



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:27 AM UTC

PDB ID : 2QFI / pdb_00002qfi
Title : Structure of the zinc transporter YiiP
Authors : Lu, M.
Deposited on : 2007-06-27
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

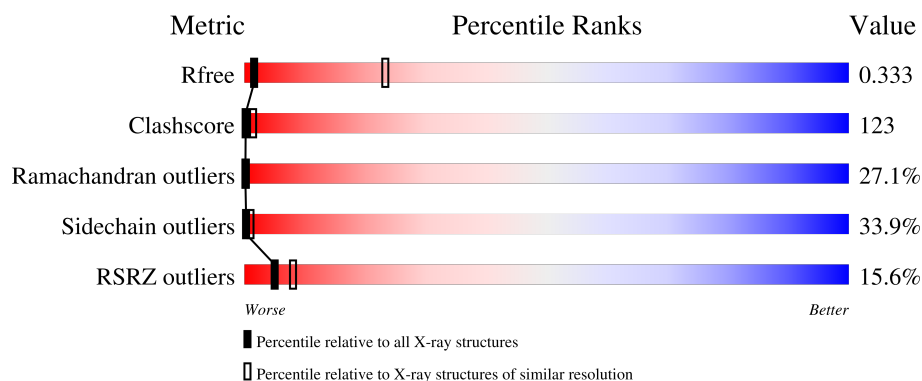
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	300	16% 10% 33% 34% 18% 5%
1	B	300	13% 14% 36% 29% 16% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4417 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 Ferrous-iron efflux pump fieF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2205	1419	378	397	11			
1	B	286	Total	C	N	O	S	0	0	0
			2205	1419	378	397	11			

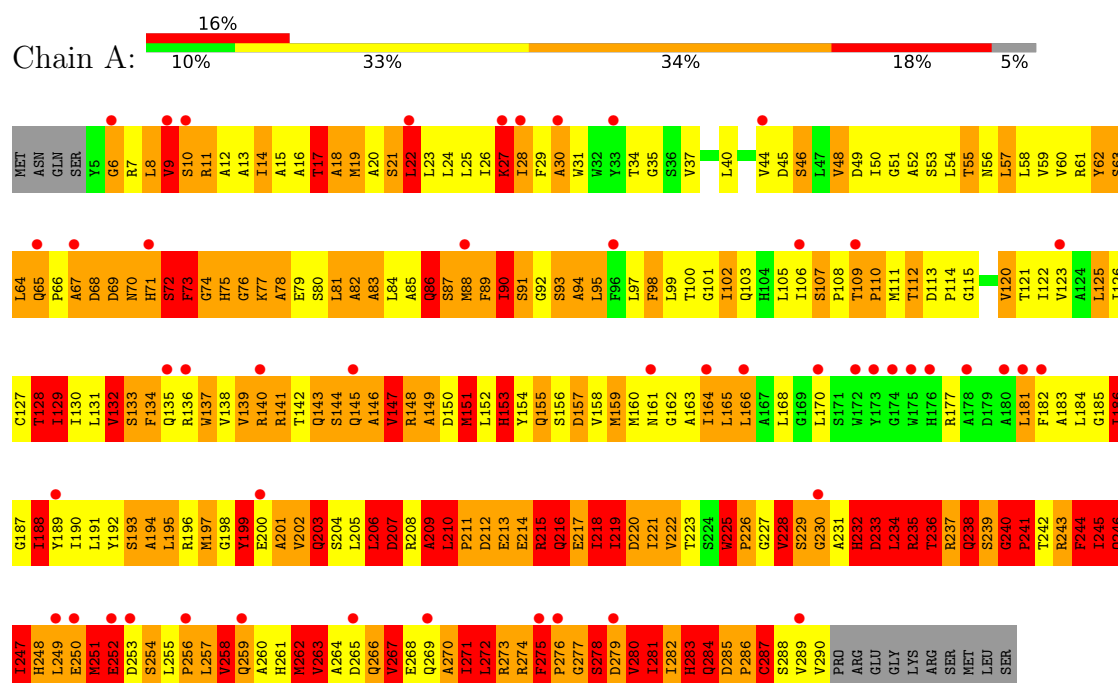
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	B	3	Total	Zn	0	0
			3	3		

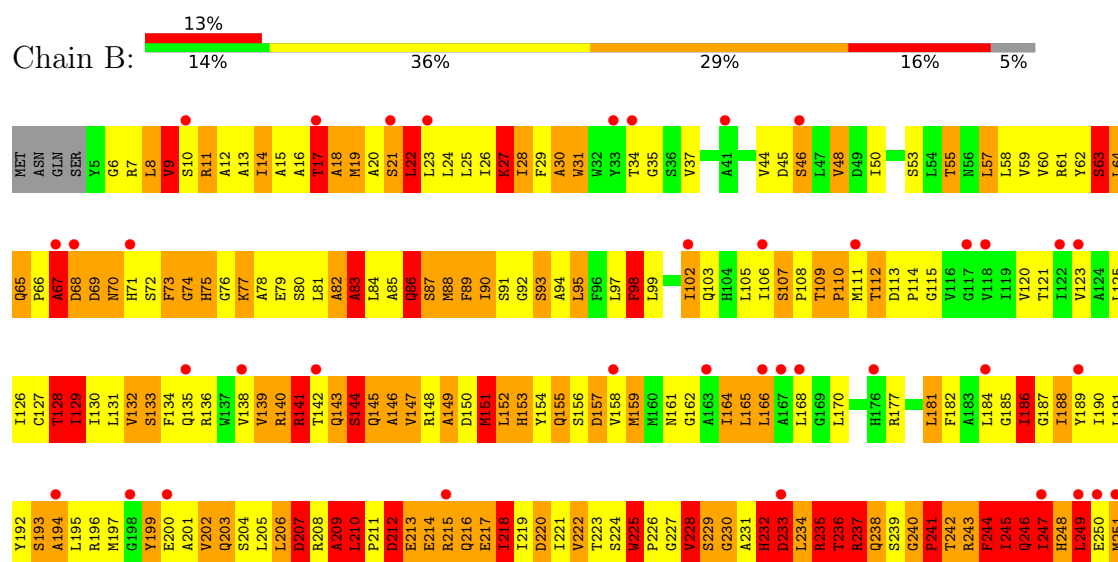
3 Residue-property plots

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: Ferrous-iron efflux pump fieF



• Molecule 1: Ferrous-iron efflux pump fieF



E252	D253	S254	L255	P256	L257	V258	Q259	A260	H261	N262	V263	A264	D265	Q266	V267	E268	Q269	A270	L271	L272	R273	R274	F275	P276	G277	S278	D279	V280	I281	I282	H283	Q284	D285	P286	C287	S288	V289	V290	PRO	ARG	GLU	GLY	LYS	ARG	SER	MET	LEU	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.66Å 110.84Å 130.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.80 12.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-3.80) 94.1 (12.00-3.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.322 , 0.329 0.348 , 0.333	Depositor DCC
R_{free} test set	772 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	118.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , 90.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.086 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4417	wwPDB-VP
Average B, all atoms (Å ²)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.77	47/2252 (2.1%)	1.87	78/3069 (2.5%)
1	B	1.42	26/2252 (1.2%)	1.65	54/3069 (1.8%)
All	All	1.61	73/4504 (1.6%)	1.76	132/6138 (2.2%)

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	24
