



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:53 PM UTC

PDB ID : 4TWH / pdb_00004twh
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) mutant F16'S
Authors : Ulens, C.; Spurny, R.; Thompson, A.J.; Alqazzaz, M.; Debaveye, S.; Lu, H.; Price, K.; Villalgordo, J.M.; Tresadern, G.; Lynch, J.W.; Lummis, S.C.R.
Deposited on : 2014-06-30
Resolution : 3.60 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

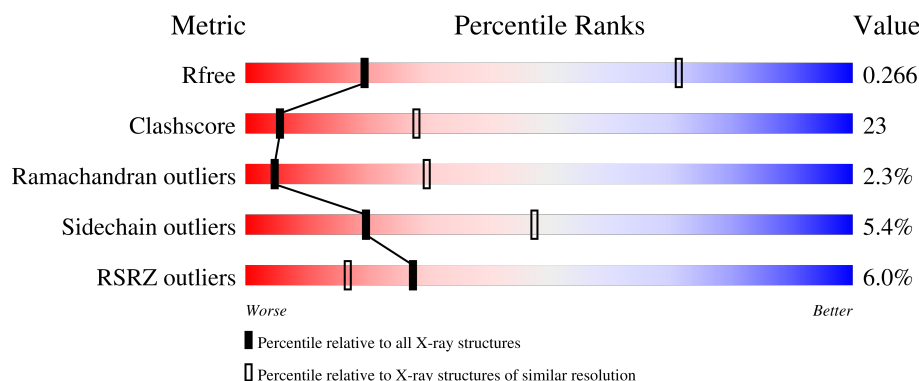
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	307	5% 62% 33% • •
1	B	307	8% 56% 36% 7% •
1	C	307	5% 57% 36% 6% •
1	D	307	4% 55% 37% 7% •
1	E	307	6% 53% 42% 6% •

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Mol	Chain	Length	Quality of chain
1	F	307	4% 57% 38% 5%
1	G	307	7% 53% 39% 7%
1	H	307	7% 59% 36% 5%
1	I	307	8% 61% 31% 6%
1	J	307	7% 55% 37% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24970 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	B	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	C	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	D	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	E	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	F	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	G	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	H	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	I	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	J	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	152	ALA	ILE	conflict	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	164	GLY	-	insertion	UNP P0C7B7
C	247	SER	PHE	engineered mutation	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	152	ALA	ILE	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	247	SER	PHE	engineered mutation	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	152	ALA	ILE	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7
E	247	SER	PHE	engineered mutation	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
F	152	ALA	ILE	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	247	SER	PHE	engineered mutation	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	152	ALA	ILE	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	247	SER	PHE	engineered mutation	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	152	ALA	ILE	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	247	SER	PHE	engineered mutation	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	152	ALA	ILE	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	247	SER	PHE	engineered mutation	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	152	ALA	ILE	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	247	SER	PHE	engineered mutation	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

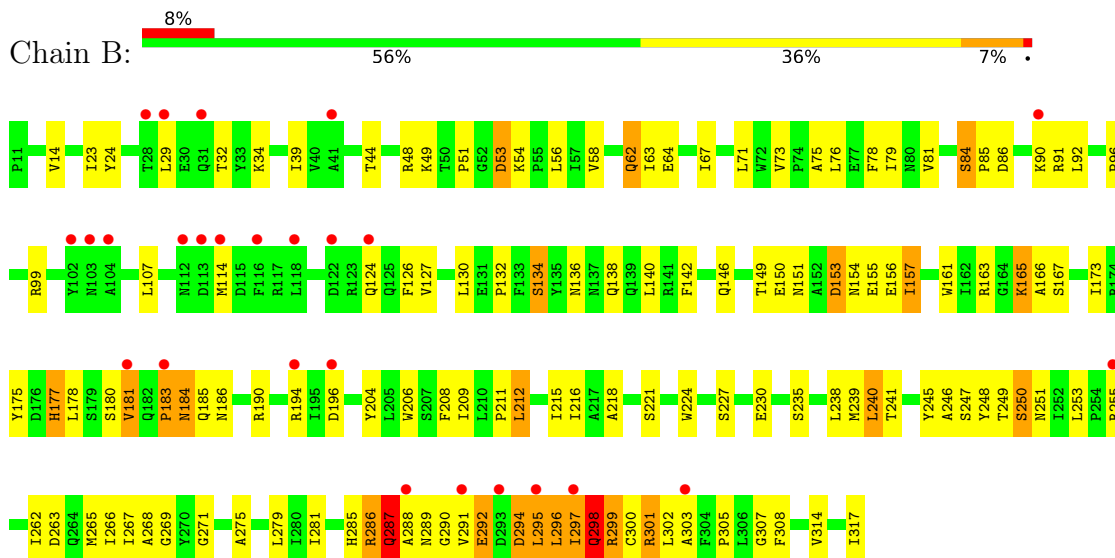
3 Residue-property plots

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: Cys-loop ligand-gated ion channel

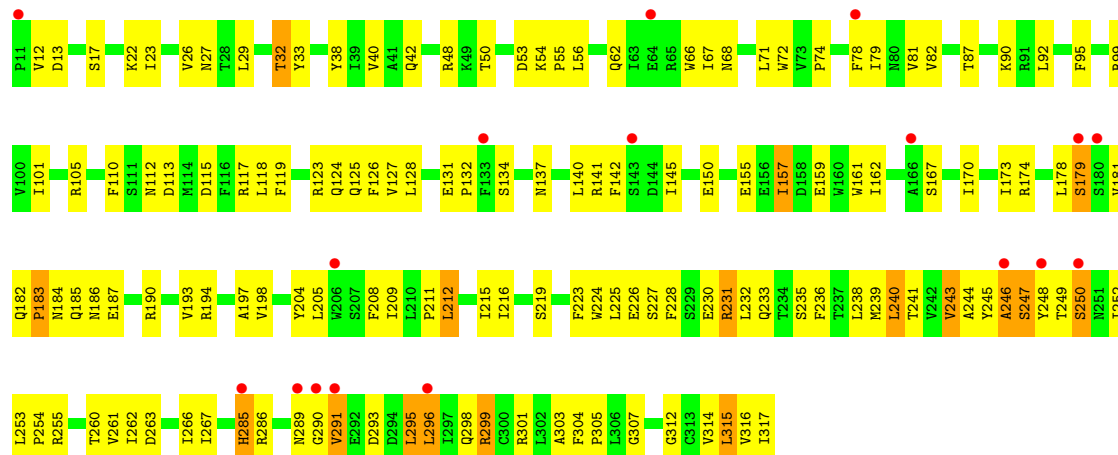


• Molecule 1: Cys-loop ligand-gated ion channel

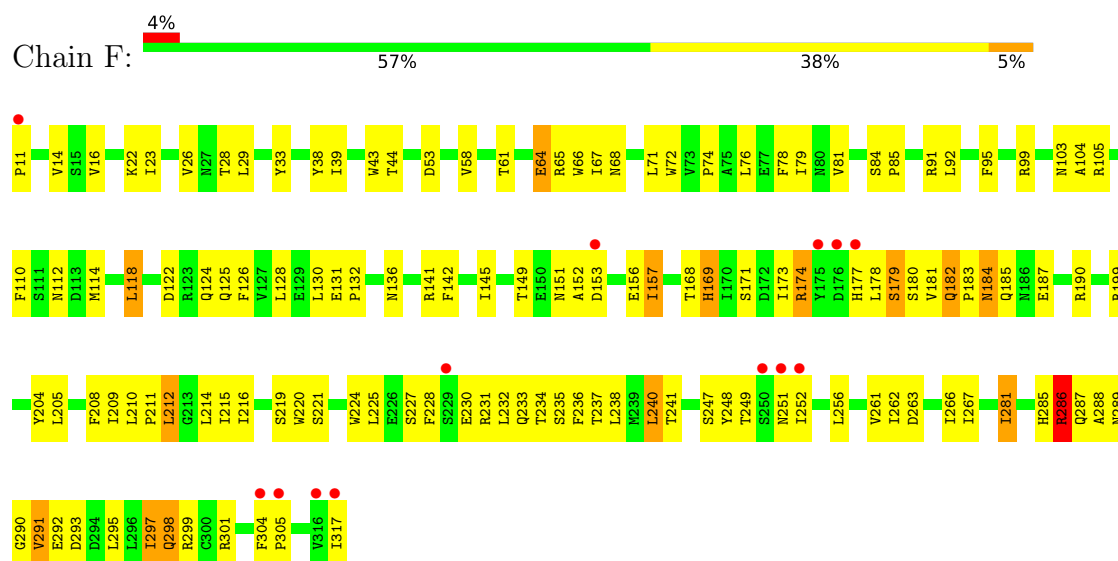


• Molecule 1: Cys-loop ligand-gated ion channel

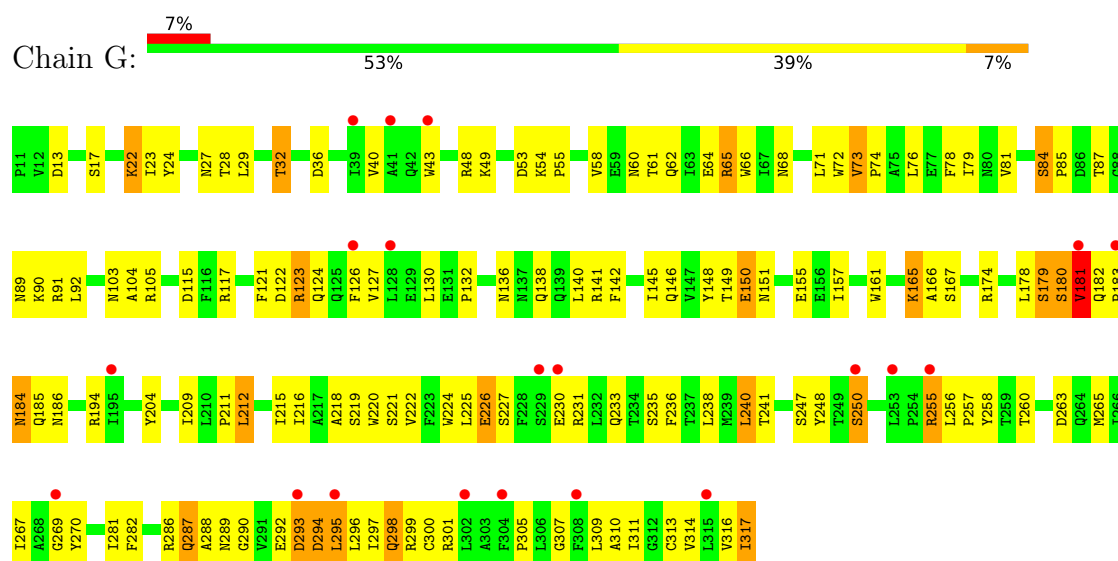




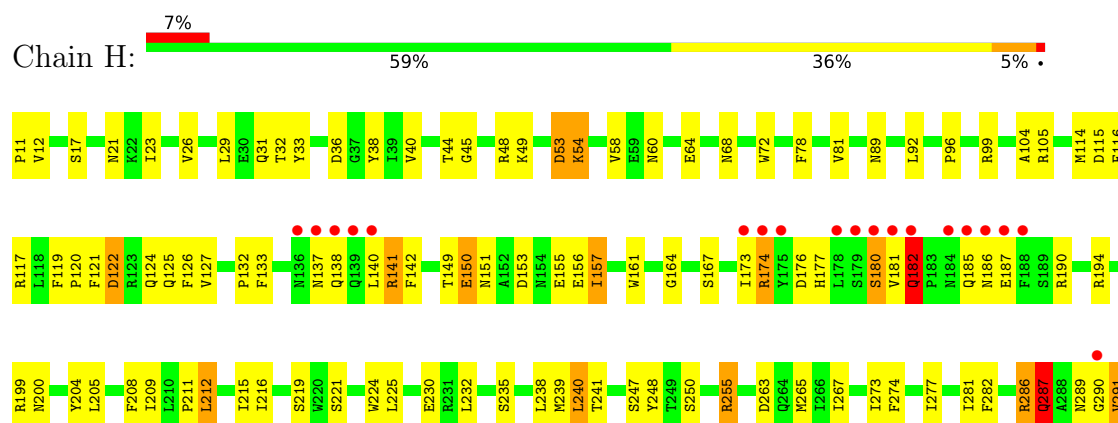
• Molecule 1: Cys-loop ligand-gated ion channel



• Molecule 1: Cys-loop ligand-gated ion channel

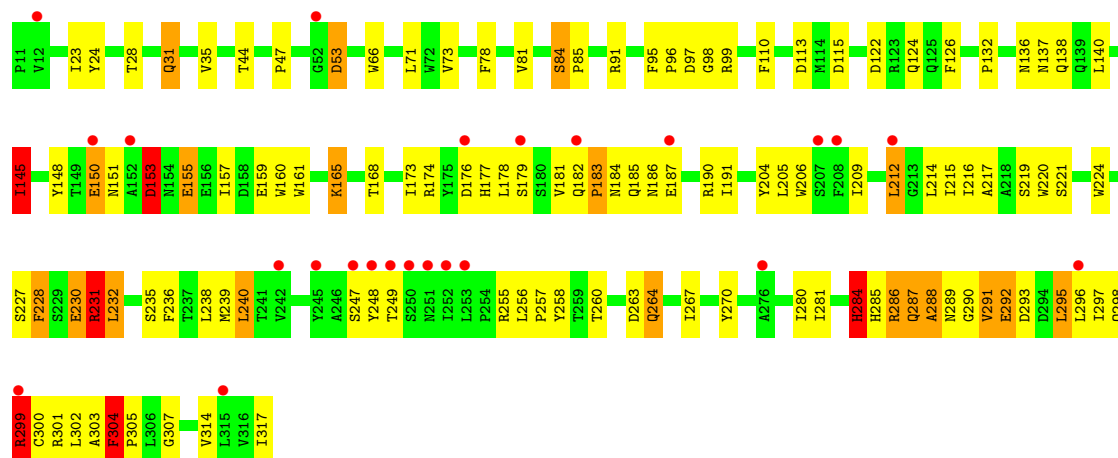


• Molecule 1: Cys-loop ligand-gated ion channel

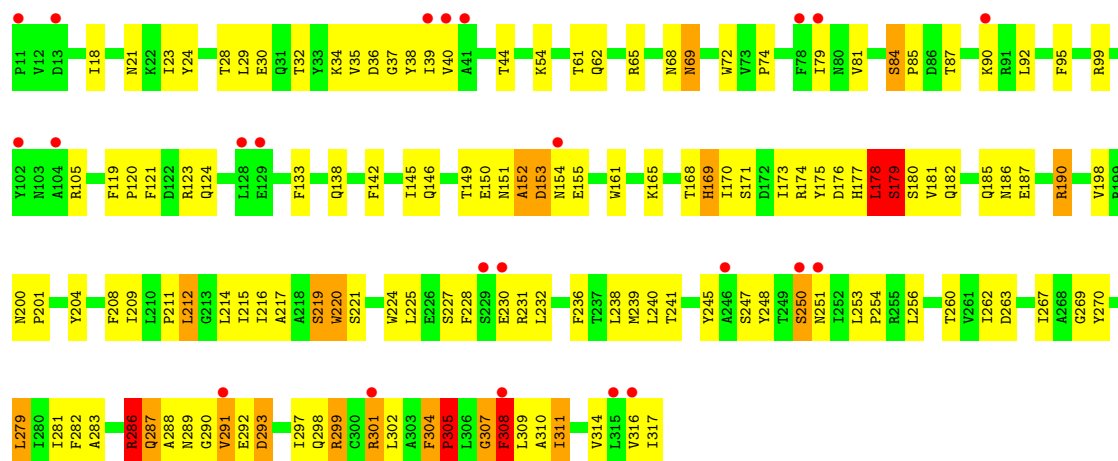




• Molecule 1: Cys-loop ligand-gated ion channel



• Molecule 1: Cys-loop ligand-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.90Å 264.97Å 111.33Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	48.62 – 3.60 48.62 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.62-3.60) 90.2 (48.62-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.220 , 0.263 0.227 , 0.266	Depositor DCC
R_{free} test set	3361 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	91.3	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	24970	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/2564	1.11	14/3495 (0.4%)
1	B	0.61	0/2564	1.16	16/3495 (0.5%)
1	C	0.54	0/2564	1.09	9/3495 (0.3%)
1	D	0.60	1/2564 (0.0%)	1.19	17/3495 (0.5%)
1	E	0.57	0/2564	1.15	13/3495 (0.4%)
1	F	0.49	0/2564	1.03	3/3495 (0.1%)
1	G	0.53	0/2564	1.09	15/3495 (0.4%)
1	H	0.53	0/2564	1.07	10/3495 (0.3%)
1	I	0.60	1/2564 (0.0%)	1.20	24/3495 (0.7%)
1	J	0.60	2/2564 (0.1%)	1.17	16/3495 (0.5%)
All	All	0.56	4/25640 (0.0%)	1.13	137/34950 (0.4%)

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	2
1	B	0	4
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	3
1	G	0	2
1	I	0	3
1	J	0	5
All	All	0	23

