H:176:LEU:HA	1.92	0.40
1:A:117:GLU:HB2	1:A:356:ALA:HB2	2.04	0.40
1:A:159:ILE:HG12	1:A:189:ILE:HG21	2.02	0.40
1:A:324:ASN:HA	1:A:329:ILE:HD11	2.04	0.40
1:C:85:ASP:OD1	1:C:87:THR:OG1	2.36	0.40
1:D:165:TYR:CZ	1:D:169:LYS:HD2	2.57	0.40
1:F:196:PHE:N	1:F:196:PHE:CD2	2.90	0.40

All (1) 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:B:327:LYS:NZ	1:C:364:LYS:O[4_455]	2.11	0.09

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	305/328 (93%)	290 (95%)	12 (4%)	3 (1%)	15	32
1	B	269/328 (82%)	230 (86%)	20 (7%)	19 (7%)	1	1
1	C	306/328 (93%)	290 (95%)	12 (4%)	4 (1%)	12	24
1	D	305/328 (93%)	279 (92%)	22 (7%)	4 (1%)	12	24
1	E	316/328 (96%)	294 (93%)	18 (6%)	4 (1%)	12	24
1	F	316/328 (96%)	293 (93%)	17 (5%)	6 (2%)	8	15
1	G	289/328 (88%)	241 (83%)	33 (11%)	15 (5%)	2	2
1	H	271/328 (83%)	237 (88%)	25 (9%)	9 (3%)	4	6
All	All	2377/2624 (91%)	2154 (91%)	159 (7%)	64 (3%)	5	8

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	93	SER
1	B	94	LEU
1	B	301	ASP
1	B	306	VAL
1	B	313	LEU
1	C	87	THR
1	D	202	VAL
1	E	142	VAL
1	F	204	ASN
1	F	205	LYS
1	G	57	LYS
1	G	87	THR
1	G	201	THR
1	G	217	ALA
1	G	230	GLU
1	G	253	GLN

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Mol	Chain	Res	Type
1	A	185	GLY
1	A	229	PRO
1	B	51	GLY
1	B	91	PRO
1	B	174	ARG
1	B	232	ASP
1	B	304	MET
1	B	351	TYR
1	E	88	GLN
1	F	57	LYS
1	F	203	GLY
1	G	165	TYR
1	G	214	PRO
1	H	57	LYS
1	H	146	ARG
1	H	232	ASP
1	H	286	VAL
1	H	301	ASP
1	B	235	SER
1	B	315	PRO
1	B	353	GLU
1	C	57	LYS
1	D	122	GLU
1	D	176	LEU
1	F	121	THR
1	G	311	GLU
1	H	51	GLY
1	H	88	GLN
1	H	273	MET
1	H	285	LEU
1	B	121	THR
1	B	165	TYR
1	F	222	GLN
1	G	157	ARG
1	G	166	CYS
1	G	251	ASP
1	A	105	LYS
1	C	86	LYS
1	D	311	GLU
1	E	311	GLU
1	E	351	TYR
1	G	148	LYS

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Mol	Chain	Res	Type
1	G	310	GLU
1	B	164	GLN
1	C	88	GLN
1	G	170	TYR
1	B	298	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/290 (93%)	237 (88%)	32 (12%)	5	9
1	B	240/290 (83%)	203 (85%)	37 (15%)	2	4
1	C	272/290 (94%)	238 (88%)	34 (12%)	4	8
1	D	271/290 (93%)	231 (85%)	40 (15%)	3	5
1	E	271/290 (93%)	244 (90%)	27 (10%)	7	14
1	F	277/290 (96%)	247 (89%)	30 (11%)	6	12
1	G	249/290 (86%)	208 (84%)	41 (16%)	2	3
1	H	232/290 (80%)	205 (88%)	27 (12%)	5	10
All	All	2081/2320 (90%)	1813 (87%)	268 (13%)	4	7

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	86	LYS
1	A	94	LEU
1	A	95	GLN
1	A	106	ILE
1	A	114	LYS
1	A	129	MET
1	A	146	ARG
1	A	148	LYS
1	A	150	LYS

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Mol	Chain	Res	Type
1	A	155	LYS
1	A	169	LYS
1	A	175	ASP
1	A	201	THR
1	A	202	VAL
1	A	236	LEU
1	A	240	LEU
1	A	251	ASP
1	A	253	GLN
1	A	255	LEU
1	A	261	ARG
1	A	275	THR
1	A	280	LEU
1	A	286	VAL
1	A	288	ASN
1	A	290	ILE
1	A	301	ASP
1	A	302	ARG
1	A	314	LYS
1	A	326	THR
1	A	347	ILE
1	A	364	LYS
1	B	57	LYS
1	B	58	THR
1	B	61	LYS
1	B	63	ASN
1	B	71	ARG
1	B	73	VAL
1	B	83	ILE
1	B	86	LYS
1	B	92	THR
1	B	93	SER
1	B	95	GLN
1	B	96	LYS
1	B	114	LYS
1	B	120	GLU
1	B	155	LYS
1	B	168	GLN
1	B	197	SER
1	B	235	SER
1	B	236	LEU
1	B	240	LEU