1	B	0	23
All	All	0	47

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	ILE	CA-CB	14.70	1.74	1.54
1	A	247	ILE	CA-CB	13.21	1.72	1.54
1	B	247	ILE	CA-CB	13.13	1.72	1.54
1	A	233	ASP	CA-C	12.09	1.66	1.52
1	A	238	GLN	N-CA	11.29	1.60	1.46
1	A	238	GLN	CA-C	10.66	1.66	1.52
1	A	90	ILE	CA-CB	10.52	1.68	1.54
1	A	245	ILE	CA-CB	9.75	1.64	1.54
1	B	286	PRO	N-CA	-9.03	1.35	1.47
1	A	278	SER	CA-C	8.70	1.64	1.52
1	B	238	GLN	N-CA	8.67	1.56	1.46
1	A	232	HIS	CA-CB	8.17	1.65	1.53
1	A	206	LEU	CA-C	-8.04	1.42	1.52
1	A	283	HIS	CA-C	-8.01	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	HIS	CA-C	7.99	1.58	1.52
1	A	237	ARG	N-CA	7.91	1.56	1.46
1	B	279	ASP	N-CA	7.88	1.56	1.46
1	B	258	VAL	CA-CB	-7.60	1.46	1.54
1	B	247	ILE	N-CA	7.58	1.55	1.46
1	A	279	ASP	N-CA	7.48	1.56	1.46
1	A	147	VAL	CA-CB	-7.17	1.44	1.54
1	A	219	ILE	N-CA	-7.11	1.38	1.46
1	A	209	ALA	CA-CB	7.06	1.65	1.53
1	A	247	ILE	N-CA	7.06	1.55	1.46
1	A	90	ILE	CA-C	7.06	1.61	1.52
1	B	232	HIS	CA-CB	6.89	1.63	1.53
1	A	81	LEU	CA-C	6.88	1.61	1.52
1	A	75	HIS	N-CA	6.73	1.55	1.45
1	A	279	ASP	CB-CG	6.59	1.68	1.52
1	A	199	TYR	N-CA	-6.55	1.37	1.46
1	B	284	GLN	N-CA	-6.48	1.38	1.46
1	B	278	SER	CA-C	6.43	1.61	1.52
1	A	279	ASP	CA-CB	6.37	1.62	1.53
1	A	239	SER	CA-C	6.17	1.60	1.52
1	B	67	ALA	CA-C	6.11	1.60	1.52
1	A	270	ALA	CA-C	6.06	1.60	1.52
1	B	9	VAL	CA-CB	6.04	1.64	1.54
1	B	236	THR	CA-C	5.98	1.59	1.52
1	A	197	MET	N-CA	-5.91	1.39	1.46
1	A	266	GLN	CG-CD	5.88	1.66	1.52
1	A	285	ASP	CA-C	5.74	1.59	1.52
1	A	9	VAL	CA-CB	5.73	1.63	1.54
1	A	275	PHE	CB-CG	5.71	1.63	1.50
1	A	250	GLU	N-CA	5.71	1.53	1.46
1	B	253	ASP	N-CA	5.69	1.53	1.46
1	A	235	ARG	CA-C	5.63	1.60	1.52
1	A	249	LEU	CA-CB	5.63	1.61	1.53
1	A	284	GLN	CA-C	-5.61	1.45	1.53
1	A	10	SER	CA-C	5.56	1.59	1.52
1	A	244	PHE	N-CA	5.55	1.53	1.46
1	A	241	PRO	N-CA	5.50	1.54	1.47
1	B	245	ILE	CA-C	5.49	1.59	1.52
1	A	287	CYS	N-CA	5.47	1.52	1.46
1	B	279	ASP	CB-CG	5.45	1.65	1.52
1	A	267	VAL	CA-CB	-5.41	1.47	1.54
1	B	235	ARG	CA-C	5.36	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	LEU	CA-CB	5.36	1.61	1.53
1	A	249	LEU	CB-CG	5.32	1.64	1.53