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	228	PHE	C-O	-8.62	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	305	PRO	C-O	-7.21	1.14	1.24
1	D	283	ALA	C-O	-6.29	1.16	1.24
1	J	291	VAL	CA-C	5.19	1.58	1.52

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	228	PHE	N-CA-C	-11.19	98.61	111.03
1	H	291	VAL	N-CA-C	10.83	123.36	111.88
1	B	296	LEU	N-CA-C	10.36	123.56	110.61
1	D	284	HIS	N-CA-C	10.24	123.70	111.82
1	D	84	SER	CA-C-N	10.03	129.98	119.85
1	D	84	SER	C-N-CA	10.03	129.98	119.85
1	E	243	VAL	N-CA-C	-9.98	100.62	110.30
1	G	295	LEU	N-CA-C	-9.56	100.19	113.20
1	E	179	SER	N-CA-C	-9.46	97.29	110.35
1	B	285	HIS	N-CA-C	9.18	125.66	113.72
1	D	286	ARG	CA-C-N	-9.00	107.44	122.29
1	D	286	ARG	C-N-CA	-9.00	107.44	122.29
1	F	285	HIS	CA-C-N	-8.91	110.92	122.77
1	F	285	HIS	C-N-CA	-8.91	110.92	122.77
1	D	287	GLN	N-CA-C	8.78	122.84	109.23
1	B	294	ASP	N-CA-C	-8.60	97.40	110.30
1	J	304	PHE	CA-C-N	-8.44	109.29	119.84
1	J	304	PHE	C-N-CA	-8.44	109.29	119.84
1	D	198	VAL	CB-CA-C	-8.29	98.21	110.81
1	A	182	GLN	CA-C-N	-8.25	109.53	119.84
1	A	182	GLN	C-N-CA	-8.25	109.53	119.84
1	I	176	ASP	CA-C-N	-8.01	111.48	122.77
1	I	176	ASP	C-N-CA	-8.01	111.48	122.77
1	B	300	CYS	N-CA-C	-7.86	102.51	113.20
1	E	179	SER	CA-C-N	-7.77	111.26	122.06
1	E	179	SER	C-N-CA	-7.77	111.26	122.06
1	I	284	HIS	CB-CA-C	-7.77	98.91	110.95
1	J	307	GLY	N-CA-C	-7.68	104.17	113.99
1	G	73	VAL	CA-C-N	7.43	127.19	119.76
1	G	73	VAL	C-N-CA	7.43	127.19	119.76
1	B	84	SER	CA-C-N	7.34	127.34	119.78
1	B	84	SER	C-N-CA	7.34	127.34	119.78
1	I	84	SER	CA-C-N	7.24	127.16	119.85
1	I	84	SER	C-N-CA	7.24	127.16	119.85
1	G	256	LEU	N-CA-C	7.21	114.48	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	LYS	CA-C-N	7.18	127.22	119.90
1	C	46	LYS	C-N-CA	7.18	127.22	119.90
1	E	314	VAL	N-CA-C	-7.14	103.36	113.07
1	I	304	PHE	CA-C-N	-7.11	111.16	119.05
1	I	304	PHE	C-N-CA	-7.11	111.16	119.05
1	C	300	CYS	N-CA-C	-7.07	105.48	112.97
1	B	300	CYS	CA-C-N	7.02	130.38	120.28
1	B	300	CYS	C-N-CA	7.02	130.38	120.28
1	I	165	LYS	N-CA-C	-7.00	99.43	109.29
1	I	231	ARG	N-CA-C	6.97	125.64	110.80
1	H	304	PHE	CA-C-N	-6.88	111.41	119.05
1	H	304	PHE	C-N-CA	-6.88	111.41	119.05
1	A	293	ASP	N-CA-C	-6.88	99.85	110.10
1	G	300	CYS	N-CA-C	-6.83	105.35	113.21
1	G	84	SER	CA-C-N	6.80	126.72	119.85
1	G	84	SER	C-N-CA	6.80	126.72	119.85
1	G	287	GLN	N-CA-C	6.80	118.90	108.42
1	J	178	LEU	CB-CA-C	-6.67	106.06	114.40
1	J	299	ARG	N-CA-C	-6.65	105.92	112.97
1	B	287	GLN	N-CA-C	6.55	117.78	108.74
1	A	182	GLN	N-CA-C	6.55	124.28	109.81
1	E	62	GLN	CA-CB-CG	6.50	127.11	114.10
1	H	291	VAL	CB-CA-C	-6.45	103.52	112.36
1	D	300	CYS	N-CA-C	-6.44	106.14	112.97
1	I	296	LEU	N-CA-C	-6.42	103.52	112.45
1	H	45	GLY	N-CA-C	-6.33	103.90	112.57
1	A	179	SER	N-CA-C	-6.29	97.40	110.80
1	J	310	ALA	N-CA-C	-6.29	104.35	111.14
1	C	298	GLN	N-CA-C	-6.28	104.88	112.54
1	J	308	PHE	CB-CA-C	-6.28	97.93	110.42
1	A	300	CYS	CA-C-N	6.24	128.65	120.28
1	A	300	CYS	C-N-CA	6.24	128.65	120.28
1	I	153	ASP	N-CA-C	6.24	124.09	110.80
1	I	299	ARG	N-CA-C	-6.18	103.84	112.25
1	I	73	VAL	CB-CA-C	-6.15	105.23	111.08
1	A	297	ILE	N-CA-C	-6.10	104.02	112.50
1	E	285	HIS	N-CA-C	6.00	120.76	113.38
1	B	290	GLY	N-CA-C	-5.97	99.02	113.18
1	F	286	ARG	CA-CB-CG	-5.97	102.16	114.10
1	D	180	SER	N-CA-C	5.96	123.48	110.80
1	C	169	HIS	CB-CA-C	-5.89	101.64	110.24
1	D	46	LYS	CA-C-N	5.88	127.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	LYS	C-N-CA	5.88	127.19	119.84
1	G	181	VAL	N-CA-C	-5.85	99.97	108.17
1	G	293	ASP	N-CA-C	-5.84	100.73	109.15
1	D	155	GLU	N-CA-C	5.83	118.86	111.69
1	G	165	LYS	N-CA-C	-5.83	106.15	113.72
1	B	298	GLN	CA-CB-CG	-5.79	102.53	114.10
1	I	287	GLN	CA-CB-CG	5.79	125.67	114.10
1	A	285	HIS	CA-C-N	-5.73	114.81	122.72
1	A	285	HIS	C-N-CA	-5.73	114.81	122.72
1	D	299	ARG	N-CA-C	-5.70	106.93	112.97
1	J	190	ARG	N-CA-C	5.68	118.17	108.90
1	H	182	GLN	N-CA-C	5.67	122.35	109.81
1	J	287	GLN	N-CA-C	5.63	117.40	108.79
1	C	286	ARG	N-CA-C	-5.58	100.09	108.96
1	C	182	GLN	N-CA-C	5.57	122.11	109.81
1	E	246	ALA	N-CA-C	5.57	117.03	111.07
1	G	145	ILE	N-CA-C	5.56	115.89	108.27
1	J	84	SER	CA-C-N	5.53	125.44	119.85
1	J	84	SER	C-N-CA	5.53	125.44	119.85
1	A	179	SER	CA-C-N	-5.53	115.38	122.79
1	A	179	SER	C-N-CA	-5.53	115.38	122.79
1	D	292	GLU	CB-CA-C	-5.51	101.74	111.05
1	G	250	SER	N-CA-C	5.48	118.01	111.71
1	D	283	ALA	N-CA-C	-5.47	104.55	111.11
1	G	28	THR	N-CA-C	5.47	117.05	111.14
1	E	12	VAL	N-CA-C	5.45	116.03	108.84
1	B	297	ILE	N-CA-C	-5.42	105.42	113.39
1	H	287	GLN	N-CA-C	5.39	122.29	110.80
1	B	253	LEU	CA-C-N	5.38	125.29	119.85
1	B	253	LEU	C-N-CA	5.38	125.29	119.85
1	B	299	ARG	N-CA-C	-5.38	99.34	110.80
1	D	163	ARG	CG-CD-NE	5.38	123.84	112.00
1	A	298	GLN	CA-CB-CG	5.37	124.83	114.10
1	G	316	VAL	N-CA-C	-5.36	104.54	112.04
1	I	249	THR	N-CA-C	5.35	116.80	110.97
1	J	68	ASN	CA-C-N	-5.34	114.13	122.73
1	J	68	ASN	C-N-CA	-5.34	114.13	122.73
1	H	164	GLY	CA-C-N	-5.34	113.29	122.79
1	H	164	GLY	C-N-CA	-5.34	113.29	122.79
1	D	286	ARG	O-C-N	-5.34	115.49	122.59
1	I	228	PHE	CA-C-O	-5.31	115.43	120.90
1	C	165	LYS	N-CA-C	-5.31	106.82	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	206	TRP	N-CA-C	5.29	117.12	111.36
1	I	151	ASN	N-CA-C	5.25	118.56	110.42
1	E	285	HIS	CA-C-N	-5.21	115.84	122.77
1	E	285	HIS	C-N-CA	-5.21	115.84	122.77
1	I	231	ARG	CA-C-N	5.19	133.32	122.58
1	I	231	ARG	C-N-CA	5.19	133.32	122.58
1	J	279	LEU	CB-CA-C	-5.16	102.78	110.88
1	I	177	HIS	N-CA-C	5.16	116.80	108.34
1	I	232	LEU	N-CA-C	-5.15	106.94	113.43
1	E	250	SER	N-CA-C	5.10	117.50	111.33
1	I	145	ILE	N-CA-C	5.09	115.25	108.27
1	J	178	LEU	N-CA-C	5.08	116.45	109.29
1	E	247	SER	CB-CA-C	-5.07	102.89	110.90
1	B	298	GLN	CB-CG-CD	5.05	121.18	112.60
1	J	169	HIS	N-CA-C	5.05	116.26	107.93
1	A	165	LYS	N-CA-C	-5.03	106.45	112.59
1	H	287	GLN	CB-CG-CD	-5.01	104.08	112.60
1	C	154	ASN	N-CA-C	5.01	118.11	111.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	VAL	Peptide
1	A	286	ARG	Peptide
1	B	177	HIS	Peptide
1	B	286	ARG	Peptide
1	B	288	ALA	Peptide
1	B	298	GLN	Peptide
1	C	286	ARG	Peptide
1	D	285	HIS	Peptide
1	E	181	VAL	Peptide
1	E	286	ARG	Peptide
1	F	177	HIS	Peptide
1	F	179	SER	Peptide
1	F	288	ALA	Peptide
1	G	178	LEU	Peptide
1	G	182	GLN	Peptide
1	I	153	ASP	Peptide
1	I	230	GLU	Peptide
1	I	286	ARG	Peptide
1	J	178	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	J	182	GLN	Peptide
1	J	219	SER	Peptide
1	J	286	ARG	Peptide
1	J	308	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2497	0	2468	127	0
1	B	2497	0	2468	145	0
1	C	2497	0	2468	143	0
1	D	2497	0	2468	143	0
1	E	2497	0	2468	123	0
1	F	2497	0	2468	119	0
1	G	2497	0	2468	116	0
1	H	2497	0	2468	111	0
1	I	2497	0	2468	117	0
1	J	2497	0	2468	148	0
All	All	24970	0	24680	1164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ARG:O	1:C:299:ARG:NH1	1.82	1.13
1:C:286:ARG:NH1	1:C:294:ASP:OD2	1.90	1.04
1:F:174:ARG:NH1	1:F:187:GLU:OE2	1.89	1.03
1:J:224:TRP:HE1	1:J:301:ARG:HG2	1.22	1.02
1:D:252:ILE:O	1:E:255:ARG:NH1	1.97	0.97
1:B:286:ARG:HG3	1:B:286:ARG:HH11	1.27	0.97
1:C:286:ARG:HH12	1:C:297:ILE:HD12	1.30	0.95
1:H:287:GLN:HB2	1:H:292:GLU:HB2	1.47	0.95
1:A:183:PRO:C	1:A:184:ASN:HD22	1.76	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD22	1:E:225:LEU:HD21	1.52	0.91
1:B:287:GLN:HG3	1:B:289:ASN:H	1.35	0.91
1:H:255:ARG:HG3	1:H:255:ARG:HH11	1.35	0.91
1:E:301:ARG:HH11	1:E:301:ARG:HG2	1.37	0.90
1:B:292:GLU:O	1:B:292:GLU:HG2	1.69	0.90
1:J:224:TRP:NE1	1:J:301:ARG:HG2	1.86	0.89
1:F:286:ARG:HG3	1:F:286:ARG:HH11	1.35	0.89
1:G:121:PHE:O	1:G:123:ARG:NH1	2.06	0.89
1:A:59:GLU:HG3	1:A:91:ARG:CZ	2.02	0.89
1:F:91:ARG:HH12	1:F:103:ASN:ND2	1.71	0.88
1:C:286:ARG:NH1	1:C:297:ILE:HD12	1.87	0.87
1:A:240:LEU:HD11	1:E:240:LEU:HD12	1.55	0.86
1:J:175:TYR:HB2	1:J:178:LEU:HD11	1.57	0.86
1:J:224:TRP:HE1	1:J:301:ARG:CG	1.88	0.86
1:A:181:VAL:HG13	1:A:185:GLN:HG3	1.57	0.85
1:F:76:LEU:HB3	1:F:130:LEU:HD21	1.56	0.85
1:D:286:ARG:O	1:D:286:ARG:HG3	1.74	0.85
1:J:287:GLN:HG3	1:J:289:ASN:H	1.39	0.84
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.57	0.84
1:B:298:GLN:HG3	1:B:299:ARG:N	1.92	0.83
1:A:231:ARG:HH22	1:A:298:GLN:HG2	1.44	0.83
1:J:288:ALA:H	1:J:289:ASN:HD22	1.27	0.83
1:C:223:PHE:O	1:C:301:ARG:NH1	2.12	0.83
1:B:230:GLU:OE2	1:C:229:SER:HB3	1.79	0.82
1:D:48:ARG:HG3	1:D:48:ARG:HH11	1.44	0.81
1:F:287:GLN:HB2	1:F:292:GLU:HB3	1.61	0.81
1:I:228:PHE:O	1:I:231:ARG:HB2	1.80	0.81
1:B:221:SER:HA	1:B:224:TRP:CZ3	2.17	0.80
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.62	0.80
1:I:159:GLU:HG3	1:I:160:TRP:CD1	2.17	0.80
1:B:286:ARG:HG3	1:B:286:ARG:NH1	1.85	0.79
1:A:219:SER:HA	1:A:238:LEU:HD23	1.64	0.79
1:B:299:ARG:C	1:B:301:ARG:H	1.87	0.79
1:C:122:ASP:HB3	1:C:124:GLN:HE22	1.48	0.79
1:B:167:SER:HB3	1:B:194:ARG:HB2	1.65	0.79
1:C:219:SER:HA	1:C:238:LEU:HD23	1.64	0.79
1:G:289:ASN:OD1	1:G:290:GLY:N	2.15	0.79
1:J:288:ALA:H	1:J:289:ASN:ND2	1.80	0.79
1:G:294:ASP:C	1:G:296:LEU:H	1.91	0.78
1:B:138:GLN:NE2	1:B:184:ASN:O	2.17	0.78
1:D:286:ARG:CZ	1:D:293:ASP:HA	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:HH11	1:B:163:ARG:HG2	1.50	0.77
1:E:223:PHE:C	1:E:301:ARG:HH12	1.92	0.77
1:D:250:SER:O	1:D:255:ARG:NH2	2.17	0.77
1:E:295:LEU:HA	1:E:298:GLN:HG2	1.66	0.77
1:C:63:ILE:HD13	1:C:90:LYS:HG3	1.66	0.76
1:G:219:SER:HA	1:G:238:LEU:HD23	1.66	0.76
1:C:251:ASN:HD21	1:D:251:ASN:HD22	1.34	0.76
1:I:238:LEU:HD21	1:J:236:PHE:CD2	2.21	0.76
1:A:99:ARG:HH21	1:B:180:SER:HB3	1.51	0.75
1:D:248:TYR:HE2	1:E:243:VAL:O	1.70	0.75
1:A:252:ILE:O	1:B:255:ARG:NH2	2.19	0.75
1:J:44:THR:HA	1:J:99:ARG:HA	1.67	0.75
1:D:289:ASN:CG	1:D:290:GLY:H	1.94	0.75
1:G:287:GLN:OE1	1:G:289:ASN:N	2.20	0.75
1:J:287:GLN:CG	1:J:289:ASN:H	1.99	0.75
1:C:58:VAL:HG12	1:C:63:ILE:HG13	1.68	0.74
1:J:289:ASN:CG	1:J:292:GLU:H	1.95	0.74
1:I:232:LEU:HA	1:I:235:SER:OG	1.86	0.74
1:C:63:ILE:HD13	1:C:90:LYS:NZ	2.01	0.74
1:C:179:SER:OG	1:C:180:SER:N	2.17	0.74
1:E:95:PHE:HB2	1:E:99:ARG:HB2	1.68	0.74
1:G:167:SER:HB3	1:G:194:ARG:HB2	1.68	0.73
1:H:174:ARG:HG3	1:H:174:ARG:HH11	1.51	0.73
1:J:289:ASN:OD1	1:J:292:GLU:N	2.19	0.73
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.70	0.73
1:I:136:ASN:ND2	1:I:187:GLU:OE2	2.22	0.73
1:I:231:ARG:NH1	1:I:232:LEU:HD22	2.03	0.73
1:I:289:ASN:OD1	1:I:290:GLY:N	2.22	0.73
1:H:287:GLN:CD	1:H:292:GLU:H	1.96	0.73
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.70	0.73
1:J:208:PHE:CE2	1:J:262:ILE:HG23	2.24	0.73
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.71	0.72
1:I:31:GLN:HE21	1:I:113:ASP:HA	1.51	0.72
1:A:223:PHE:O	1:A:301:ARG:NH2	2.21	0.72
1:D:287:GLN:NE2	1:D:289:ASN:OD1	2.22	0.72
1:G:248:TYR:HB2	1:H:247:SER:HB3	1.71	0.72
1:H:225:LEU:HD22	1:H:230:GLU:CD	2.13	0.72
1:C:223:PHE:C	1:C:301:ARG:HH12	1.97	0.72
1:D:157:ILE:HD11	1:E:117:ARG:NH2	2.04	0.72
1:C:44:THR:HA	1:C:99:ARG:HA	1.71	0.72
1:H:287:GLN:HB2	1:H:292:GLU:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:301:ARG:O	1:J:301:ARG:HD3	1.89	0.72
1:J:179:SER:OG	1:J:180:SER:N	2.20	0.71
1:C:90:LYS:HZ3	1:C:92:LEU:N	1.88	0.71
1:C:248:TYR:HB2	1:D:247:SER:HB3	1.70	0.71
1:A:59:GLU:HG3	1:A:91:ARG:NE	2.04	0.71
1:F:44:THR:HA	1:F:99:ARG:HA	1.72	0.71
1:H:219:SER:HA	1:H:238:LEU:HD22	1.71	0.71
1:I:314:VAL:O	1:I:317:ILE:HG22	1.90	0.71
1:H:248:TYR:HB2	1:I:247:SER:HB3	1.72	0.71
1:D:44:THR:HA	1:D:99:ARG:HA	1.72	0.71
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.72	0.71
1:A:174:ARG:HG2	1:A:187:GLU:HG2	1.70	0.71
1:G:87:THR:HG21	1:G:90:LYS:HE2	1.72	0.71
1:D:31:GLN:HE21	1:D:114:MET:H	1.39	0.70
1:J:174:ARG:HB2	1:J:187:GLU:HG2	1.72	0.70
1:A:299:ARG:C	1:A:301:ARG:H	1.98	0.70
1:F:208:PHE:HE2	1:F:249:THR:HA	1.55	0.70
1:C:122:ASP:HB3	1:C:124:GLN:NE2	2.06	0.70
1:E:296:LEU:HA	1:E:299:ARG:HD2	1.74	0.70
1:I:299:ARG:C	1:I:301:ARG:H	1.97	0.70
1:D:289:ASN:OD1	1:D:292:GLU:HG2	1.91	0.69
1:E:167:SER:HB3	1:E:194:ARG:HB2	1.72	0.69
1:C:169:HIS:CE1	1:C:171:SER:HB3	2.27	0.69
1:F:236:PHE:CD2	1:J:238:LEU:HD11	2.28	0.69
1:D:64:GLU:O	1:D:68:ASN:ND2	2.25	0.69
1:E:299:ARG:C	1:E:301:ARG:H	2.00	0.69
1:F:91:ARG:HH12	1:F:103:ASN:HD22	1.39	0.69
1:A:61:THR:HG21	1:B:64:GLU:OE2	1.93	0.69
1:A:215:ILE:HD13	1:B:239:MET:HE3	1.75	0.69
1:H:293:ASP:OD2	1:H:298:GLN:HB3	1.93	0.69
1:D:286:ARG:O	1:D:287:GLN:NE2	2.25	0.68
1:H:286:ARG:O	1:H:287:GLN:HB3	1.92	0.68
1:D:14:VAL:HG22	1:D:43:TRP:HB3	1.75	0.68
1:G:27:ASN:HB3	1:G:32:THR:HB	1.72	0.68
1:F:286:ARG:HG3	1:F:286:ARG:NH1	2.05	0.68
1:A:111:SER:OG	1:E:22:LYS:NZ	2.27	0.68
1:G:212:LEU:O	1:G:216:ILE:HG12	1.93	0.68
1:G:13:ASP:OD1	1:G:141:ARG:NH1	2.23	0.68
1:J:253:LEU:HD21	1:J:262:ILE:HG21	1.76	0.68
1:A:182:GLN:N	1:A:182:GLN:OE1	2.26	0.68
1:I:178:LEU:HD23	1:I:186:ASN:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:ASP:HB3	1:G:296:LEU:HG	1.76	0.67
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.76	0.67
1:I:44:THR:HA	1:I:99:ARG:HA	1.76	0.67
1:J:301:ARG:O	1:J:305:PRO:HG2	1.94	0.67
1:B:221:SER:HA	1:B:224:TRP:CE3	2.29	0.67
1:G:299:ARG:HA	1:G:301:ARG:HG3	1.75	0.67
1:I:299:ARG:HA	1:I:301:ARG:HG3	1.76	0.67
1:D:287:GLN:HG3	1:D:289:ASN:H	1.57	0.67
1:G:226:GLU:O	1:G:231:ARG:NH1	2.27	0.67
1:J:221:SER:HA	1:J:301:ARG:NH2	2.10	0.67
1:C:151:ASN:OD1	1:C:152:ALA:N	2.28	0.67
1:J:169:HIS:NE2	1:J:171:SER:HB3	2.09	0.67
1:I:219:SER:HA	1:I:238:LEU:HD13	1.77	0.67
1:I:264:GLN:HA	1:I:267:ILE:HG12	1.77	0.67
1:C:299:ARG:HH11	1:C:299:ARG:C	2.02	0.67
1:I:291:VAL:O	1:I:293:ASP:N	2.26	0.67
1:I:148:TYR:CE1	1:J:177:HIS:ND1	2.62	0.67
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.77	0.66
1:H:316:VAL:HG23	1:H:317:ILE:HD12	1.75	0.66
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.78	0.66
1:J:282:PHE:CZ	1:J:286:ARG:HD3	2.31	0.66
1:C:229:SER:O	1:C:233:GLN:HG2	1.95	0.66
1:J:289:ASN:CG	1:J:290:GLY:H	2.02	0.66
1:E:295:LEU:O	1:E:299:ARG:HD2	1.96	0.66
1:F:287:GLN:HG2	1:F:289:ASN:H	1.59	0.66
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.76	0.66
1:A:61:THR:HG21	1:B:64:GLU:CD	2.21	0.65
1:C:63:ILE:HD13	1:C:90:LYS:HZ2	1.62	0.65
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.79	0.65
1:I:287:GLN:HE22	1:I:290:GLY:N	1.93	0.65
1:F:212:LEU:O	1:F:216:ILE:HG12	1.96	0.65
1:E:289:ASN:OD1	1:E:290:GLY:N	2.30	0.65
1:J:208:PHE:CZ	1:J:262:ILE:HG23	2.32	0.65
1:G:27:ASN:OD1	1:G:255:ARG:NH1	2.26	0.65
1:H:241:THR:HA	1:I:240:LEU:HD23	1.78	0.65
1:F:68:ASN:OD1	1:J:62:GLN:NE2	2.28	0.65
1:I:299:ARG:O	1:I:299:ARG:HG3	1.96	0.65
1:J:305:PRO:O	1:J:308:PHE:N	2.19	0.65
1:B:153:ASP:CG	1:B:154:ASN:H	2.05	0.65
1:C:153:ASP:OD2	1:C:154:ASN:ND2	2.30	0.65
1:F:295:LEU:HA	1:F:298:GLN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:289:ASN:ND2	1:J:292:GLU:HB2	2.12	0.64
1:C:294:ASP:OD1	1:C:294:ASP:N	2.28	0.64
1:D:65:ARG:NH1	1:E:68:ASN:O	2.30	0.64