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Mol	Chain	Res	Type
1	B	244	VAL
1	B	263	LEU
1	B	275	THR
1	B	280	LEU
1	B	282	LYS
1	B	286	VAL
1	B	287	LEU
1	B	288	ASN
1	B	302	ARG
1	B	304	MET
1	B	312	GLU
1	B	317	THR
1	B	326	THR
1	B	340	ASP
1	B	343	ASN
1	B	347	ILE
1	B	364	LYS
1	C	47	GLN
1	C	50	ILE
1	C	57	LYS
1	C	66	LYS
1	C	82	LYS
1	C	88	GLN
1	C	106	ILE
1	C	114	LYS
1	C	122	GLU
1	C	129	MET
1	C	146	ARG
1	C	150	LYS
1	C	153	ARG
1	C	155	LYS
1	C	220	LEU
1	C	225	LYS
1	C	236	LEU
1	C	240	LEU
1	C	253	GLN
1	C	257	GLU
1	C	258	LEU
1	C	261	ARG
1	C	264	ARG
1	C	275	THR
1	C	280	LEU

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Mol	Chain	Res	Type
1	C	291	LYS
1	C	292	ARG
1	C	301	ASP
1	C	302	ARG
1	C	310	GLU
1	C	344	ASP
1	C	353	GLU
1	C	363	ARG
1	C	364	LYS
1	D	49	HIS
1	D	58	THR
1	D	61	LYS
1	D	71	ARG
1	D	83	ILE
1	D	92	THR
1	D	94	LEU
1	D	95	GLN
1	D	113	VAL
1	D	114	LYS
1	D	123	LYS
1	D	150	LYS
1	D	155	LYS
1	D	161	SER
1	D	174	ARG
1	D	175	ASP
1	D	176	LEU
1	D	191	ILE
1	D	197	SER
1	D	198	ASN
1	D	199	GLU
1	D	201	THR
1	D	202	VAL
1	D	220	LEU
1	D	222	GLN
1	D	224	LYS
1	D	225	LYS
1	D	236	LEU
1	D	240	LEU
1	D	245	SER
1	D	251	ASP
1	D	258	LEU
1	D	261	ARG

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Mol	Chain	Res	Type
1	D	264	ARG
1	D	280	LEU
1	D	302	ARG
1	D	308	HIS
1	D	317	THR
1	D	324	ASN
1	D	363	ARG
1	E	58	THR
1	E	71	ARG
1	E	85	ASP
1	E	86	LYS
1	E	93	SER
1	E	94	LEU
1	E	113	VAL
1	E	114	LYS
1	E	148	LYS
1	E	155	LYS
1	E	168	GLN
1	E	206	LEU
1	E	208	THR
1	E	236	LEU
1	E	240	LEU
1	E	244	VAL
1	E	251	ASP
1	E	256	LYS
1	E	260	GLU
1	E	266	LYS
1	E	275	THR
1	E	280	LEU
1	E	286	VAL
1	E	326	THR
1	E	343	ASN
1	E	344	ASP
1	E	347	ILE
1	F	57	LYS
1	F	61	LYS
1	F	63	ASN
1	F	64	PHE
1	F	88	GLN
1	F	90	ASN
1	F	96	LYS
1	F	146	ARG

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Mol	Chain	Res	Type
1	F	150	LYS
1	F	155	LYS
1	F	187	MET
1	F	224	LYS
1	F	225	LYS
1	F	235	SER
1	F	236	LEU
1	F	240	LEU
1	F	258	LEU
1	F	259	ARG
1	F	261	ARG
1	F	275	THR
1	F	280	LEU
1	F	286	VAL
1	F	291	LYS
1	F	292	ARG
1	F	310	GLU
1	F	312	GLU
1	F	314	LYS
1	F	317	THR
1	F	347	ILE
1	F	355	MET
1	G	61	LYS
1	G	82	LYS
1	G	87	THR
1	G	88	GLN
1	G	93	SER
1	G	94	LEU
1	G	96	LYS
1	G	106	ILE
1	G	112	ILE
1	G	114	LYS
1	G	123	LYS
1	G	146	ARG
1	G	155	LYS
1	G	157	ARG
1	G	164	GLN
1	G	168	GLN
1	G	174	ARG
1	G	175	ASP
1	G	177	LYS
1	G	201	THR