1	A	233	ASP	C-O	5.29	1.30	1.24
1	A	251	MET	N-CA	-5.26	1.39	1.46
1	A	188	ILE	CA-CB	5.24	1.61	1.54
1	A	226	PRO	CA-C	5.24	1.60	1.52
1	B	285	ASP	CA-C	5.20	1.59	1.52
1	B	279	ASP	CA-CB	5.19	1.62	1.53
1	B	289	VAL	CA-CB	5.18	1.61	1.53
1	A	238	GLN	CB-CG	5.16	1.68	1.52
1	B	287	CYS	N-CA	5.14	1.52	1.46
1	B	275	PHE	CA-CB	5.14	1.61	1.53
1	B	231	ALA	CA-CB	-5.13	1.46	1.53
1	A	125	LEU	CA-C	-5.12	1.50	1.53
1	A	229	SER	CA-C	-5.09	1.46	1.52
1	B	237	ARG	N-CA	5.05	1.52	1.46
1	A	231	ALA	CA-CB	-5.05	1.46	1.53

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	N-CA-C	15.77	133.95	107.93
1	B	233	ASP	N-CA-C	14.99	131.09	108.46
1	A	240	GLY	CA-C-N	13.85	137.16	119.84
1	A	240	GLY	C-N-CA	13.85	137.16	119.84
1	A	238	GLN	N-CA-C	13.22	129.68	110.24
1	A	141	ARG	N-CA-C	-12.74	97.19	113.12
1	B	252	GLU	N-CA-C	-12.61	99.61	112.97
1	B	240	GLY	CA-C-N	12.35	135.28	119.84
1	B	240	GLY	C-N-CA	12.35	135.28	119.84
1	A	279	ASP	N-CA-C	-11.70	95.90	110.65
1	A	22	LEU	N-CA-C	-11.31	98.70	111.82
1	A	68	ASP	N-CA-C	-10.93	96.07	111.81
1	A	287	CYS	N-CA-C	10.58	125.98	108.73
1	A	75	HIS	N-CA-C	10.47	126.50	109.96
1	A	248	HIS	N-CA-C	10.43	126.50	107.73
1	B	248	HIS	N-CA-C	10.32	123.77	109.11
1	A	247	ILE	N-CA-CB	10.32	128.26	111.23
1	B	68	ASP	N-CA-C	-10.11	96.62	110.68
1	B	247	ILE	N-CA-CB	10.04	127.79	111.23
1	B	141	ARG	N-CA-C	-9.88	101.10	113.55
1	A	281	ILE	CB-CA-C	-9.87	97.07	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	HIS	N-CA-C	-9.61	93.58	109.24
1	A	206	LEU	N-CA-C	-9.52	95.69	109.96
1	A	252	GLU	CA-C-N	9.20	137.65	122.66
1	A	252	GLU	C-N-CA	9.20	137.65	122.66
1	B	238	GLN	N-CA-C	9.03	123.65	110.28
1	A	244	PHE	N-CA-C	8.98	129.93	110.80
1	B	279	ASP	N-CA-C	-8.60	92.49	110.80
1	B	244	PHE	N-CA-C	8.59	129.10	110.80
1	B	252	GLU	CA-C-N	8.43	137.64	121.54
1	B	252	GLU	C-N-CA	8.43	137.64	121.54
1	A	91	SER	N-CA-C	-8.34	96.13	107.88
1	A	280	VAL	N-CA-C	-8.26	92.17	109.34
1	A	232	HIS	CB-CA-C	8.13	123.36	111.65
1	A	210	LEU	CA-C-N	8.08	129.94	119.84
1	A	210	LEU	C-N-CA	8.08	129.94	119.84
1	B	287	CYS	N-CA-C	8.08	121.41	108.41
1	B	289	VAL	N-CA-C	-8.02	98.11	108.93