1:J:176:ASP:HB2	1:J:177:HIS:CD2	2.33	0.64
1:J:221:SER:HA	1:J:301:ARG:HH22	1.62	0.64
1:D:211:PRO:O	1:D:215:ILE:HG12	1.98	0.64
1:F:11:PRO:C	1:F:141:ARG:HH12	2.06	0.64
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.78	0.64
1:B:54:LYS:H	1:B:54:LYS:HD2	1.63	0.64
1:D:286:ARG:HH12	1:D:298:GLN:HE21	1.45	0.64
1:G:219:SER:HA	1:G:238:LEU:CD2	2.27	0.63
1:H:38:TYR:CZ	1:H:105:ARG:HD2	2.33	0.63
1:H:235:SER:HA	1:H:238:LEU:HD12	1.80	0.63
1:I:231:ARG:CZ	1:I:232:LEU:HD13	2.28	0.63
1:C:63:ILE:CD1	1:C:90:LYS:NZ	2.60	0.63
1:C:251:ASN:ND2	1:D:251:ASN:HD22	1.96	0.63
1:H:167:SER:HB2	1:H:194:ARG:HB2	1.79	0.63
1:D:123:ARG:HH21	1:D:198:VAL:HG22	1.63	0.63
1:F:11:PRO:CA	1:F:141:ARG:HH12	2.11	0.63
1:F:11:PRO:CB	1:F:141:ARG:HH12	2.10	0.63
1:C:63:ILE:HG12	1:C:90:LYS:HZ1	1.64	0.63
1:C:90:LYS:HD2	1:C:91:ARG:N	2.14	0.63
1:B:241:THR:HA	1:C:240:LEU:HD23	1.80	0.63
1:A:184:ASN:HD22	1:A:184:ASN:N	1.95	0.63
1:A:248:TYR:HB2	1:B:247:SER:HB3	1.81	0.63
1:D:212:LEU:O	1:D:216:ILE:HG12	1.99	0.63
1:A:19:PHE:CZ	1:B:178:LEU:HD11	2.33	0.63
1:D:215:ILE:HD13	1:E:239:MET:HE3	1.80	0.63
1:H:44:THR:HA	1:H:99:ARG:HA	1.79	0.63
1:C:14:VAL:HG22	1:C:43:TRP:HB3	1.81	0.63
1:D:248:TYR:OH	1:E:244:ALA:HA	1.99	0.62
1:F:91:ARG:NH1	1:F:103:ASN:HB3	2.13	0.62
1:J:123:ARG:HG3	1:J:198:VAL:HG22	1.79	0.62
1:B:298:GLN:HG3	1:B:299:ARG:CB	2.29	0.62
1:A:287:GLN:HG3	1:A:289:ASN:H	1.64	0.62
1:F:240:LEU:HD23	1:J:241:THR:HA	1.80	0.62
1:A:183:PRO:C	1:A:184:ASN:ND2	2.52	0.62
1:C:90:LYS:HD2	1:C:91:ARG:H	1.64	0.62
1:J:149:THR:O	1:J:151:ASN:N	2.31	0.62
1:B:177:HIS:CD2	1:B:178:LEU:HA	2.35	0.62
1:E:42:GLN:HB2	1:E:101:ILE:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:O	1:A:216:ILE:HG12	1.99	0.62
1:D:248:TYR:CE2	1:E:243:VAL:O	2.52	0.62
1:F:287:GLN:HG3	1:F:290:GLY:H	1.65	0.62
1:C:54:LYS:HD2	1:C:55:PRO:HD2	1.82	0.62
1:D:225:LEU:HD21	1:E:232:LEU:HD22	1.81	0.62
1:H:157:ILE:C	1:I:258:TYR:OH	2.43	0.62
1:A:165:LYS:O	1:A:165:LYS:HG3	2.00	0.62
1:F:248:TYR:CD1	1:G:247:SER:HA	2.35	0.62
1:B:24:TYR:CE2	1:B:34:LYS:HD3	2.33	0.61
1:I:301:ARG:O	1:I:305:PRO:HG2	2.00	0.61
1:A:178:LEU:HB2	1:A:179:SER:O	1.99	0.61
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.82	0.61
1:C:311:ILE:O	1:C:314:VAL:HG22	2.00	0.61
1:J:24:TYR:CE2	1:J:34:LYS:HD3	2.35	0.61
1:C:223:PHE:C	1:C:301:ARG:NH1	2.58	0.61
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.82	0.61
1:G:293:ASP:O	1:G:295:LEU:N	2.34	0.61
1:I:286:ARG:O	1:I:292:GLU:HB3	1.99	0.61
1:D:286:ARG:NH2	1:D:293:ASP:OD1	2.33	0.61
1:F:252:ILE:HD11	1:G:250:SER:HB3	1.81	0.61
1:I:224:TRP:CH2	1:I:301:ARG:HB3	2.35	0.61
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.36	0.61
1:C:169:HIS:ND1	1:C:171:SER:HB3	2.16	0.61
1:F:236:PHE:HD2	1:J:238:LEU:HD11	1.64	0.61
1:G:299:ARG:C	1:G:301:ARG:H	2.06	0.61
1:C:295:LEU:HA	1:C:298:GLN:HG2	1.81	0.61
1:A:95:PHE:HB2	1:A:99:ARG:HB3	1.81	0.61
1:C:289:ASN:OD1	1:C:290:GLY:N	2.27	0.61
1:I:216:ILE:O	1:I:219:SER:HB3	2.01	0.61
1:A:174:ARG:HD3	1:A:187:GLU:OE2	2.01	0.61
1:A:91:ARG:NH1	1:B:134:SER:HB2	2.16	0.60
1:E:225:LEU:HD13	1:E:230:GLU:HG2	1.83	0.60
1:F:224:TRP:CD1	1:F:301:ARG:HH11	2.19	0.60
1:E:208:PHE:O	1:E:245:TYR:OH	2.18	0.60
1:G:260:THR:H	1:G:263:ASP:HB2	1.64	0.60
1:I:289:ASN:OD1	1:I:291:VAL:N	2.32	0.60
1:I:295:LEU:CD2	1:I:298:GLN:HB2	2.32	0.60
1:C:90:LYS:HD3	1:C:102:TYR:CE1	2.36	0.60
1:E:301:ARG:HG2	1:E:301:ARG:NH1	2.12	0.60
1:B:76:LEU:HB3	1:B:130:LEU:HD21	1.82	0.60
1:G:179:SER:OG	1:G:180:SER:N	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:LEU:CD2	1:I:186:ASN:HB3	2.31	0.60
1:E:223:PHE:C	1:E:301:ARG:NH1	2.60	0.60
1:J:232:LEU:HD23	1:J:236:PHE:HE1	1.66	0.60
1:B:208:PHE:HE2	1:B:249:THR:HA	1.67	0.60
1:C:241:THR:HA	1:D:240:LEU:HD23	1.82	0.60
1:E:228:PHE:HA	1:E:231:ARG:HG3	1.83	0.60
1:J:23:ILE:HG12	1:J:35:VAL:HG22	1.83	0.60
1:C:63:ILE:HG21	1:C:90:LYS:HE3	1.83	0.60
1:I:204:TYR:O	1:I:209:ILE:HG12	2.02	0.60
1:B:149:THR:O	1:B:151:ASN:N	2.34	0.59
1:C:298:GLN:HG3	1:C:299:ARG:N	2.17	0.59
1:J:219:SER:HA	1:J:238:LEU:HD21	1.84	0.59
1:B:224:TRP:CD2	1:B:301:ARG:HD3	2.37	0.59
1:C:224:TRP:HA	1:C:301:ARG:NH1	2.17	0.59
1:G:127:VAL:HG22	1:G:194:ARG:HG2	1.83	0.59
1:I:159:GLU:HG3	1:I:160:TRP:HD1	1.67	0.59
1:C:124:GLN:N	1:C:124:GLN:OE1	2.34	0.59
1:G:209:ILE:HG23	1:G:265:MET:HE1	1.83	0.59
1:G:288:ALA:N	1:G:292:GLU:OE2	2.30	0.59
1:I:155:GLU:HG2	1:I:161:TRP:CD1	2.37	0.59
1:J:291:VAL:O	1:J:293:ASP:N	2.35	0.59
1:B:127:VAL:HG22	1:B:194:ARG:HG2	1.84	0.59
1:D:284:HIS:C	1:D:286:ARG:HG2	2.27	0.59
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.84	0.59
1:H:221:SER:HB2	1:I:281:ILE:HD11	1.84	0.59
1:I:260:THR:O	1:I:264:GLN:HG2	2.03	0.59
1:B:287:GLN:HG3	1:B:289:ASN:N	2.13	0.59
1:E:296:LEU:HA	1:E:299:ARG:CD	2.32	0.59
1:I:137:ASN:HA	1:I:140:LEU:O	2.03	0.59
1:D:123:ARG:NH2	1:D:198:VAL:HG22	2.16	0.59
1:J:220:TRP:CZ2	1:J:301:ARG:NH1	2.71	0.59
1:A:227:SER:O	1:A:231:ARG:HD2	2.03	0.59
1:A:300:CYS:HG	1:A:304:PHE:HE2	1.51	0.59
1:G:181:VAL:HG12	1:G:183:PRO:HD2	1.83	0.59
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.83	0.59
1:B:296:LEU:HD23	1:B:298:GLN:HE22	1.68	0.58
1:A:247:SER:HB3	1:E:248:TYR:HB2	1.83	0.58
1:D:31:GLN:HE21	1:D:113:ASP:HA	1.66	0.58
1:F:287:GLN:HG2	1:F:289:ASN:N	2.17	0.58
1:I:215:ILE:HD13	1:J:239:MET:HE3	1.84	0.58
1:I:240:LEU:HD13	1:J:240:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:228:PHE:HA	1:J:231:ARG:CZ	2.34	0.58
1:C:211:PRO:O	1:C:215:ILE:HG12	2.03	0.58
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.39	0.58
1:C:90:LYS:HD3	1:C:102:TYR:CZ	2.38	0.58
1:D:286:ARG:HD2	1:D:292:GLU:C	2.28	0.58
1:F:112:ASN:ND2	1:F:125:GLN:O	2.37	0.58
1:E:174:ARG:HH12	1:E:187:GLU:CD	2.11	0.58
1:H:53:ASP:O	1:H:96:PRO:HG3	2.03	0.58
1:D:216:ILE:O	1:D:219:SER:HB3	2.04	0.58
1:D:248:TYR:HD1	1:D:248:TYR:N	2.00	0.58
1:A:239:MET:HE3	1:E:215:ILE:HD13	1.86	0.58
1:G:314:VAL:O	1:G:317:ILE:HG12	2.04	0.58
1:H:33:TYR:OH	1:H:127:VAL:N	2.26	0.58
1:J:289:ASN:ND2	1:J:292:GLU:OE1	2.37	0.58
1:B:54:LYS:HD2	1:B:54:LYS:N	2.19	0.58
1:G:211:PRO:O	1:G:215:ILE:HG12	2.04	0.58
1:A:241:THR:HA	1:B:240:LEU:HD23	1.85	0.58
1:E:183:PRO:HD2	1:E:184:ASN:H	1.68	0.58
1:F:169:HIS:NE2	1:F:171:SER:HB3	2.19	0.58
1:A:142:PHE:HB3	1:A:170:ILE:HD13	1.85	0.57
1:D:123:ARG:HE	1:D:198:VAL:HG22	1.69	0.57
1:H:200:ASN:ND2	1:I:258:TYR:HE1	2.02	0.57
1:A:289:ASN:OD1	1:A:290:GLY:N	2.31	0.57
1:C:251:ASN:HD21	1:D:251:ASN:ND2	2.01	0.57
1:D:46:LYS:HD2	1:D:46:LYS:N	2.18	0.57
1:D:123:ARG:HH21	1:D:198:VAL:CG2	2.17	0.57
1:E:174:ARG:HA	1:E:186:ASN:O	2.04	0.57
1:J:153:ASP:CG	1:J:154:ASN:H	2.11	0.57
1:B:299:ARG:C	1:B:301:ARG:N	2.60	0.57
1:C:208:PHE:O	1:C:245:TYR:OH	2.21	0.57
1:E:301:ARG:HH11	1:E:301:ARG:CG	2.14	0.57
1:G:204:TYR:O	1:G:209:ILE:HG12	2.04	0.57
1:B:39:ILE:HD11	1:B:130:LEU:HD11	1.86	0.57
1:B:212:LEU:O	1:B:216:ILE:HG12	2.03	0.57
1:D:31:GLN:NE2	1:D:114:MET:H	2.03	0.57
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.86	0.57
1:H:215:ILE:HD13	1:I:239:MET:HE3	1.87	0.57
1:C:63:ILE:CD1	1:C:90:LYS:HZ2	2.17	0.57
1:F:64:GLU:O	1:F:64:GLU:HG3	2.05	0.57
1:A:182:GLN:CD	1:A:183:PRO:HD3	2.30	0.57
1:D:284:HIS:HA	1:D:286:ARG:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ASN:CG	1:D:290:GLY:N	2.63	0.57
1:H:176:ASP:OD1	1:H:177:HIS:N	2.38	0.57
1:A:224:TRP:HA	1:A:301:ARG:HH21	1.69	0.56
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.40	0.56
1:A:231:ARG:NH2	1:A:298:GLN:HG2	2.19	0.56
1:F:263:ASP:O	1:F:267:ILE:HG12	2.06	0.56
1:H:287:GLN:NE2	1:H:290:GLY:C	2.64	0.56
1:I:228:PHE:CE1	1:I:284:HIS:HB2	2.41	0.56
1:J:299:ARG:C	1:J:301:ARG:H	2.13	0.56
1:J:301:ARG:HD3	1:J:302:LEU:HD23	1.88	0.56
1:A:295:LEU:HA	1:A:298:GLN:HG3	1.87	0.56
1:C:90:LYS:NZ	1:C:92:LEU:HG	2.20	0.56
1:A:181:VAL:O	1:A:185:GLN:NE2	2.38	0.56
1:I:212:LEU:O	1:I:216:ILE:HG12	2.05	0.56
1:D:123:ARG:NE	1:D:198:VAL:HG22	2.21	0.56
1:I:257:PRO:HG2	1:I:258:TYR:CZ	2.41	0.56
1:C:149:THR:O	1:C:151:ASN:N	2.39	0.56
1:D:274:PHE:O	1:D:278:LEU:HD13	2.06	0.56
1:E:17:SER:HB2	1:E:40:VAL:HB	1.88	0.56
1:H:122:ASP:OD2	1:H:199:ARG:NE	2.33	0.56
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.87	0.56
1:I:228:PHE:CZ	1:I:284:HIS:CD2	2.94	0.56
1:J:204:TYR:O	1:J:209:ILE:HG12	2.06	0.56
1:A:148:TYR:HH	1:B:177:HIS:CE1	2.23	0.56
1:A:228:PHE:HA	1:A:231:ARG:HD3	1.87	0.56
1:C:212:LEU:O	1:C:216:ILE:HG12	2.06	0.56
1:C:289:ASN:CG	1:C:290:GLY:H	2.14	0.56
1:D:263:ASP:O	1:D:267:ILE:HG12	2.05	0.56
1:F:251:ASN:HD22	1:J:251:ASN:ND2	2.04	0.56
1:G:62:GLN:NE2	1:H:68:ASN:OD1	2.37	0.56
1:H:216:ILE:O	1:H:219:SER:HB3	2.05	0.56
1:H:224:TRP:CD1	1:H:301:ARG:HH11	2.24	0.56
1:D:248:TYR:N	1:D:248:TYR:CD1	2.73	0.56
1:F:173:ILE:HD13	1:F:190:ARG:HB3	1.87	0.55
1:G:36:ASP:OD2	1:G:105:ARG:NH2	2.34	0.55
1:G:150:GLU:HG3	1:G:150:GLU:O	2.07	0.55
1:B:181:VAL:HG23	1:B:183:PRO:HD2	1.87	0.55
1:J:289:ASN:OD1	1:J:291:VAL:N	2.40	0.55
1:A:148:TYR:OH	1:B:177:HIS:CE1	2.59	0.55
1:A:181:VAL:CG1	1:A:185:GLN:HG3	2.34	0.55
1:A:216:ILE:O	1:A:219:SER:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:VAL:HG22	1:I:183:PRO:HD2	1.88	0.55
1:J:208:PHE:CE1	1:J:245:TYR:HE2	2.25	0.55
1:E:224:TRP:HA	1:E:301:ARG:NH1	2.21	0.55
1:G:91:ARG:HB3	1:G:103:ASN:HB3	1.89	0.55
1:B:71:LEU:HD22	1:B:73:VAL:HG22	1.89	0.55
1:B:212:LEU:HD12	1:B:265:MET:HB3	1.88	0.55
1:B:298:GLN:HG3	1:B:299:ARG:HB2	1.88	0.55
1:J:279:LEU:HD11	1:J:304:PHE:CZ	2.42	0.55
1:A:19:PHE:CE1	1:B:178:LEU:HD11	2.42	0.55
1:B:44:THR:HA	1:B:99:ARG:HA	1.88	0.55
1:E:26:VAL:HG22	1:E:33:TYR:HB3	1.88	0.55
1:H:125:GLN:OE1	1:H:194:ARG:HD3	2.07	0.55
1:H:212:LEU:O	1:H:216:ILE:HG12	2.07	0.55
1:I:231:ARG:HH12	1:I:232:LEU:HD22	1.69	0.55
1:A:28:THR:HB	1:A:256:LEU:HD21	1.88	0.55
1:B:163:ARG:HG2	1:B:163:ARG:NH1	2.15	0.55
1:H:181:VAL:HG21	1:H:185:GLN:HB2	1.88	0.55
1:E:247:SER:HA	1:E:250:SER:HB2	1.88	0.55
1:J:279:LEU:HD11	1:J:304:PHE:CE2	2.41	0.55
1:B:218:ALA:O	1:B:221:SER:OG	2.23	0.54
1:D:286:ARG:NH1	1:D:298:GLN:HE21	2.04	0.54
1:H:255:ARG:HG3	1:H:255:ARG:NH1	2.13	0.54
1:I:286:ARG:HD3	1:I:287:GLN:H	1.72	0.54
1:D:174:ARG:NH1	1:D:187:GLU:OE2	2.40	0.54
1:E:212:LEU:O	1:E:216:ILE:HG12	2.06	0.54
1:H:287:GLN:CD	1:H:290:GLY:H	2.15	0.54
1:J:28:THR:HB	1:J:256:LEU:HD21	1.88	0.54
1:D:174:ARG:CZ	1:D:187:GLU:HG2	2.36	0.54
1:E:263:ASP:O	1:E:267:ILE:HG12	2.08	0.54
1:G:136:ASN:HD21	1:G:185:GLN:HG3	1.72	0.54
1:H:180:SER:O	1:H:180:SER:OG	2.21	0.54
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.88	0.54
1:D:229:SER:O	1:D:233:GLN:HB2	2.07	0.54
1:J:231:ARG:NH2	1:J:298:GLN:HE22	2.05	0.54
1:B:81:VAL:HG21	1:B:85:PRO:HG3	1.89	0.54
1:D:289:ASN:CG	1:D:292:GLU:HG2	2.32	0.54
1:E:247:SER:OG	1:E:248:TYR:N	2.39	0.54
1:G:289:ASN:HD21	1:G:292:GLU:HB3	1.71	0.54
1:J:81:VAL:HG21	1:J:85:PRO:HG3	1.89	0.54
1:J:179:SER:OG	1:J:181:VAL:N	2.39	0.54
1:D:183:PRO:HB2	1:D:185:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:HA	1:D:286:ARG:NE	2.22	0.54
1:F:178:LEU:HD11	1:F:181:VAL:O	2.08	0.54
1:C:122:ASP:CG	1:C:199:ARG:HE	2.15	0.54
1:I:122:ASP:N	1:I:122:ASP:OD1	2.41	0.54
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.42	0.54
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.88	0.54
1:I:53:ASP:O	1:I:96:PRO:HG3	2.08	0.54
1:I:295:LEU:HD22	1:I:298:GLN:HB2	1.90	0.54
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.89	0.54
1:A:302:LEU:C	1:A:305:PRO:HD2	2.34	0.53
1:E:178:LEU:HD21	1:E:185:GLN:O	2.08	0.53
1:G:295:LEU:HA	1:G:298:GLN:HB2	1.91	0.53
1:G:305:PRO:O	1:G:309:LEU:HG	2.08	0.53
1:A:150:GLU:O	1:A:150:GLU:HG3	2.08	0.53
1:D:123:ARG:HG2	1:D:197:ALA:O	2.08	0.53
1:D:286:ARG:NH1	1:D:293:ASP:HA	2.24	0.53
1:H:174:ARG:HA	1:H:186:ASN:O	2.08	0.53
1:J:176:ASP:C	1:J:177:HIS:HD2	2.16	0.53
1:B:156:GLU:HG3	1:C:117:ARG:HH22	1.71	0.53
1:D:224:TRP:HD1	1:E:285:HIS:CD2	2.27	0.53
1:F:78:PHE:HB3	1:F:81:VAL:HB	1.89	0.53
1:F:228:PHE:HA	1:F:231:ARG:NH1	2.22	0.53
1:B:298:GLN:CG	1:B:299:ARG:N	2.69	0.53
1:D:176:ASP:HB2	1:D:177:HIS:CD2	2.44	0.53
1:D:181:VAL:HG21	1:D:185:GLN:O	2.09	0.53
1:F:91:ARG:HH12	1:F:103:ASN:CG	2.16	0.53
1:F:299:ARG:C	1:F:301:ARG:H	2.16	0.53
1:G:294:ASP:C	1:G:296:LEU:N	2.58	0.53
1:I:228:PHE:CZ	1:I:231:ARG:NE	2.76	0.53
1:B:58:VAL:HG13	1:B:62:GLN:HB2	1.90	0.53
1:D:48:ARG:HH11	1:D:48:ARG:CG	2.17	0.53
1:I:228:PHE:CE1	1:I:231:ARG:NE	2.77	0.53
1:C:90:LYS:NZ	1:C:92:LEU:N	2.56	0.53
1:C:301:ARG:HG2	1:C:301:ARG:HH11	1.74	0.53
1:D:135:TYR:HD2	1:D:139:GLN:OE1	1.92	0.53
1:E:66:TRP:CE3	1:E:71:LEU:HD12	2.44	0.53
1:E:178:LEU:HB3	1:E:179:SER:O	2.08	0.53
1:G:241:THR:HA	1:H:240:LEU:HD23	1.89	0.53
1:J:224:TRP:CE2	1:J:301:ARG:HG2	2.44	0.53
1:A:293:ASP:HB2	1:A:295:LEU:HD12	1.91	0.53
1:D:27:ASN:HB3	1:D:32:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:PRO:HG3	1:I:97:ASP:O	2.09	0.53
1:I:228:PHE:CE2	1:I:284:HIS:CD2	2.97	0.53
1:C:90:LYS:HZ3	1:C:91:ARG:C	2.16	0.53
1:J:174:ARG:HA	1:J:186:ASN:O	2.08	0.53
1:A:219:SER:HA	1:A:238:LEU:CD2	2.37	0.52
1:C:18:ILE:HB	1:C:147:VAL:HG22	1.90	0.52
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.45	0.52
1:B:114:MET:HA	1:B:124:GLN:HE22	1.74	0.52
1:B:153:ASP:OD1	1:B:154:ASN:N	2.33	0.52
1:G:136:ASN:ND2	1:G:185:GLN:HA	2.25	0.52
1:A:71:LEU:HD22	1:A:73:VAL:HG23	1.91	0.52
1:A:208:PHE:O	1:A:245:TYR:OH	2.27	0.52
1:H:156:GLU:OE1	1:H:156:GLU:N	2.25	0.52
1:E:246:ALA:O	1:E:250:SER:N	2.40	0.52
1:G:294:ASP:O	1:G:296:LEU:N	2.43	0.52
1:A:62:GLN:NE2	1:B:67:ILE:HG22	2.25	0.52
1:A:263:ASP:O	1:A:267:ILE:HG12	2.09	0.52
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.44	0.52
1:C:301:ARG:O	1:C:305:PRO:HG2	2.10	0.52
1:E:117:ARG:O	1:E:260:THR:HA	2.09	0.52
1:A:284:HIS:HE1	1:E:226:GLU:OE2	1.93	0.52
1:B:301:ARG:NH1	1:B:302:LEU:HD12	2.24	0.52
1:D:144:ASP:OD2	1:D:146:GLN:NE2	2.43	0.52
1:J:153:ASP:OD1	1:J:154:ASN:N	2.33	0.52
1:A:91:ARG:NH1	1:B:134:SER:CB	2.73	0.52
1:C:63:ILE:CG1	1:C:90:LYS:HZ1	2.23	0.52
1:C:292:GLU:HG3	1:C:292:GLU:O	2.09	0.52
1:G:149:THR:HB	1:G:151:ASN:ND2	2.24	0.52
1:B:295:LEU:O	1:B:296:LEU:HG	2.10	0.52
1:G:13:ASP:CG	1:G:141:ARG:NH1	2.68	0.52
1:H:122:ASP:HB3	1:H:124:GLN:HE21	1.75	0.52
1:H:225:LEU:HD22	1:H:230:GLU:OE2	2.10	0.52
1:D:299:ARG:C	1:D:301:ARG:H	2.16	0.52
1:E:246:ALA:O	1:E:249:THR:HB	2.09	0.52
1:D:241:THR:HA	1:E:240:LEU:HD23	1.91	0.51
1:F:289:ASN:HB2	1:F:292:GLU:HB2	1.92	0.51
1:H:287:GLN:HE22	1:H:290:GLY:C	2.18	0.51
1:D:62:GLN:HE21	1:E:67:ILE:HG22	1.75	0.51
1:E:211:PRO:O	1:E:215:ILE:HG12	2.09	0.51
1:I:95:PHE:HB2	1:I:99:ARG:HG2	1.92	0.51
1:A:185:GLN:OE1	1:A:185:GLN:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ARG:HH11	1:B:286:ARG:CG	2.09	0.51
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.92	0.51
1:F:181:VAL:HG23	1:F:183:PRO:HD2	1.93	0.51
1:J:314:VAL:O	1:J:317:ILE:HG22	2.10	0.51
1:A:289:ASN:CG	1:A:290:GLY:H	2.17	0.51
1:D:295:LEU:HD12	1:D:295:LEU:H	1.75	0.51