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Mol	Chain	Res	Type
1	G	202	VAL
1	G	212	SER
1	G	240	LEU
1	G	242	THR
1	G	253	GLN
1	G	266	LYS
1	G	269	ILE
1	G	280	LEU
1	G	285	LEU
1	G	287	LEU
1	G	294	SER
1	G	295	LEU
1	G	304	MET
1	G	308	HIS
1	G	320	ASP
1	G	326	THR
1	G	339	ARG
1	G	340	ASP
1	G	350	LYS
1	G	353	GLU
1	G	363	ARG
1	H	50	ILE
1	H	63	ASN
1	H	90	ASN
1	H	92	THR
1	H	102	ARG
1	H	110	PRO
1	H	114	LYS
1	H	124	THR
1	H	137	VAL
1	H	146	ARG
1	H	155	LYS
1	H	174	ARG
1	H	177	LYS
1	H	201	THR
1	H	202	VAL
1	H	236	LEU
1	H	240	LEU
1	H	242	THR
1	H	245	SER
1	H	269	ILE
1	H	276	ASP

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Mol	Chain	Res	Type
1	H	278	GLU
1	H	280	LEU
1	H	314	LYS
1	H	326	THR
1	H	340	ASP
1	H	347	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	279	ASN
1	B	56	GLN
1	B	95	GLN
1	B	144	HIS
1	B	173	HIS
1	B	297	GLN
1	C	52	ASN
1	C	56	GLN
1	C	63	ASN
1	C	88	GLN
1	C	167	HIS
1	C	222	GLN
1	C	253	GLN
1	C	279	ASN
1	D	56	GLN
1	D	88	GLN
1	D	95	GLN
1	D	167	HIS
1	E	56	GLN
1	E	63	ASN
1	E	90	ASN
1	E	279	ASN
1	E	308	HIS
1	E	343	ASN
1	F	49	HIS
1	F	52	ASN
1	F	88	GLN
1	F	90	ASN
1	F	253	GLN
1	F	279	ASN
1	G	49	HIS

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Mol	Chain	Res	Type
1	G	56	GLN
1	G	88	GLN
1	G	109	HIS
1	G	164	GLN
1	G	180	ASN
1	G	198	ASN
1	G	279	ASN
1	H	144	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	309/328 (94%)	-0.15	0 100 100	25, 42, 77, 89	0
1	B	279/328 (85%)	0.03	7 (2%) 57 51	25, 52, 81, 93	0
1	C	310/328 (94%)	-0.22	0 100 100	20, 36, 62, 73	0
1	D	309/328 (94%)	-0.12	4 (1%) 77 73	26, 43, 72, 84	0
1	E	318/328 (96%)	-0.22	1 (0%) 94 93	23, 40, 59, 72	0
1	F	318/328 (96%)	-0.18	2 (0%) 89 88	20, 39, 64, 75	0
1	G	297/328 (90%)	0.14	10 (3%) 45 38	38, 62, 95, 101	0
1	H	277/328 (84%)	0.14	16 (5%) 23 17	34, 60, 87, 94	0
All	All	2417/2624 (92%)	-0.08	40 (1%) 70 66	20, 46, 81, 101	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	286	VAL	6.0
1	H	250	PHE	5.2
1	H	284	LEU	4.5
1	H	285	LEU	4.3
1	G	63	ASN	4.3
1	G	64	PHE	4.1
1	B	88	GLN	4.0
1	F	207	ASP	3.5
1	B	262	VAL	3.5
1	H	234	TRP	3.3
1	G	253	GLN	3.2
1	G	88	GLN	3.2
1	F	208	THR	3.0
1	B	286	VAL	2.8
1	H	287	LEU	2.8
1	H	271	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	89	LEU	2.5
1	H	298	ILE	2.5
1	H	289	PRO	2.4
1	B	264	ARG	2.4
1	G	344	ASP	2.4
1	E	138	PHE	2.3
1	B	293	GLY	2.3
1	G	212	SER	2.3
1	H	275	THR	2.3
1	G	309	GLU	2.2
1	G	300	LYS	2.2
1	G	315	PRO	2.2
1	H	142	VAL	2.2
1	D	63	ASN	2.2
1	H	63	ASN	2.2
1	H	288	ASN	2.2
1	G	218	PRO	2.2
1	D	255	LEU	2.1
1	H	138	PHE	2.1
1	B	265	GLY	2.1
1	D	94	LEU	2.1
1	H	248	LEU	2.0
1	B	83	ILE	2.0
1	H	251	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.