1	A	83	ALA	N-CA-C	-7.88	94.02	110.80
1	A	197	MET	N-CA-C	-7.88	102.70	111.28
1	B	241	PRO	N-CA-C	7.87	128.68	112.47
1	A	241	PRO	N-CA-C	7.80	128.54	112.47
1	B	232	HIS	CB-CA-C	7.76	122.82	111.65
1	B	214	GLU	N-CA-C	-7.59	103.11	112.38
1	A	214	GLU	N-CA-C	-7.56	103.16	112.38
1	A	247	ILE	CA-C-N	-7.50	111.72	123.12
1	A	247	ILE	C-N-CA	-7.50	111.72	123.12
1	B	233	ASP	CA-C-N	7.42	130.54	120.44
1	B	233	ASP	C-N-CA	7.42	130.54	120.44
1	A	232	HIS	CA-C-N	-7.38	109.62	121.58
1	A	232	HIS	C-N-CA	-7.38	109.62	121.58
1	B	112	THR	N-CA-C	7.35	119.29	111.28
1	A	112	THR	N-CA-C	7.08	119.00	111.28
1	A	279	ASP	N-CA-CB	6.98	118.37	110.35
1	A	236	THR	N-CA-CB	-6.90	100.66	111.56
1	A	90	ILE	CB-CA-C	6.90	122.60	111.29
1	B	120	VAL	N-CA-C	6.87	117.13	107.37
1	A	75	HIS	CB-CA-C	-6.85	99.34	112.43
1	B	22	LEU	N-CA-C	-6.85	103.87	111.82
1	B	285	ASP	CA-C-N	6.84	128.39	119.84
1	B	285	ASP	C-N-CA	6.84	128.39	119.84
1	B	207	ASP	N-CA-C	-6.82	96.28	110.80
1	A	285	ASP	CA-C-N	6.81	128.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASP	C-N-CA	6.81	128.35	119.84
1	A	73	PHE	CB-CA-C	-6.77	99.56	110.79
1	A	221	ILE	N-CA-C	-6.71	104.32	110.82
1	B	94	ALA	N-CA-C	-6.66	105.02	113.01
1	A	157	ASP	N-CA-C	-6.61	104.96	113.16
1	A	132	VAL	N-CA-C	-6.60	105.88	111.56
1	B	254	SER	N-CA-C	-6.57	96.80	110.80
1	B	281	ILE	CA-C-N	-6.56	114.37	123.10
1	B	281	ILE	C-N-CA	-6.56	114.37	123.10
1	A	51	GLY	N-CA-C	-6.47	104.81	112.64
1	A	120	VAL	N-CA-C	6.46	116.55	107.37
1	A	281	ILE	CA-C-N	-6.44	114.71	123.14
1	A	281	ILE	C-N-CA	-6.44	114.71	123.14
1	B	28	ILE	N-CA-C	-6.43	103.28	112.35
1	A	232	HIS	CA-CB-CG	6.36	120.16	113.80
1	B	247	ILE	CA-C-N	-6.34	114.30	122.79
1	B	247	ILE	C-N-CA	-6.34	114.30	122.79
1	B	75	HIS	N-CA-C	6.32	118.80	109.69
1	A	204	SER	N-CA-C	-6.28	103.71	111.75
1	B	283	HIS	N-CA-C	-6.25	99.01	108.96
1	A	233	ASP	CA-C-O	6.25	127.61	119.98
1	B	232	HIS	CA-C-N	-6.25	108.31	121.81
1	B	232	HIS	C-N-CA	-6.25	108.31	121.81
1	B	109	THR	CA-C-N	6.23	127.62	119.84
1	B	109	THR	C-N-CA	6.23	127.62	119.84
1	A	199	TYR	CA-CB-CG	-6.22	102.71	113.90
1	A	28	ILE	N-CA-C	-6.15	103.68	112.35