1:F:224:TRP:CD1	1:F:301:ARG:NH1	2.78	0.51
1:H:89:ASN:O	1:H:104:ALA:HA	2.11	0.51
1:J:212:LEU:O	1:J:216:ILE:HG12	2.11	0.51
1:B:48:ARG:O	1:B:96:PRO:HA	2.11	0.51
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.92	0.51
1:F:211:PRO:O	1:F:215:ILE:HG12	2.11	0.51
1:G:29:LEU:HD13	1:G:257:PRO:HD3	1.93	0.51
1:J:219:SER:HA	1:J:238:LEU:CD2	2.41	0.51
1:F:122:ASP:OD1	1:F:122:ASP:N	2.43	0.51
1:G:216:ILE:O	1:G:219:SER:HB3	2.11	0.51
1:J:311:ILE:O	1:J:314:VAL:HG22	2.11	0.51
1:A:149:THR:O	1:A:151:ASN:N	2.43	0.51
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.45	0.51
1:B:271:GLY:O	1:B:275:ALA:N	2.41	0.51
1:C:284:HIS:HD2	1:C:285:HIS:NE2	2.08	0.51
1:J:176:ASP:C	1:J:177:HIS:CD2	2.89	0.51
1:C:219:SER:HA	1:C:238:LEU:CD2	2.37	0.50
1:G:65:ARG:HA	1:G:68:ASN:HD22	1.74	0.50
1:G:149:THR:O	1:G:151:ASN:N	2.43	0.50
1:A:38:TYR:CZ	1:A:105:ARG:HD2	2.47	0.50
1:A:91:ARG:CD	1:B:134:SER:OG	2.60	0.50
1:F:28:THR:HB	1:F:256:LEU:HD21	1.93	0.50
1:G:54:LYS:HB3	1:G:55:PRO:HD2	1.93	0.50
1:I:66:TRP:HB3	1:I:71:LEU:HD13	1.94	0.50
1:B:296:LEU:HD23	1:B:298:GLN:NE2	2.25	0.50
1:H:225:LEU:HB3	1:H:230:GLU:HG2	1.93	0.50
1:C:284:HIS:HD2	1:C:285:HIS:CD2	2.29	0.50
1:E:50:THR:HB	1:E:56:LEU:HB2	1.93	0.50
1:F:248:TYR:HD1	1:G:247:SER:HA	1.75	0.50
1:D:286:ARG:HD2	1:D:292:GLU:O	2.11	0.50
1:C:129:GLU:HA	1:C:191:ILE:O	2.11	0.50
1:C:287:GLN:HG2	1:C:289:ASN:H	1.77	0.50
1:E:115:ASP:OD1	1:E:117:ARG:HG3	2.12	0.50
1:E:301:ARG:O	1:E:305:PRO:HG2	2.11	0.50
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:GLN:OE1	1:G:148:TYR:OH	2.30	0.50
1:A:155:GLU:OE2	1:A:161:TRP:HB3	2.11	0.50
1:B:173:ILE:HG12	1:B:190:ARG:CZ	2.41	0.50
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.46	0.50
1:H:174:ARG:HG3	1:H:174:ARG:NH1	2.24	0.50
1:H:299:ARG:O	1:H:299:ARG:HD3	2.11	0.50
1:A:229:SER:HA	1:E:230:GLU:OE2	2.12	0.50
1:C:264:GLN:HA	1:C:267:ILE:HG12	1.92	0.50
1:H:138:GLN:HA	1:H:141:ARG:CZ	2.42	0.50
1:A:175:TYR:O	1:A:178:LEU:HD21	2.11	0.49
1:B:153:ASP:CG	1:B:154:ASN:N	2.70	0.49
1:F:76:LEU:HB3	1:F:130:LEU:CD2	2.35	0.49
1:H:140:LEU:C	1:H:141:ARG:HD3	2.37	0.49
1:J:227:SER:HB3	1:J:230:GLU:HG3	1.94	0.49
1:C:167:SER:HB2	1:C:194:ARG:HB2	1.94	0.49
1:F:183:PRO:O	1:F:184:ASN:HB2	2.12	0.49
1:G:72:TRP:CZ2	1:G:74:PRO:HB3	2.48	0.49
1:H:122:ASP:CG	1:H:199:ARG:HE	2.20	0.49
1:A:183:PRO:O	1:A:184:ASN:ND2	2.45	0.49
1:C:216:ILE:O	1:C:219:SER:HB3	2.11	0.49
1:D:205:LEU:O	1:D:209:ILE:HB	2.12	0.49
1:F:216:ILE:O	1:F:219:SER:HB3	2.12	0.49
1:G:13:ASP:CG	1:G:141:ARG:HH11	2.17	0.49
1:G:155:GLU:HB3	1:G:161:TRP:NE1	2.26	0.49
1:I:299:ARG:C	1:I:301:ARG:N	2.69	0.49
1:B:146:GLN:N	1:B:146:GLN:OE1	2.45	0.49
1:D:307:GLY:O	1:D:311:ILE:HD12	2.12	0.49
1:E:112:ASN:OD1	1:E:113:ASP:N	2.46	0.49
1:I:264:GLN:HA	1:I:267:ILE:CG1	2.42	0.49
1:J:311:ILE:HA	1:J:314:VAL:HG13	1.95	0.49
1:A:294:ASP:O	1:A:298:GLN:HG3	2.12	0.49
1:E:128:LEU:HB2	1:E:193:VAL:HB	1.94	0.49
1:J:287:GLN:HG3	1:J:289:ASN:N	2.18	0.49
1:D:48:ARG:HG3	1:D:48:ARG:NH1	2.21	0.49
1:D:185:GLN:OE1	1:D:185:GLN:N	2.44	0.49
1:F:122:ASP:CG	1:F:199:ARG:HE	2.20	0.49
1:B:298:GLN:HG3	1:B:299:ARG:CA	2.43	0.49
1:D:290:GLY:O	1:D:291:VAL:HG13	2.12	0.49
1:E:299:ARG:C	1:E:301:ARG:N	2.69	0.49
1:G:215:ILE:HD13	1:H:239:MET:HE3	1.93	0.49
1:H:26:VAL:HG22	1:H:33:TYR:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:O	1:B:250:SER:OG	2.30	0.49
1:B:297:ILE:O	1:B:299:ARG:N	2.46	0.49
1:C:299:ARG:C	1:C:301:ARG:H	2.21	0.49
1:D:123:ARG:CZ	1:D:198:VAL:HG22	2.43	0.49
1:G:76:LEU:HB3	1:G:130:LEU:HD21	1.94	0.49
1:A:57:ILE:HG22	1:A:91:ARG:NH2	2.27	0.49
1:A:250:SER:HG	1:E:248:TYR:HE1	1.61	0.49
1:C:33:TYR:CE2	1:C:110:PHE:HB2	2.48	0.49
1:G:282:PHE:O	1:G:286:ARG:HB3	2.13	0.49
1:I:248:TYR:CE1	1:J:250:SER:HB2	2.48	0.49
1:J:151:ASN:OD1	1:J:152:ALA:N	2.46	0.49
1:J:220:TRP:CE2	1:J:301:ARG:CZ	2.96	0.49
1:B:238:LEU:HD21	1:C:236:PHE:CE2	2.48	0.48
1:F:262:ILE:O	1:F:266:ILE:HG12	2.13	0.48
1:D:145:ILE:HD12	1:D:191:ILE:HG21	1.94	0.48
1:G:165:LYS:O	1:G:165:LYS:HG3	2.12	0.48
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.43	0.48
1:J:220:TRP:CE3	1:J:221:SER:HB3	2.48	0.48
1:B:287:GLN:HB2	1:B:292:GLU:OE1	2.13	0.48
1:D:227:SER:HB3	1:D:230:GLU:HG2	1.96	0.48
1:E:13:ASP:OD2	1:E:141:ARG:HD3	2.14	0.48
1:G:17:SER:HB2	1:G:40:VAL:HB	1.94	0.48
1:D:31:GLN:HE21	1:D:114:MET:N	2.09	0.48
1:F:61:THR:HG21	1:G:64:GLU:CD	2.38	0.48
1:F:145:ILE:HG23	1:F:168:THR:HG21	1.93	0.48
1:J:173:ILE:HD13	1:J:190:ARG:HB3	1.95	0.48
1:C:212:LEU:HD12	1:C:265:MET:HB3	1.95	0.48
1:C:294:ASP:OD2	1:C:297:ILE:HD12	2.13	0.48
1:H:287:GLN:OE1	1:H:292:GLU:N	2.36	0.48
1:A:78:PHE:CE2	1:A:130:LEU:HD12	2.48	0.48
1:B:132:PRO:HD3	1:B:142:PHE:CE2	2.48	0.48
1:C:224:TRP:HA	1:C:301:ARG:HH12	1.76	0.48
1:F:204:TYR:O	1:F:209:ILE:HG12	2.13	0.48
1:F:241:THR:HA	1:G:240:LEU:HD23	1.95	0.48
1:H:23:ILE:HG21	1:H:126:PHE:CD1	2.48	0.48
1:H:204:TYR:O	1:H:208:PHE:HB2	2.13	0.48
1:G:48:ARG:NH1	1:G:48:ARG:HB2	2.28	0.48
1:J:283:ALA:HB1	1:J:298:GLN:HE21	1.78	0.48
1:C:204:TYR:O	1:C:209:ILE:HG12	2.14	0.48
1:E:29:LEU:HD12	1:E:29:LEU:HA	1.57	0.48
1:E:223:PHE:O	1:E:301:ARG:NH1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.49	0.48
1:H:119:PHE:HA	1:H:122:ASP:OD1	2.13	0.48
1:A:19:PHE:O	1:A:37:GLY:HA3	2.14	0.48
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.96	0.48
1:F:174:ARG:HB2	1:F:187:GLU:HG2	1.96	0.48
1:J:305:PRO:O	1:J:307:GLY:N	2.47	0.48
1:A:115:ASP:OD2	1:E:157:ILE:HD11	2.14	0.48
1:B:224:TRP:CZ2	1:B:301:ARG:CZ	2.97	0.48
1:B:248:TYR:HD1	1:C:247:SER:HA	1.78	0.48
1:F:65:ARG:HD2	1:G:68:ASN:OD1	2.14	0.48
1:H:137:ASN:HB3	1:H:187:GLU:O	2.13	0.48
1:H:248:TYR:HD1	1:I:247:SER:HA	1.78	0.48
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.49	0.47
1:G:218:ALA:HB2	1:H:274:PHE:CD1	2.50	0.47
1:H:11:PRO:HB3	1:H:141:ARG:CZ	2.44	0.47
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.97	0.47
1:J:95:PHE:HB2	1:J:99:ARG:HG2	1.96	0.47
1:J:289:ASN:ND2	1:J:292:GLU:CD	2.73	0.47
1:A:289:ASN:CG	1:A:290:GLY:N	2.72	0.47
1:B:91:ARG:HB2	1:C:133:PHE:HE2	1.80	0.47
1:B:235:SER:HA	1:B:238:LEU:HD12	1.95	0.47
1:A:185:GLN:N	1:A:185:GLN:CD	2.73	0.47
1:C:60:ASN:O	1:C:63:ILE:HD12	2.14	0.47
1:D:175:TYR:O	1:D:178:LEU:HD21	2.15	0.47
1:E:295:LEU:HA	1:E:298:GLN:CG	2.39	0.47
1:J:227:SER:O	1:J:231:ARG:NH1	2.48	0.47
1:J:247:SER:HA	1:J:250:SER:HB3	1.97	0.47
1:J:289:ASN:CG	1:J:290:GLY:N	2.73	0.47
1:B:165:LYS:O	1:B:165:LYS:HG3	2.14	0.47
1:G:181:VAL:HG12	1:G:183:PRO:CD	2.44	0.47
1:H:287:GLN:HE22	1:H:291:VAL:N	2.11	0.47
1:A:73:VAL:HG21	1:A:92:LEU:HD11	1.94	0.47
1:C:90:LYS:NZ	1:C:91:ARG:C	2.72	0.47
1:D:62:GLN:OE1	1:D:62:GLN:HA	2.15	0.47
1:E:315:LEU:HG	1:E:316:VAL:N	2.29	0.47
1:F:235:SER:HA	1:F:238:LEU:HG	1.95	0.47
1:J:224:TRP:HE1	1:J:301:ARG:CD	2.26	0.47
1:A:228:PHE:HA	1:A:231:ARG:CD	2.45	0.47
1:B:51:PRO:HD2	1:B:56:LEU:HD13	1.97	0.47
1:B:53:ASP:H	1:B:54:LYS:HD2	1.79	0.47
1:B:298:GLN:CD	1:B:299:ARG:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:SER:HB3	1:C:230:GLU:HG3	1.96	0.47
1:G:29:LEU:HB2	1:G:255:ARG:HD2	1.96	0.47
1:I:302:LEU:C	1:I:305:PRO:HD2	2.39	0.47
1:B:78:PHE:HB3	1:B:81:VAL:HB	1.97	0.47
1:C:77:GLU:O	1:C:130:LEU:HD12	2.15	0.47
1:E:27:ASN:HB3	1:E:32:THR:HB	1.96	0.47
1:G:286:ARG:HD2	1:G:287:GLN:N	2.30	0.47
1:I:47:PRO:HB3	1:I:96:PRO:O	2.15	0.47
1:J:178:LEU:HD12	1:J:178:LEU:N	2.30	0.47
1:A:302:LEU:HA	1:A:305:PRO:HG2	1.97	0.47
1:E:225:LEU:HD22	1:E:230:GLU:OE2	2.15	0.47
1:J:92:LEU:HD23	1:J:92:LEU:HA	1.78	0.47
1:A:65:ARG:HA	1:A:68:ASN:HD22	1.79	0.46
1:C:105:ARG:HD3	1:D:77:GLU:OE2	2.14	0.46
1:I:132:PRO:HG3	1:I:140:LEU:HD22	1.97	0.46
1:I:145:ILE:HD12	1:I:191:ILE:CG2	2.45	0.46
1:I:232:LEU:HA	1:I:235:SER:HG	1.76	0.46
1:A:268:ALA:HB1	1:A:308:PHE:HE1	1.79	0.46
1:A:295:LEU:HA	1:A:298:GLN:CG	2.44	0.46
1:B:224:TRP:CD1	1:C:281:ILE:HG23	2.50	0.46
1:D:286:ARG:O	1:D:287:GLN:CD	2.57	0.46
1:D:302:LEU:HD12	1:D:305:PRO:HG2	1.97	0.46
1:E:227:SER:O	1:E:231:ARG:HG2	2.15	0.46
1:F:26:VAL:HG13	1:F:114:MET:HE1	1.97	0.46
1:F:64:GLU:CD	1:J:61:THR:HG21	2.41	0.46
1:J:293:ASP:CG	1:J:298:GLN:NE2	2.73	0.46
1:C:122:ASP:HB3	1:C:124:GLN:CD	2.40	0.46
1:D:122:ASP:CG	1:D:199:ARG:HE	2.23	0.46
1:E:182:GLN:OE1	1:E:182:GLN:N	2.42	0.46
1:I:214:LEU:HD12	1:J:270:TYR:HB3	1.96	0.46
1:C:66:TRP:CE3	1:C:71:LEU:HD22	2.49	0.46
1:F:149:THR:O	1:F:151:ASN:N	2.46	0.46
1:A:64:GLU:OE2	1:A:67:ILE:HD12	2.16	0.46
1:C:294:ASP:OD2	1:C:297:ILE:HB	2.16	0.46
1:F:181:VAL:CG2	1:F:183:PRO:HD2	2.45	0.46
1:F:227:SER:HB3	1:F:230:GLU:HG3	1.98	0.46
1:F:248:TYR:HE1	1:G:250:SER:HG	1.61	0.46
1:F:281:ILE:HG23	1:J:224:TRP:CZ3	2.50	0.46
1:A:87:THR:HG21	1:A:90:LYS:HE2	1.96	0.46
1:C:63:ILE:CD1	1:C:90:LYS:HG3	2.42	0.46
1:C:157:ILE:HD11	1:D:115:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:PHE:HB2	1:F:99:ARG:HG2	1.98	0.46
1:F:182:GLN:N	1:F:182:GLN:OE1	2.49	0.46
1:F:232:LEU:HD23	1:F:236:PHE:HE1	1.80	0.46
1:G:122:ASP:N	1:G:122:ASP:OD1	2.48	0.46
1:G:233:GLN:O	1:G:236:PHE:HB2	2.16	0.46
1:I:217:ALA:HA	1:I:220:TRP:CE3	2.50	0.46
1:J:227:SER:C	1:J:231:ARG:NH1	2.74	0.46
1:J:247:SER:O	1:J:250:SER:HB3	2.16	0.46
1:J:289:ASN:HD21	1:J:292:GLU:HB2	1.80	0.46
1:B:49:LYS:HD2	1:B:49:LYS:N	2.30	0.46
1:B:136:ASN:ND2	1:B:185:GLN:HA	2.31	0.46
1:B:208:PHE:O	1:B:245:TYR:OH	2.34	0.46
1:B:248:TYR:HB2	1:C:247:SER:HB3	1.96	0.46
1:D:62:GLN:O	1:D:66:TRP:HD1	1.98	0.46
1:E:312:GLY:O	1:E:315:LEU:HD23	2.16	0.46
1:F:23:ILE:HG21	1:F:126:PHE:CD1	2.51	0.46
1:A:95:PHE:HB2	1:A:99:ARG:CB	2.43	0.46
1:B:211:PRO:O	1:B:215:ILE:HG12	2.15	0.46
1:I:231:ARG:HG2	1:I:280:ILE:HG21	1.98	0.46
1:F:233:GLN:HE21	1:J:230:GLU:HB3	1.80	0.46
1:H:225:LEU:CD2	1:I:231:ARG:NH1	2.79	0.46
1:I:84:SER:HA	1:I:85:PRO:HD3	1.67	0.46
1:B:48:ARG:HG2	1:B:48:ARG:HH11	1.80	0.46
1:B:297:ILE:C	1:B:299:ARG:H	2.24	0.46
1:C:248:TYR:O	1:C:252:ILE:HG12	2.16	0.46
1:D:97:ASP:OD2	1:D:99:ARG:NH1	2.49	0.46
1:D:295:LEU:H	1:D:295:LEU:CD1	2.29	0.46
1:E:291:VAL:O	1:E:293:ASP:N	2.49	0.46
1:G:29:LEU:CB	1:G:255:ARG:HD2	2.45	0.46
1:I:185:GLN:OE1	1:I:185:GLN:N	2.41	0.46
1:A:182:GLN:CG	1:A:183:PRO:HD3	2.45	0.45
1:D:48:ARG:CG	1:D:48:ARG:NH1	2.76	0.45
1:F:16:VAL:HG12	1:F:145:ILE:HD13	1.98	0.45
1:H:36:ASP:CG	1:H:105:ARG:HH21	2.23	0.45
1:A:50:THR:OG1	1:A:54:LYS:O	2.26	0.45
1:B:130:LEU:HD22	1:B:142:PHE:CZ	2.51	0.45
1:D:225:LEU:CD2	1:E:232:LEU:HD22	2.47	0.45
1:D:293:ASP:C	1:D:298:GLN:HE22	2.24	0.45
1:E:48:ARG:NH1	1:E:48:ARG:HB2	2.31	0.45
1:F:293:ASP:O	1:F:295:LEU:N	2.49	0.45
1:G:260:THR:HG23	1:G:263:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:ILE:HD12	1:I:191:ILE:HG23	1.97	0.45
1:J:179:SER:OG	1:J:181:VAL:HG12	2.17	0.45
1:B:136:ASN:HD22	1:B:185:GLN:HA	1.81	0.45
1:E:142:PHE:HB3	1:E:170:ILE:HD13	1.97	0.45
1:I:28:THR:HB	1:I:256:LEU:HD21	1.98	0.45
1:J:65:ARG:O	1:J:69:ASN:ND2	2.49	0.45
1:A:295:LEU:HA	1:A:298:GLN:CD	2.41	0.45
1:C:19:PHE:CE2	1:C:148:TYR:CD2	3.05	0.45
1:E:205:LEU:HD23	1:E:205:LEU:HA	1.88	0.45
1:E:262:ILE:O	1:E:266:ILE:HG12	2.17	0.45
1:F:179:SER:OG	1:F:180:SER:N	2.50	0.45
1:G:48:ARG:HB2	1:G:48:ARG:CZ	2.47	0.45
1:J:24:TYR:O	1:J:34:LYS:HG2	2.16	0.45
1:J:142:PHE:HB3	1:J:170:ILE:HD13	1.98	0.45
1:A:286:ARG:HA	1:A:286:ARG:HD2	1.50	0.45
1:C:58:VAL:O	1:C:63:ILE:HD11	2.16	0.45
1:C:178:LEU:HD23	1:C:181:VAL:O	2.16	0.45
1:E:66:TRP:HE3	1:E:71:LEU:HD12	1.81	0.45
1:E:241:THR:O	1:E:244:ALA:HB3	2.17	0.45
1:F:67:ILE:HG22	1:J:62:GLN:NE2	2.31	0.45
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.79	0.45
1:G:29:LEU:HB3	1:G:255:ARG:HH11	1.81	0.45
1:J:177:HIS:CD2	1:J:177:HIS:N	2.84	0.45
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.82	0.45
1:B:291:VAL:O	1:B:291:VAL:HG22	2.16	0.45
1:C:174:ARG:HA	1:C:186:ASN:O	2.17	0.45
1:C:212:LEU:HD23	1:C:245:TYR:CD2	2.52	0.45
1:D:287:GLN:NE2	1:D:292:GLU:H	2.15	0.45
1:F:220:TRP:CD1	1:F:304:PHE:HE2	2.34	0.45
1:H:149:THR:C	1:H:151:ASN:H	2.25	0.45
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.76	0.45
1:C:263:ASP:O	1:C:267:ILE:HG12	2.17	0.45
1:D:302:LEU:HD12	1:D:302:LEU:HA	1.60	0.45
1:G:132:PRO:HD3	1:G:142:PHE:CE2	2.51	0.45
1:H:224:TRP:CD1	1:H:301:ARG:NH1	2.84	0.45
1:J:24:TYR:OH	1:J:34:LYS:HE2	2.17	0.45
1:J:146:GLN:N	1:J:146:GLN:OE1	2.50	0.45
1:J:175:TYR:HB2	1:J:178:LEU:CD1	2.39	0.45
1:J:289:ASN:HD22	1:J:292:GLU:CD	2.25	0.45
1:D:31:GLN:HG3	1:D:114:MET:HB2	1.98	0.45
1:F:110:PHE:CE2	1:F:128:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:ASP:OD1	1:H:117:ARG:HG3	2.17	0.45
1:H:132:PRO:CG	1:H:140:LEU:HD22	2.47	0.45
1:H:209:ILE:HG23	1:H:265:MET:HE1	1.99	0.45
1:A:284:HIS:CE1	1:E:226:GLU:OE2	2.69	0.45
1:B:84:SER:HA	1:B:85:PRO:HD3	1.75	0.45
1:B:86:ASP:HB3	1:B:107:LEU:HB3	1.97	0.45
1:C:81:VAL:HG21	1:C:85:PRO:HG3	1.98	0.45
1:D:23:ILE:HG21	1:D:126:PHE:CD1	2.52	0.45
1:D:123:ARG:NH2	1:D:163:ARG:HD3	2.32	0.45
1:E:253:LEU:HB3	1:E:254:PRO:HD2	1.99	0.45
1:G:136:ASN:ND2	1:G:185:GLN:HG3	2.30	0.45
1:H:157:ILE:HD11	1:I:115:ASP:OD2	2.17	0.45
1:I:248:TYR:CD1	1:J:247:SER:HA	2.52	0.45
1:I:287:GLN:HE22	1:I:290:GLY:CA	2.30	0.45
1:J:291:VAL:O	1:J:291:VAL:HG12	2.17	0.45
1:B:263:ASP:O	1:B:267:ILE:HG12	2.17	0.45
1:C:317:ILE:HD12	1:C:317:ILE:HA	1.78	0.45
1:D:289:ASN:ND2	1:D:291:VAL:H	2.13	0.45
1:E:81:VAL:HA	1:E:110:PHE:HA	1.97	0.45
1:H:122:ASP:OD1	1:H:122:ASP:N	2.49	0.45
1:J:176:ASP:CB	1:J:177:HIS:CD2	3.00	0.45
1:A:16:VAL:HA	1:A:40:VAL:O	2.17	0.44
1:E:216:ILE:O	1:E:219:SER:HB3	2.18	0.44
1:E:223:PHE:CE1	1:E:304:PHE:HD2	2.35	0.44
1:A:78:PHE:O	1:A:81:VAL:HG12	2.18	0.44
1:B:173:ILE:HD13	1:B:190:ARG:CB	2.45	0.44
1:B:178:LEU:HA	1:B:178:LEU:HD23	1.62	0.44
1:B:204:TYR:O	1:B:209:ILE:HG12	2.17	0.44
1:C:63:ILE:CD1	1:C:90:LYS:HZ1	2.29	0.44
1:C:277:ILE:HG22	1:C:281:ILE:HD12	2.00	0.44
1:D:264:GLN:HA	1:D:267:ILE:HG12	1.99	0.44
1:G:136:ASN:HD22	1:G:185:GLN:HA	1.82	0.44
1:I:78:PHE:O	1:I:81:VAL:HG12	2.16	0.44
1:I:295:LEU:HA	1:I:295:LEU:HD23	1.56	0.44
1:J:21:ASN:ND2	1:J:37:GLY:HA2	2.33	0.44
1:J:24:TYR:CZ	1:J:34:LYS:HE2	2.52	0.44
1:A:91:ARG:HD3	1:B:134:SER:OG	2.18	0.44
1:B:209:ILE:HG23	1:B:265:MET:HE1	1.98	0.44
1:B:216:ILE:HD12	1:B:269:GLY:HA2	1.99	0.44
1:B:251:ASN:HD21	1:C:251:ASN:CG	2.24	0.44
1:D:299:ARG:O	1:D:299:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ARG:CZ	1:E:198:VAL:HG22	2.47	0.44
1:E:132:PRO:HG2	1:E:140:LEU:HD22	2.00	0.44
1:I:115:ASP:O	1:I:124:GLN:NE2	2.45	0.44
1:I:224:TRP:CZ2	1:I:301:ARG:HB3	2.52	0.44
1:I:288:ALA:HB3	1:I:292:GLU:CD	2.42	0.44
1:A:21:ASN:ND2	1:A:37:GLY:HA2	2.32	0.44
1:A:248:TYR:HD1	1:B:250:SER:HG	1.58	0.44
1:E:224:TRP:HA	1:E:301:ARG:CZ	2.47	0.44
1:C:304:PHE:HB3	1:C:305:PRO:HD3	1.99	0.44
1:E:295:LEU:HA	1:E:298:GLN:HE21	1.83	0.44
1:G:22:LYS:HG3	1:G:24:TYR:HD1	1.83	0.44
1:G:66:TRP:CE3	1:G:71:LEU:HD12	2.53	0.44
1:G:157:ILE:HD11	1:H:115:ASP:OD2	2.17	0.44
1:H:157:ILE:HA	1:H:157:ILE:HD13	1.66	0.44
1:I:205:LEU:HD23	1:I:205:LEU:HA	1.86	0.44
1:J:288:ALA:N	1:J:289:ASN:ND2	2.57	0.44
1:C:58:VAL:HB	1:C:92:LEU:HB2	2.00	0.44
1:C:291:VAL:O	1:C:293:ASP:N	2.50	0.44
1:D:84:SER:HA	1:D:85:PRO:HD3	1.62	0.44
1:D:294:ASP:N	1:D:298:GLN:HE22	2.15	0.44
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.86	0.44
1:E:118:LEU:HA	1:E:261:VAL:HG23	2.00	0.44
1:E:119:PHE:HZ	1:E:204:TYR:CZ	2.36	0.44
1:H:21:ASN:ND2	1:H:36:ASP:OD2	2.35	0.44
1:J:208:PHE:HE1	1:J:245:TYR:HE2	1.66	0.44
1:J:220:TRP:CE2	1:J:301:ARG:NH1	2.85	0.44
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.53	0.44
1:E:247:SER:HA	1:E:250:SER:CB	2.48	0.44
1:F:64:GLU:OE2	1:J:61:THR:HG21	2.18	0.44
1:G:307:GLY:O	1:G:311:ILE:HG13	2.18	0.44
1:H:282:PHE:CZ	1:H:286:ARG:HD2	2.52	0.44
1:I:228:PHE:O	1:I:231:ARG:CB	2.59	0.44
1:J:200:ASN:HA	1:J:201:PRO:HD3	1.84	0.44
1:J:216:ILE:HD12	1:J:269:GLY:HA2	1.99	0.44
1:A:145:ILE:HG23	1:A:168:THR:HG21	2.00	0.44
1:A:151:ASN:ND2	1:A:162:ILE:HG21	2.33	0.44
1:B:185:GLN:OE1	1:B:185:GLN:N	2.50	0.44
1:B:298:GLN:NE2	1:B:299:ARG:HB2	2.33	0.44
1:C:61:THR:HG21	1:D:64:GLU:HG3	2.00	0.44
1:C:182:GLN:H	1:C:183:PRO:CD	2.30	0.44
1:D:28:THR:HB	1:D:256:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:TRP:CD1	1:E:285:HIS:CD2	3.05	0.44
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.52	0.44
1:E:235:SER:HA	1:E:238:LEU:HD12	1.98	0.44
1:E:299:ARG:HA	1:E:301:ARG:HG3	2.00	0.44
1:F:227:SER:HB3	1:F:230:GLU:CG	2.48	0.44
1:F:291:VAL:O	1:F:293:ASP:N	2.51	0.44
1:C:279:LEU:HD13	1:C:300:CYS:SG	2.58	0.44
1:D:112:ASN:ND2	1:D:125:GLN:O	2.51	0.44
1:D:208:PHE:O	1:D:245:TYR:OH	2.35	0.44
1:F:230:GLU:O	1:F:234:THR:OG1	2.29	0.44
1:H:225:LEU:HD23	1:I:231:ARG:NH1	2.33	0.44
1:I:231:ARG:HG2	1:I:280:ILE:CG2	2.48	0.44
1:J:21:ASN:HB2	1:J:36:ASP:O	2.18	0.44
1:J:214:LEU:HA	1:J:217:ALA:HB3	2.00	0.44
1:A:59:GLU:OE2	1:B:75:ALA:HB3	2.17	0.43
1:B:48:ARG:HG2	1:B:48:ARG:NH1	2.33	0.43
1:C:122:ASP:OD2	1:C:199:ARG:NE	2.36	0.43
1:C:182:GLN:H	1:C:183:PRO:HD3	1.83	0.43
1:D:137:ASN:HB3	1:D:187:GLU:O	2.18	0.43
1:H:310:ALA:O	1:H:314:VAL:HG23	2.17	0.43
1:B:224:TRP:CG	1:C:281:ILE:HG12	2.52	0.43
1:B:287:GLN:HB2	1:B:292:GLU:HB3	2.00	0.43
1:E:162:ILE:HD13	1:E:197:ALA:HB2	2.00	0.43
1:F:29:LEU:HD12	1:F:29:LEU:HA	1.86	0.43
1:F:130:LEU:HD23	1:F:131:GLU:N	2.33	0.43
1:H:287:GLN:HE22	1:H:291:VAL:CA	2.31	0.43
1:A:268:ALA:HB1	1:A:308:PHE:CE1	2.53	0.43
1:B:181:VAL:HG21	1:B:185:GLN:CD	2.43	0.43
1:C:84:SER:HA	1:C:85:PRO:HD3	1.87	0.43
1:C:273:ILE:O	1:C:277:ILE:HG12	2.19	0.43
1:F:287:GLN:HG3	1:F:290:GLY:N	2.30	0.43
1:F:297:ILE:HA	1:F:297:ILE:HD13	1.58	0.43
1:I:221:SER:HB2	1:J:281:ILE:HD11	1.99	0.43
1:J:149:THR:C	1:J:151:ASN:N	2.76	0.43
1:C:58:VAL:O	1:C:91:ARG:HA	2.19	0.43
1:C:182:GLN:O	1:C:183:PRO:C	2.60	0.43
1:E:183:PRO:CD	1:E:184:ASN:H	2.32	0.43
1:F:287:GLN:CG	1:F:290:GLY:H	2.30	0.43
1:G:89:ASN:HB2	1:H:133:PHE:CE1	2.54	0.43
1:G:91:ARG:N	1:G:103:ASN:O	2.51	0.43
1:I:35:VAL:HB	1:I:110:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:GLN:N	1:J:185:GLN:OE1	2.52	0.43
1:E:72:TRP:CZ2	1:E:74:PRO:HB3	2.53	0.43
1:I:285:HIS:O	1:I:285:HIS:ND1	2.51	0.43
1:A:84:SER:HA	1:A:85:PRO:HD3	1.87	0.43
1:B:183:PRO:C	1:B:184:ASN:OD1	2.61	0.43
1:F:118:LEU:HA	1:F:261:VAL:HG23	2.01	0.43
1:G:235:SER:HA	1:G:238:LEU:HD13	2.00	0.43
1:H:255:ARG:HH11	1:H:255:ARG:CG	2.15	0.43
1:A:59:GLU:OE2	1:B:75:ALA:CB	2.66	0.43
1:A:81:VAL:O	1:E:105:ARG:NH2	2.51	0.43
1:C:216:ILE:HD12	1:C:269:GLY:HA2	1.99	0.43
1:D:123:ARG:CZ	1:D:163:ARG:HD3	2.49	0.43
1:D:160:TRP:HA	1:D:198:VAL:O	2.18	0.43
1:E:233:GLN:O	1:E:236:PHE:HB2	2.18	0.43
1:H:287:GLN:HG3	1:H:289:ASN:H	1.84	0.43
1:A:59:GLU:OE2	1:A:91:ARG:NH1	2.51	0.43
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.54	0.43
1:C:142:PHE:HB3	1:C:170:ILE:HD13	2.00	0.43
1:D:123:ARG:NH2	1:D:163:ARG:HG3	2.34	0.43
1:E:54:LYS:HB3	1:E:55:PRO:HD2	2.01	0.43
1:F:14:VAL:HG22	1:F:43:TRP:HB3	2.01	0.43
1:F:33:TYR:CE2	1:F:110:PHE:HB2	2.53	0.43
1:F:38:TYR:CZ	1:F:105:ARG:HD2	2.54	0.43
1:F:287:GLN:CB	1:F:292:GLU:HB3	2.41	0.43
1:J:145:ILE:O	1:J:168:THR:HG21	2.19	0.43
1:J:178:LEU:HB3	1:J:179:SER:H	1.56	0.43
1:A:145:ILE:HG22	1:A:170:ILE:HD11	2.01	0.43
1:B:301:ARG:O	1:B:305:PRO:HG2	2.19	0.43
1:D:22:LYS:HE3	1:D:24:TYR:CG	2.53	0.43
1:D:31:GLN:NE2	1:D:113:ASP:HA	2.33	0.43
1:E:289:ASN:OD1	1:E:291:VAL:N	2.50	0.43
1:E:301:ARG:NH1	1:E:301:ARG:CG	2.77	0.43
1:B:14:VAL:HG21	1:B:140:LEU:HD21	2.01	0.43
1:C:230:GLU:HB3	1:D:233:GLN:NE2	2.34	0.43
1:D:287:GLN:NE2	1:D:287:GLN:HA	2.33	0.43
1:E:157:ILE:HD13	1:E:157:ILE:HA	1.79	0.43
1:F:228:PHE:HA	1:F:231:ARG:CZ	2.48	0.43
1:G:61:THR:HG21	1:H:64:GLU:HG3	2.00	0.43
1:A:289:ASN:ND2	1:A:291:VAL:HG12	2.34	0.42
1:D:91:ARG:HD2	1:E:134:SER:HB3	2.00	0.42
1:F:58:VAL:HB	1:F:92:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ASN:OD1	1:F:104:ALA:N	2.52	0.42
1:G:84:SER:HA	1:G:85:PRO:HD3	1.69	0.42
1:G:225:LEU:HD21	1:H:232:LEU:HD22	2.02	0.42
1:H:17:SER:HB2	1:H:40:VAL:HB	2.00	0.42
1:B:268:ALA:HB1	1:B:308:PHE:HZ	1.84	0.42
1:D:296:LEU:HD13	1:D:299:ARG:HD3	2.00	0.42
1:F:136:ASN:ND2	1:F:185:GLN:HB3	2.33	0.42
1:G:89:ASN:O	1:G:104:ALA:HA	2.19	0.42
1:I:231:ARG:NH1	1:I:232:LEU:HD13	2.34	0.42
1:I:248:TYR:HD1	1:J:247:SER:HA	1.84	0.42
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.54	0.42
1:D:137:ASN:ND2	1:D:187:GLU:OE1	2.47	0.42
1:G:227:SER:HB3	1:G:230:GLU:HG3	2.02	0.42
1:H:12:VAL:HG11	1:H:72:TRP:HZ3	1.84	0.42
1:H:49:LYS:HE3	1:H:49:LYS:HA	2.01	0.42
1:H:138:GLN:HA	1:H:141:ARG:NH2	2.34	0.42
1:I:78:PHE:CD2	1:I:110:PHE:CE2	3.07	0.42
1:I:238:LEU:HA	1:I:238:LEU:HD23	1.73	0.42
1:I:260:THR:N	1:I:263:ASP:HB2	2.34	0.42
1:J:153:ASP:CG	1:J:154:ASN:N	2.77	0.42
1:B:215:ILE:HD13	1:C:239:MET:HE3	2.01	0.42
1:B:296:LEU:HA	1:B:298:GLN:CD	2.44	0.42
1:B:296:LEU:HA	1:B:298:GLN:HG2	2.00	0.42
1:B:298:GLN:HB2	1:B:299:ARG:HG3	2.00	0.42
1:C:23:ILE:HG12	1:C:35:VAL:HG22	2.00	0.42
1:D:114:MET:HE2	1:D:124:GLN:HG2	2.01	0.42
1:D:304:PHE:HB3	1:D:305:PRO:HD3	2.02	0.42
1:E:125:GLN:OE1	1:E:194:ARG:HD3	2.18	0.42
1:G:260:THR:N	1:G:263:ASP:HB2	2.32	0.42
1:I:47:PRO:HA	1:I:98:GLY:HA2	2.02	0.42
1:I:136:ASN:OD1	1:I:136:ASN:N	2.53	0.42
1:J:28:THR:HG21	1:J:254:PRO:HB2	2.00	0.42
1:A:59:GLU:CG	1:A:91:ARG:CZ	2.87	0.42
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.87	0.42
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.83	0.42
1:E:303:ALA:O	1:E:307:GLY:N	2.48	0.42
1:F:220:TRP:CD1	1:F:304:PHE:CE2	3.07	0.42
1:F:232:LEU:CD2	1:F:236:PHE:HE1	2.33	0.42
1:H:48:ARG:O	1:H:96:PRO:HA	2.20	0.42
1:J:151:ASN:O	1:J:152:ALA:HB2	2.20	0.42
1:J:279:LEU:HD22	1:J:297:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HD2	1:B:134:SER:OG	2.19	0.42
1:D:81:VAL:HG21	1:D:85:PRO:HG3	2.02	0.42
1:E:174:ARG:NH1	1:E:187:GLU:CG	2.82	0.42
1:F:228:PHE:CZ	1:F:232:LEU:HD13	2.53	0.42
1:H:120:PRO:HD2	1:H:121:PHE:CE1	2.55	0.42
1:C:19:PHE:CE2	1:C:148:TYR:HD2	2.37	0.42
1:C:90:LYS:CE	1:C:92:LEU:HG	2.50	0.42
1:C:136:ASN:OD1	1:C:138:GLN:HB2	2.20	0.42
1:F:301:ARG:O	1:F:305:PRO:HG2	2.20	0.42
1:H:78:PHE:O	1:H:81:VAL:HG12	2.20	0.42
1:H:114:MET:HB3	1:H:116:PHE:CZ	2.55	0.42
1:H:287:GLN:OE1	1:H:292:GLU:HB2	2.18	0.42
1:I:228:PHE:CE1	1:I:284:HIS:CG	3.07	0.42
1:I:289:ASN:ND2	1:I:291:VAL:HG22	2.34	0.42
1:B:301:ARG:NH1	1:B:301:ARG:O	2.53	0.42
1:D:157:ILE:N	1:D:157:ILE:HD12	2.35	0.42
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.85	0.42
1:D:306:LEU:HA	1:D:309:LEU:HB2	2.02	0.42
1:F:299:ARG:HG2	1:F:301:ARG:NE	2.34	0.42
1:I:23:ILE:HG21	1:I:126:PHE:CD1	2.54	0.42
1:I:24:TYR:HE2	1:J:30:GLU:OE2	2.02	0.42
1:J:87:THR:HG21	1:J:90:LYS:HE2	2.02	0.42
1:B:196:ASP:OD2	1:I:165:LYS:CE	2.67	0.42
1:E:137:ASN:HB3	1:E:187:GLU:O	2.20	0.42
1:G:220:TRP:C	1:G:222:VAL:H	2.26	0.42
1:A:182:GLN:HG2	1:A:183:PRO:HD3	2.02	0.42
1:A:273:ILE:O	1:A:277:ILE:HG12	2.20	0.42
1:C:78:PHE:O	1:C:81:VAL:HG12	2.19	0.42
1:D:89:ASN:O	1:D:104:ALA:HA	2.20	0.42
1:E:78:PHE:O	1:E:81:VAL:HG12	2.20	0.42
1:F:66:TRP:HB3	1:F:71:LEU:HD23	2.02	0.42
1:F:76:LEU:CB	1:F:130:LEU:HD21	2.40	0.42
1:G:58:VAL:HB	1:G:92:LEU:HB2	2.02	0.42
1:G:132:PRO:CG	1:G:140:LEU:HD22	2.50	0.42
1:H:263:ASP:O	1:H:267:ILE:HG12	2.19	0.42
1:I:145:ILE:CG2	1:I:168:THR:HG21	2.49	0.42
1:I:264:GLN:HG2	1:I:264:GLN:H	1.61	0.42
1:A:167:SER:HB3	1:A:194:ARG:HB2	2.01	0.41
1:B:286:ARG:N	1:B:292:GLU:OE2	2.52	0.41
1:C:239:MET:HA	1:C:273:ILE:HD13	2.00	0.41
1:D:119:PHE:CG	1:D:120:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:PRO:HD3	1:D:142:PHE:CE2	2.55	0.41
1:D:179:SER:HB3	1:D:180:SER:H	1.66	0.41
1:D:302:LEU:C	1:D:305:PRO:HD2	2.44	0.41
1:F:78:PHE:O	1:F:81:VAL:HG12	2.20	0.41
1:F:91:ARG:NH1	1:F:103:ASN:CB	2.82	0.41
1:F:214:LEU:HD12	1:G:270:TYR:HB3	2.00	0.41
1:J:260:THR:H	1:J:263:ASP:HB2	1.85	0.41
1:B:314:VAL:O	1:B:317:ILE:HB	2.20	0.41
1:G:155:GLU:HB3	1:G:161:TRP:CD1	2.55	0.41
1:G:221:SER:HB2	1:H:281:ILE:CD1	2.48	0.41
1:A:300:CYS:SG	1:A:304:PHE:HE2	2.43	0.41
1:B:183:PRO:HB2	1:B:184:ASN:H	1.62	0.41
1:B:262:ILE:O	1:B:266:ILE:HG12	2.21	0.41
1:F:237:THR:O	1:F:240:LEU:HB3	2.21	0.41
1:G:216:ILE:HD12	1:G:269:GLY:HA2	2.01	0.41
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.76	0.41
1:H:185:GLN:OE1	1:H:185:GLN:N	2.51	0.41
1:H:293:ASP:CG	1:H:298:GLN:HB3	2.46	0.41
1:J:72:TRP:CZ2	1:J:74:PRO:HB3	2.54	0.41
1:A:64:GLU:O	1:A:68:ASN:ND2	2.53	0.41
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.85	0.41
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.83	0.41
1:D:55:PRO:HB3	1:D:95:PHE:CD2	2.55	0.41
1:D:91:ARG:N	1:D:103:ASN:O	2.53	0.41
1:F:132:PRO:HD3	1:F:142:PHE:CE2	2.55	0.41
1:F:299:ARG:HA	1:F:301:ARG:HG3	2.02	0.41
1:G:138:GLN:H	1:G:138:GLN:HG2	1.67	0.41
1:G:224:TRP:CH2	1:G:301:ARG:HB3	2.55	0.41
1:G:310:ALA:O	1:G:314:VAL:HG23	2.19	0.41
1:H:92:LEU:HD23	1:H:92:LEU:HA	1.87	0.41
1:I:304:PHE:HA	1:I:307:GLY:HA3	2.03	0.41
1:J:38:TYR:CZ	1:J:105:ARG:HD2	2.55	0.41
1:J:177:HIS:C	1:J:178:LEU:HD12	2.45	0.41
1:A:28:THR:HB	1:A:256:LEU:CD2	2.50	0.41
1:A:257:PRO:HB3	1:E:159:GLU:CB	2.50	0.41
1:B:91:ARG:HB2	1:C:133:PHE:CE2	2.55	0.41
1:B:303:ALA:O	1:B:307:GLY:N	2.52	0.41
1:F:247:SER:HB3	1:J:248:TYR:HB2	2.03	0.41
1:G:299:ARG:C	1:G:301:ARG:N	2.74	0.41
1:H:174:ARG:NH1	1:H:174:ARG:CG	2.83	0.41
1:H:311:ILE:O	1:H:315:LEU:HD13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:TRP:CE2	1:I:301:ARG:HD3	2.55	0.41
1:A:227:SER:C	1:A:231:ARG:HD2	2.45	0.41
1:D:165:LYS:O	1:D:166:ALA:HB3	2.20	0.41
1:G:43:TRP:CH2	1:G:74:PRO:HD2	2.56	0.41
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.21	0.41
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.68	0.41
1:C:204:TYR:O	1:C:208:PHE:HB2	2.21	0.41
1:C:260:THR:HG23	1:C:263:ASP:OD2	2.20	0.41
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.56	0.41
1:F:72:TRP:CH2	1:F:74:PRO:HG3	2.56	0.41
1:G:62:GLN:O	1:G:66:TRP:HD1	2.03	0.41
1:H:238:LEU:HD21	1:I:236:PHE:CE2	2.56	0.41
1:H:273:ILE:O	1:H:277:ILE:HG12	2.21	0.41
1:I:138:GLN:HG3	1:I:187:GLU:OE1	2.21	0.41
1:I:231:ARG:HH11	1:I:231:ARG:HD3	1.62	0.41
1:J:18:ILE:HD13	1:J:39:ILE:HG22	2.03	0.41
1:J:307:GLY:O	1:J:308:PHE:C	2.63	0.41
1:C:90:LYS:HE2	1:C:102:TYR:CD1	2.56	0.41
1:D:92:LEU:HA	1:D:92:LEU:HD23	1.85	0.41
1:E:137:ASN:OD1	1:E:137:ASN:N	2.53	0.41
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.88	0.41
1:I:173:ILE:HD13	1:I:190:ARG:HB3	2.02	0.41
1:J:304:PHE:N	1:J:304:PHE:HD1	2.19	0.41
1:B:63:ILE:HD12	1:B:90:LYS:HB2	2.03	0.41
1:B:206:TRP:O	1:C:267:ILE:HD12	2.21	0.41
1:D:112:ASN:OD1	1:D:113:ASP:N	2.54	0.41
1:F:79:ILE:HD13	1:F:79:ILE:HA	1.89	0.41
1:F:81:VAL:HG21	1:F:85:PRO:HG3	2.01	0.41
1:F:84:SER:HA	1:F:85:PRO:HD3	1.84	0.41
1:F:151:ASN:O	1:F:152:ALA:HB2	2.20	0.41
1:G:71:LEU:HD22	1:G:73:VAL:CG2	2.50	0.41
1:G:117:ARG:HH11	1:G:117:ARG:HD3	1.74	0.41
1:H:54:LYS:HE2	1:H:54:LYS:HB3	1.91	0.41
1:H:58:VAL:HB	1:H:92:LEU:HB2	2.02	0.41
1:H:287:GLN:NE2	1:H:292:GLU:H	2.19	0.41
1:I:78:PHE:CD2	1:I:110:PHE:CZ	3.09	0.41
1:I:91:ARG:HB2	1:J:133:PHE:HE2	1.86	0.41
1:I:288:ALA:HB3	1:I:292:GLU:OE2	2.21	0.41
1:J:178:LEU:C	1:J:179:SER:O	2.63	0.41
1:F:156:GLU:CD	1:F:156:GLU:H	2.29	0.41
1:G:13:ASP:OD1	1:G:141:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.90	0.41
1:J:120:PRO:HD2	1:J:121:PHE:CE1	2.55	0.41
1:J:263:ASP:O	1:J:267:ILE:HG12	2.21	0.41
1:J:299:ARG:C	1:J:301:ARG:N	2.79	0.41
1:A:240:LEU:HD11	1:E:240:LEU:CD1	2.40	0.40
1:B:24:TYR:OH	1:B:34:LYS:HE2	2.20	0.40
1:C:79:ILE:HD13	1:C:79:ILE:HA	1.88	0.40
1:D:204:TYR:O	1:D:209:ILE:HG12	2.21	0.40
1:D:228:PHE:HA	1:D:231:ARG:NH1	2.36	0.40
1:F:118:LEU:HD12	1:F:122:ASP:HA	2.03	0.40
1:F:157:ILE:HD13	1:F:157:ILE:HA	1.74	0.40
1:F:205:LEU:HD23	1:F:205:LEU:HA	1.94	0.40
1:G:263:ASP:O	1:G:267:ILE:HG12	2.22	0.40
1:J:211:PRO:O	1:J:215:ILE:HG12	2.21	0.40
1:J:301:ARG:O	1:J:301:ARG:CD	2.64	0.40
1:B:287:GLN:CG	1:B:289:ASN:H	2.20	0.40
1:B:296:LEU:C	1:B:298:GLN:HG2	2.46	0.40
1:C:66:TRP:HE3	1:C:71:LEU:HD22	1.86	0.40
1:C:125:GLN:OE1	1:C:194:ARG:HD3	2.21	0.40
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.80	0.40
1:D:117:ARG:HH11	1:D:117:ARG:HD3	1.74	0.40
1:D:212:LEU:HD12	1:D:265:MET:HB3	2.04	0.40
1:F:157:ILE:HD11	1:G:115:ASP:OD2	2.22	0.40
1:H:313:CYS:O	1:H:316:VAL:HG22	2.21	0.40
1:J:79:ILE:HD13	1:J:79:ILE:HA	1.91	0.40
1:A:59:GLU:HA	1:A:91:ARG:HG2	2.03	0.40
1:A:184:ASN:N	1:A:184:ASN:ND2	2.68	0.40
1:B:175:TYR:O	1:B:186:ASN:HB2	2.22	0.40
1:C:48:ARG:HH12	1:C:94:LEU:HB3	1.86	0.40
1:G:174:ARG:HA	1:G:186:ASN:O	2.20	0.40
1:H:132:PRO:HD3	1:H:142:PHE:CE2	2.57	0.40
1:B:71:LEU:HD22	1:B:73:VAL:CG2	2.50	0.40
1:C:119:PHE:HA	1:C:122:ASP:OD1	2.22	0.40
1:D:46:LYS:HA	1:D:47:PRO:HD3	1.93	0.40
1:E:304:PHE:HB3	1:E:305:PRO:HD3	2.03	0.40
1:F:286:ARG:NH1	1:F:286:ARG:CG	2.76	0.40
1:G:78:PHE:HB3	1:G:81:VAL:HB	2.03	0.40
1:H:211:PRO:HB3	1:I:270:TYR:CD1	2.56	0.40
1:J:84:SER:HA	1:J:85:PRO:HD3	1.75	0.40
1:J:119:PHE:CD2	1:J:262:ILE:HD12	2.57	0.40
1:A:250:SER:HB3	1:E:252:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLU:O	1:B:294:ASP:N	2.54	0.40
1:C:90:LYS:HZ3	1:C:92:LEU:CA	2.35	0.40
1:C:151:ASN:O	1:C:152:ALA:HB2	2.22	0.40
1:D:123:ARG:NH2	1:D:198:VAL:CG2	2.81	0.40
1:E:87:THR:HG21	1:E:90:LYS:HE2	2.04	0.40
1:H:31:GLN:HG2	1:H:114:MET:HB2	2.04	0.40
1:I:174:ARG:HH11	1:I:174:ARG:HG3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/307 (99%)	274 (90%)	24 (8%)	7 (2%)	5	30
1	B	305/307 (99%)	272 (89%)	27 (9%)	6 (2%)	6	32
1	C	305/307 (99%)	275 (90%)	23 (8%)	7 (2%)	5	30
1	D	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	3	25
1	E	305/307 (99%)	280 (92%)	22 (7%)	3 (1%)	12	45
1	F	305/307 (99%)	277 (91%)	25 (8%)	3 (1%)	12	45
1	G	305/307 (99%)	278 (91%)	19 (6%)	8 (3%)	4	27
1	H	305/307 (99%)	277 (91%)	19 (6%)	9 (3%)	3	25
1	I	305/307 (99%)	276 (90%)	18 (6%)	11 (4%)	2	22
1	J	305/307 (99%)	271 (89%)	27 (9%)	7 (2%)	5	30
All	All	3050/3070 (99%)	2756 (90%)	224 (7%)	70 (2%)	5	30