1	A	153	HIS	N-CA-C	-6.13	103.75	111.11
1	A	249	LEU	N-CA-C	-6.11	106.08	112.93
1	A	207	ASP	N-CA-C	-6.08	97.84	110.80
1	B	17	THR	N-CA-C	6.06	120.50	111.96
1	A	244	PHE	CA-C-N	6.06	128.62	120.50
1	A	244	PHE	C-N-CA	6.06	128.62	120.50
1	A	109	THR	CA-C-N	6.05	127.40	119.84
1	A	109	THR	C-N-CA	6.05	127.40	119.84
1	B	263	VAL	N-CA-C	-6.04	104.96	110.82
1	A	215	ARG	N-CA-C	-6.01	97.99	110.80
1	B	248	HIS	CB-CA-C	6.00	120.91	111.72
1	A	72	SER	CA-C-N	5.96	128.26	120.28
1	A	72	SER	C-N-CA	5.96	128.26	120.28
1	B	266	GLN	N-CA-C	-5.94	104.44	111.03
1	A	263	VAL	N-CA-C	-5.94	105.06	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ALA	N-CA-C	-5.83	105.87	112.87
1	A	134	PHE	N-CA-C	-5.82	105.43	113.18
1	B	237	ARG	CA-C-N	5.78	129.08	120.87
1	B	237	ARG	C-N-CA	5.78	129.08	120.87
1	A	237	ARG	CA-C-N	5.75	129.27	121.05
1	A	237	ARG	C-N-CA	5.75	129.27	121.05
1	B	281	ILE	CB-CA-C	-5.75	102.63	111.31
1	B	267	VAL	CB-CA-C	-5.70	101.94	111.29
1	A	225	TRP	CA-CB-CG	-5.67	102.83	113.60
1	A	287	CYS	CA-C-O	5.62	126.38	120.36
1	B	157	ASP	N-CA-C	-5.60	106.43	113.20
1	A	254	SER	N-CA-C	-5.59	98.90	110.80
1	B	272	LEU	N-CA-C	-5.57	98.94	110.80
1	A	238	GLN	CB-CA-C	-5.56	101.50	109.84
1	A	248	HIS	CB-CA-C	5.54	120.31	111.73
1	B	252	GLU	O-C-N	5.48	129.40	122.06
1	A	137	TRP	N-CA-C	-5.47	104.96	111.69
1	A	277	GLY	N-CA-C	-5.43	100.32	113.18
1	B	83	ALA	N-CA-C	-5.36	99.39	110.80
1	A	17	THR	N-CA-C	5.27	119.62	111.56
1	B	253	ASP	CA-C-N	5.25	131.57	121.54
1	B	253	ASP	C-N-CA	5.25	131.57	121.54
1	A	40	LEU	N-CA-C	5.22	118.01	110.28
1	A	289	VAL	N-CA-C	-5.22	98.47	109.34
1	A	148	ARG	N-CA-C	-5.10	104.99	111.11
1	B	232	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	252	GLU	O-C-N	5.08	129.35	122.59

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Peptide
1	A	144	SER	Peptide
1	A	194	ALA	Peptide
1	A	195	LEU	Peptide
1	A	203	GLN	Peptide
1	A	209	ALA	Peptide
1	A	210	LEU	Peptide
1	A	225	TRP	Peptide
1	A	228	VAL	Peptide
1	A	234	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	240	GLY	Peptide
1	A	243	ARG	Peptide
1	A	246	GLN	Peptide
1	A	258	VAL	Peptide