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	A	185	GLN
1	B	166	ALA
1	B	183	PRO
1	B	298	GLN
1	C	166	ALA
1	C	182	GLN
1	D	180	SER
1	D	291	VAL
1	F	153	ASP
1	F	184	ASN
1	G	166	ALA
1	G	179	SER
1	H	287	GLN
1	I	153	ASP
1	I	179	SER
1	I	288	ALA
1	I	292	GLU
1	J	179	SER
1	J	220	TRP
1	J	308	PHE
1	B	150	GLU
1	C	122	ASP
1	C	152	ALA
1	C	153	ASP
1	C	290	GLY
1	D	183	PRO
1	E	150	GLU
1	G	184	ASN
1	G	294	ASP
1	H	150	GLU
1	A	60	ASN
1	A	153	ASP
1	B	53	ASP
1	D	286	ARG
1	D	290	GLY
1	E	53	ASP
1	G	150	GLU
1	H	180	SER
1	C	53	ASP
1	D	150	GLU
1	D	166	ALA
1	I	150	GLU

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Mol	Chain	Res	Type
1	I	184	ASN
1	I	231	ARG
1	J	150	GLU
1	J	152	ALA
1	A	304	PHE
1	B	153	ASP
1	G	53	ASP
1	G	60	ASN
1	G	180	SER
1	H	53	ASP
1	H	60	ASN
1	H	303	ALA
1	I	53	ASP
1	A	166	ALA
1	D	53	ASP
1	E	183	PRO
1	F	53	ASP
1	H	153	ASP
1	H	304	PHE
1	I	304	PHE
1	J	153	ASP
1	J	305	PRO
1	H	182	GLN
1	D	182	GLN
1	I	183	PRO
1	I	182	GLN
1	A	182	GLN