1	A	27	LYS	Peptide
1	A	271	ILE	Peptide
1	A	272	LEU	Peptide
1	A	278	SER	Peptide
1	A	280	VAL	Peptide
1	A	287	CYS	Peptide
1	A	6	GLY	Peptide
1	A	63	SER	Peptide
1	A	76	GLY	Peptide
1	A	97	LEU	Peptide
1	B	140	ARG	Peptide
1	B	141	ARG	Peptide
1	B	144	SER	Peptide
1	B	194	ALA	Peptide
1	B	203	GLN	Peptide
1	B	209	ALA	Peptide
1	B	210	LEU	Peptide
1	B	225	TRP	Peptide
1	B	228	VAL	Peptide
1	B	243	ARG	Peptide
1	B	246	GLN	Peptide
1	B	252	GLU	Peptide
1	B	258	VAL	Peptide
1	B	27	LYS	Peptide
1	B	271	ILE	Peptide
1	B	272	LEU	Peptide
1	B	276	PRO	Peptide
1	B	278	SER	Peptide
1	B	280	VAL	Peptide
1	B	287	CYS	Peptide
1	B	63	SER	Peptide
1	B	67	ALA	Peptide
1	B	97	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2205	0	2239	567	4
1	B	2205	0	2239	529	0
2	A	4	0	0	0	2
2	B	3	0	0	0	0
All	All	4417	0	4478	1092	4

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 123.

All (1092) 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:B:232:HIS:CE1	1:B:245:ILE:HG21	1.36	1.61
1:B:245:ILE:CB	1:B:245:ILE:CA	1.74	1.56
1:B:232:HIS:CE1	1:B:245:ILE:CG2	1.96	1.49
1:B:232:HIS:NE2	1:B:245:ILE:CG2	1.79	1.41
1:A:67:ALA:HB1	1:A:72:SER:O	1.31	1.30
1:B:232:HIS:NE2	1:B:245:ILE:HD12	1.47	1.30
1:B:225:TRP:CZ3	1:B:266:GLN:HB3	1.70	1.27
1:A:6:GLY:O	1:A:12:ALA:HB3	1.34	1.26
1:A:225:TRP:CZ3	1:A:266:GLN:HB3	1.67	1.26
1:A:232:HIS:CE1	1:A:245:ILE:HG21	1.71	1.25
1:A:17:THR:N	1:A:148:ARG:HH22	1.34	1.23
1:B:67:ALA:HB1	1:B:72:SER:O	1.36	1.23
1:B:232:HIS:NE2	1:B:245:ILE:HG21	0.91	1.21
1:B:235:ARG:NH1	1:B:237:ARG:HD3	1.55	1.21
1:A:209:ALA:O	1:A:236:THR:HB	1.38	1.20
1:B:276:PRO:HG2	1:B:277:GLY:O	1.40	1.18
1:A:202:VAL:O	1:A:205:LEU:HG	1.41	1.18
1:A:79:GLU:CB	1:A:147:VAL:HG21	1.75	1.17
1:A:87:SER:HB3	1:A:197:MET:HB2	1.24	1.16
1:B:87:SER:CB	1:B:197:MET:HB2	1.75	1.16
1:B:22:LEU:HD23	1:B:131:LEU:HB3	1.24	1.15
1:A:79:GLU:HB2	1:A:147:VAL:CG2	1.75	1.15
1:A:252:GLU:HB3	1:A:256:PRO:HG3	1.26	1.15
1:B:67:ALA:HB3	1:B:69:ASP:HA	1.19	1.15
1:A:232:HIS:NE2	1:A:245:ILE:HD12	1.61	1.14
1:B:87:SER:HB3	1:B:197:MET:CB	1.78	1.14
1:A:235:ARG:HH12	1:A:237:ARG:CD	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLY:HA2	1:B:249:LEU:HG	1.20	1.11
1:A:244:PHE:O	1:A:282:ILE:HG23	1.49	1.11
1:B:232:HIS:CE1	1:B:245:ILE:HG22	1.86	1.11
1:A:235:ARG:NH1	1:A:237:ARG:HD3	1.66	1.10
1:A:240:GLY:CA	1:A:277:GLY:HA2	1.80	1.10
1:B:235:ARG:HH12	1:B:237:ARG:CD	1.64	1.10
1:A:206:LEU:HD22	1:A:237:ARG:HE	0.95	1.10
1:A:67:ALA:HB3	1:A:69:ASP:HA	1.25	1.09
1:B:79:GLU:HB2	1:B:147:VAL:CG2	1.82	1.08
1:A:276:PRO:HG2	1:A:277:GLY:O	1.51	1.08
1:B:79:GLU:CB	1:B:147:VAL:HG21	1.81	1.08
1:A:22:LEU:HD23	1:A:131:LEU:HB3	1.24	1.07
1:B:206:LEU:HD22	1:B:237:ARG:HE	1.05	1.07
1:A:144:SER:CB	1:A:148:ARG:HG2	1.85	1.07
1:A:199:TYR:HA	1:A:202:VAL:CG2	1.85	1.07
1:A:230:GLY:HA2	1:A:249:LEU:HG	1.26	1.06
1:B:252:GLU:HB3	1:B:256:PRO:HG3	1.32	1.06
1:A:247:ILE:HG12	1:A:248:HIS:CD2	1.89	1.05
1:A:245:ILE:HG23	1:A:283:HIS:CD2	1.91	1.05
1:B:286:PRO:HG2	1:B:287:CYS:N	1.66	1.05
1:A:286:PRO:HG2	1:A:287:CYS:H	1.22	1.04
1:A:139:VAL:HG13	1:A:140:ARG:N	1.69	1.04
1:B:109:THR:HB	1:B:110:PRO:HD2	1.36	1.04
1:B:225:TRP:HZ3	1:B:266:GLN:CB	1.69	1.04
1:A:144:SER:HB3	1:A:148:ARG:HG2	1.36	1.04
1:B:232:HIS:NE2	1:B:245:ILE:CD1	2.20	1.04
1:B:17:THR:N	1:B:148:ARG:HH22	1.53	1.03
1:A:232:HIS:CE1	1:A:245:ILE:CG2	2.42	1.03
1:B:286:PRO:HG2	1:B:287:CYS:H	0.90	1.03
1:B:202:VAL:O	1:B:205:LEU:HG	1.57	1.03
1:A:73:PHE:C	1:A:73:PHE:CD2	2.36	1.02
1:A:87:SER:CB	1:A:197:MET:HB2	1.90	1.02
1:B:209:ALA:O	1:B:236:THR:HB	1.60	1.02
1:B:252:GLU:HB3	1:B:256:PRO:CG	1.88	1.02
1:B:87:SER:HB3	1:B:197:MET:HB2	1.05	1.01
1:B:272:LEU:HD13	1:B:273:ARG:HA	1.39	1.01
1:B:252:GLU:HA	1:B:256:PRO:HD3	1.39	1.01
1:A:209:ALA:HB1	1:A:236:THR:OG1	1.61	1.01
1:A:87:SER:HB3	1:A:197:MET:CB	1.91	1.01
1:B:199:TYR:HA	1:B:202:VAL:CG2	1.90	1.01
1:B:6:GLY:O	1:B:12:ALA:HB3	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLN:O	1:B:219:ILE:HG22	1.59	1.00
1:A:64:LEU:C	1:A:65:GLN:HE21	1.68	1.00
1:A:230:GLY:HA2	1:A:249:LEU:CG	1.90	1.00
1:A:225:TRP:HZ3	1:A:266:GLN:CB	1.74	1.00
1:A:235:ARG:HH12	1:A:237:ARG:HD3	0.84	1.00
1:A:225:TRP:CH2	1:A:266:GLN:HB3	1.96	0.99
1:A:262:MET:O	1:A:266:GLN:N	1.94	0.99
1:B:256:PRO:C	1:B:257:LEU:HD23	1.88	0.99