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	274/274 (100%)	264 (96%)	10 (4%)	31	56
1	B	274/274 (100%)	258 (94%)	16 (6%)	18	46
1	C	274/274 (100%)	260 (95%)	14 (5%)	21	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	274/274 (100%)	259 (94%)	15 (6%)	19	47
1	E	274/274 (100%)	260 (95%)	14 (5%)	21	49
1	F	274/274 (100%)	256 (93%)	18 (7%)	15	43
1	G	274/274 (100%)	258 (94%)	16 (6%)	18	46
1	H	274/274 (100%)	260 (95%)	14 (5%)	21	49
1	I	274/274 (100%)	260 (95%)	14 (5%)	21	49
1	J	274/274 (100%)	257 (94%)	17 (6%)	16	44
All	All	2740/2740 (100%)	2592 (95%)	148 (5%)	20	47

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	49	LYS
1	A	150	GLU
1	A	157	ILE
1	A	165	LYS
1	A	181	VAL
1	A	184	ASN
1	A	210	LEU
1	A	212	LEU
1	A	302	LEU
1	B	32	THR
1	B	62	GLN
1	B	79	ILE
1	B	134	SER
1	B	157	ILE
1	B	165	LYS
1	B	181	VAL
1	B	184	ASN
1	B	212	LEU
1	B	240	LEU
1	B	250	SER
1	B	279	LEU
1	B	287	GLN
1	B	292	GLU
1	B	295	LEU
1	B	301	ARG
1	C	32	THR
1	C	46	LYS

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Mol	Chain	Res	Type
1	C	48	ARG
1	C	71	LEU
1	C	157	ILE
1	C	179	SER
1	C	182	GLN
1	C	212	LEU
1	C	240	LEU
1	C	250	SER
1	C	281	ILE
1	C	292	GLU
1	C	309	LEU
1	C	317	ILE
1	D	31	GLN
1	D	32	THR
1	D	40	VAL
1	D	71	LEU
1	D	124	GLN
1	D	169	HIS
1	D	176	ASP
1	D	181	VAL
1	D	212	LEU
1	D	230	GLU
1	D	233	GLN
1	D	240	LEU
1	D	255	ARG
1	D	286	ARG
1	D	287	GLN
1	E	32	THR
1	E	82	VAL
1	E	124	GLN
1	E	145	ILE
1	E	157	ILE
1	E	212	LEU
1	E	231	ARG
1	E	240	LEU
1	E	291	VAL
1	E	295	LEU
1	E	296	LEU
1	E	299	ARG
1	E	315	LEU
1	E	317	ILE
1	F	22	LYS

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Mol	Chain	Res	Type
1	F	39	ILE
1	F	64	GLU
1	F	118	LEU
1	F	124	GLN
1	F	157	ILE
1	F	169	HIS
1	F	174	ARG
1	F	182	GLN
1	F	210	LEU
1	F	212	LEU
1	F	240	LEU
1	F	281	ILE
1	F	286	ARG
1	F	291	VAL
1	F	297	ILE
1	F	298	GLN
1	F	317	ILE
1	G	22	LYS
1	G	32	THR
1	G	49	LYS
1	G	65	ARG
1	G	123	ARG
1	G	124	GLN
1	G	181	VAL
1	G	184	ASN
1	G	212	LEU
1	G	226	GLU
1	G	240	LEU
1	G	255	ARG
1	G	297	ILE
1	G	298	GLN
1	G	313	CYS
1	G	317	ILE
1	H	32	THR
1	H	54	LYS
1	H	122	ASP
1	H	141	ARG
1	H	150	GLU
1	H	157	ILE
1	H	174	ARG
1	H	182	GLN
1	H	212	LEU

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Mol	Chain	Res	Type
1	H	240	LEU
1	H	250	SER
1	H	255	ARG
1	H	286	ARG
1	H	296	LEU
1	I	31	GLN
1	I	145	ILE
1	I	150	GLU
1	I	155	GLU
1	I	157	ILE
1	I	212	LEU
1	I	240	LEU
1	I	255	ARG
1	I	264	GLN
1	I	284	HIS
1	I	291	VAL
1	I	295	LEU
1	I	297	ILE
1	I	299	ARG
1	J	29	LEU
1	J	32	THR
1	J	40	VAL
1	J	54	LYS
1	J	69	ASN
1	J	124	GLN
1	J	138	GLN
1	J	165	LYS
1	J	179	SER
1	J	212	LEU
1	J	250	SER
1	J	286	ARG
1	J	293	ASP
1	J	301	ARG
1	J	309	LEU
1	J	311	ILE
1	J	316	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	124	GLN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	151	ASN
1	A	184	ASN
1	A	264	GLN
1	A	285	HIS
1	B	124	GLN
1	B	169	HIS
1	B	177	HIS
1	B	251	ASN
1	B	287	GLN
1	B	298	GLN
1	C	62	GLN
1	C	251	ASN
1	C	264	GLN
1	C	284	HIS
1	D	31	GLN
1	D	62	GLN
1	D	68	ASN
1	D	285	HIS
1	D	287	GLN
1	D	298	GLN
1	E	233	GLN
1	E	285	HIS
1	E	298	GLN
1	F	124	GLN
1	F	233	GLN
1	F	284	HIS
1	G	136	ASN
1	G	151	ASN
1	H	124	GLN
1	H	151	ASN
1	H	182	GLN
1	H	233	GLN
1	H	289	ASN
1	H	298	GLN
1	I	31	GLN
1	I	89	ASN
1	I	284	HIS
1	I	287	GLN
1	J	21	ASN
1	J	69	ASN
1	J	124	GLN

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Mol	Chain	Res	Type
1	J	182	GLN
1	J	251	ASN
1	J	285	HIS
1	J	287	GLN
1	J	298	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	307/307 (100%)	0.18	14 (4%)	37	21	69, 114, 205, 266	0
1	B	307/307 (100%)	0.45	26 (8%)	16	12	67, 100, 210, 287	0
1	C	307/307 (100%)	0.23	14 (4%)	37	21	64, 99, 199, 276	0
1	D	307/307 (100%)	0.25	12 (3%)	43	24	71, 102, 210, 290	0
1	E	307/307 (100%)	0.35	17 (5%)	30	18	70, 109, 203, 258	0
1	F	307/307 (100%)	0.19	13 (4%)	40	22	70, 110, 211, 306	0
1	G	307/307 (100%)	0.46	20 (6%)	25	16	70, 101, 201, 258	0
1	H	307/307 (100%)	0.27	22 (7%)	21	14	67, 108, 206, 301	0
1	I	307/307 (100%)	0.47	24 (7%)	19	13	62, 103, 206, 335	0
1	J	307/307 (100%)	0.38	23 (7%)	20	14	75, 111, 230, 307	0
All	All	3070/3070 (100%)	0.32	185 (6%)	27	17	62, 106, 208, 335	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	245	TYR	9.7
1	I	248	TYR	8.9
1	E	291	VAL	8.4
1	E	290	GLY	7.3
1	I	251	ASN	7.0
1	B	113	ASP	6.5
1	F	176	ASP	6.4
1	H	185	GLN	6.0
1	I	208	PHE	5.9
1	G	126	PHE	5.7
1	A	175	TYR	5.6
1	B	255	ARG	5.5
1	H	174	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
1	J	39	ILE	5.4
1	F	252	ILE	5.3
1	A	176	ASP	5.1
1	A	177	HIS	5.1
1	J	250	SER	4.9
1	B	28	THR	4.8
1	I	252	ILE	4.8
1	C	313	CYS	4.8
1	A	153	ASP	4.8
1	H	173	ILE	4.8
1	I	247	SER	4.7
1	I	52	GLY	4.5
1	B	303	ALA	4.5
1	J	251	ASN	4.4
1	D	248	TYR	4.4
1	F	251	ASN	4.2
1	G	315	LEU	4.2
1	J	315	LEU	4.1
1	D	245	TYR	4.1
1	C	251	ASN	4.1
1	F	175	TYR	4.0
1	D	226	GLU	4.0
1	J	104	ALA	4.0
1	H	137	ASN	4.0
1	B	102	TYR	3.9
1	A	252	ILE	3.9
1	D	179	SER	3.9
1	I	182	GLN	3.9
1	H	186	ASN	3.8
1	G	181	VAL	3.8
1	C	314	VAL	3.8
1	G	308	PHE	3.7
1	B	31	GLN	3.7
1	H	184	ASN	3.7
1	H	181	VAL	3.7
1	H	188	PHE	3.6
1	C	316	VAL	3.5
1	G	255	ARG	3.5
1	I	249	THR	3.5
1	G	41	ALA	3.5
1	I	315	LEU	3.4
1	E	250	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	314	VAL	3.4
1	B	112	ASN	3.4
1	G	250	SER	3.3
1	F	11	PRO	3.3
1	C	172	ASP	3.3
1	A	64	GLU	3.3
1	B	114	MET	3.2
1	C	308	PHE	3.2
1	J	11	PRO	3.2
1	A	102	TYR	3.2
1	I	242	VAL	3.1
1	B	29	LEU	3.1
1	H	136	ASN	3.0
1	B	116	PHE	3.0
1	I	212	LEU	3.0
1	G	195	ILE	2.9
1	B	288	ALA	2.9
1	G	293	ASP	2.9
1	J	154	ASN	2.9
1	F	316	VAL	2.9
1	H	138	GLN	2.9
1	E	248	TYR	2.9
1	B	194	ARG	2.9
1	C	32	THR	2.9
1	B	297	ILE	2.8
1	I	296	LEU	2.8
1	F	177	HIS	2.8
1	A	157	ILE	2.8
1	F	250	SER	2.8
1	B	103	ASN	2.8
1	J	129	GLU	2.8
1	J	291	VAL	2.8
1	C	255	ARG	2.7
1	I	187	GLU	2.7
1	J	246	ALA	2.7
1	H	311	ILE	2.7
1	A	88	GLY	2.7
1	G	253	LEU	2.7
1	H	175	TYR	2.7
1	G	39	ILE	2.7
1	J	308	PHE	2.7
1	I	253	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	246	ALA	2.7
1	E	289	ASN	2.7
1	A	158	ASP	2.7
1	B	183	PRO	2.7
1	G	304	PHE	2.6
1	E	180	SER	2.6
1	G	229	SER	2.6
1	G	230	GLU	2.6
1	J	78	PHE	2.6
1	B	104	ALA	2.6
1	E	179	SER	2.6
1	F	305	PRO	2.6
1	E	133	PHE	2.6
1	B	118	LEU	2.6
1	H	179	SER	2.5
1	I	276	ALA	2.5
1	A	91	ARG	2.5
1	J	229	SER	2.5
1	C	64	GLU	2.5
1	J	230	GLU	2.5
1	D	208	PHE	2.5
1	A	254	PRO	2.5
1	G	269	GLY	2.5
1	I	250	SER	2.5
1	A	154	ASN	2.4
1	H	140	LEU	2.4
1	A	118	LEU	2.4
1	E	296	LEU	2.4
1	I	152	ALA	2.4
1	E	11	PRO	2.4
1	J	102	TYR	2.4
1	D	227	SER	2.4
1	B	196	ASP	2.4
1	E	166	ALA	2.4
1	I	176	ASP	2.4
1	H	180	SER	2.4
1	B	295	LEU	2.4
1	D	302	LEU	2.3
1	I	207	SER	2.3
1	G	295	LEU	2.3
1	E	64	GLU	2.3
1	B	122	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	190	ARG	2.3
1	H	182	GLN	2.3
1	C	30	GLU	2.3
1	E	143	SER	2.2
1	J	90	LYS	2.2
1	I	179	SER	2.2
1	G	128	LEU	2.2
1	J	79	ILE	2.2
1	J	301	ARG	2.2
1	D	173	ILE	2.2
1	H	187	GLU	2.2
1	C	133	PHE	2.2
1	B	293	ASP	2.2
1	F	153	ASP	2.2
1	E	206	TRP	2.2
1	F	229	SER	2.2
1	G	302	LEU	2.2
1	J	13	ASP	2.1
1	H	139	GLN	2.1
1	B	90	LYS	2.1
1	E	78	PHE	2.1
1	F	304	PHE	2.1
1	H	290	GLY	2.1
1	B	181	VAL	2.1
1	J	41	ALA	2.1
1	C	289	ASN	2.1
1	J	40	VAL	2.1
1	H	294	ASP	2.1
1	G	183	PRO	2.1
1	B	41	ALA	2.1
1	H	178	LEU	2.1
1	G	43	TRP	2.1
1	I	150	GLU	2.1
1	D	299	ARG	2.1
1	D	188	PHE	2.1
1	B	291	VAL	2.1
1	C	291	VAL	2.1
1	J	128	LEU	2.1
1	I	299	ARG	2.0
1	F	317	ILE	2.0
1	E	285	HIS	2.0
1	C	28	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	124	GLN	2.0
1	I	12	VAL	2.0
1	J	316	VAL	2.0
1	D	89	ASN	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.