1:A:216:GLN:O	1:A:219:ILE:HG22	1.63	0.98
1:A:251:MET:C	1:A:253:ASP:H	1.68	0.98
1:B:244:PHE:CD1	1:B:245:ILE:O	2.16	0.98
1:A:139:VAL:HG13	1:A:140:ARG:H	1.25	0.98
1:A:244:PHE:CD1	1:A:245:ILE:O	2.16	0.98
1:A:245:ILE:HA	1:A:283:HIS:O	1.61	0.98
1:A:240:GLY:HA3	1:A:277:GLY:HA2	1.46	0.98
1:A:109:THR:HB	1:A:110:PRO:HD2	1.42	0.98
1:A:6:GLY:C	1:A:12:ALA:HB3	1.89	0.97
1:B:159:MET:HG3	1:B:184:LEU:HD11	1.44	0.97
1:A:247:ILE:HG12	1:A:248:HIS:HD2	1.20	0.97
1:B:14:ILE:HD11	1:B:138:VAL:HA	1.43	0.97
1:A:143:GLN:H	1:A:143:GLN:CD	1.70	0.96
1:B:234:LEU:CD1	1:B:234:LEU:H	1.78	0.96
1:A:199:TYR:HA	1:A:202:VAL:HG23	1.44	0.96
1:A:225:TRP:CZ3	1:A:266:GLN:CB	2.46	0.96
1:A:242:THR:H	1:A:280:VAL:HG12	1.31	0.95
1:A:240:GLY:HA2	1:A:277:GLY:HA2	1.48	0.95
1:A:63:SER:HA	1:A:76:GLY:HA2	1.49	0.95
1:A:272:LEU:HD13	1:A:273:ARG:HA	1.49	0.95
1:B:230:GLY:HA2	1:B:249:LEU:CG	1.96	0.95
1:A:17:THR:H	1:A:148:ARG:HH22	1.09	0.94
1:B:62:TYR:HA	1:B:65:GLN:HE22	1.29	0.94
1:A:256:PRO:C	1:A:257:LEU:HD23	1.92	0.94
1:B:248:HIS:HB2	1:B:252:GLU:C	1.93	0.94
1:A:85:ALA:O	1:A:89:PHE:O	1.86	0.94
1:A:206:LEU:HD22	1:A:237:ARG:NE	1.81	0.94
1:B:225:TRP:HZ3	1:B:266:GLN:HB3	1.13	0.94
1:A:261:HIS:O	1:A:263:VAL:N	2.01	0.93
1:A:11:ARG:HH22	1:A:239:SER:HA	1.33	0.93
1:A:14:ILE:HD11	1:A:138:VAL:HA	1.48	0.93
1:A:138:VAL:O	1:A:139:VAL:O	1.84	0.93
1:B:240:GLY:CA	1:B:277:GLY:HA2	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:HB3	1:B:75:HIS:HD2	1.33	0.92
1:B:261:HIS:O	1:B:263:VAL:N	2.03	0.92
1:A:21:SER:HA	1:A:24:LEU:HB2	1.53	0.91
1:B:240:GLY:HA2	1:B:277:GLY:HA2	1.52	0.91
1:B:11:ARG:HH22	1:B:239:SER:HA	1.34	0.91
1:B:225:TRP:CZ3	1:B:266:GLN:CB	2.49	0.91
1:A:17:THR:N	1:A:148:ARG:NH2	2.19	0.90
1:B:67:ALA:CB	1:B:69:ASP:HA	1.99	0.90
1:B:272:LEU:O	1:B:274:ARG:N	2.04	0.90
1:A:23:LEU:HD11	1:A:154:TYR:OH	1.72	0.90
1:A:159:MET:HG3	1:A:184:LEU:HD11	1.54	0.89
1:B:17:THR:H	1:B:148:ARG:HH22	1.13	0.89
1:B:262:MET:O	1:B:266:GLN:N	2.05	0.89
1:B:144:SER:CB	1:B:148:ARG:HG2	2.01	0.89
1:B:248:HIS:O	1:B:253:ASP:HB2	1.73	0.89
1:B:225:TRP:CH2	1:B:266:GLN:HB3	2.06	0.89
1:A:243:ARG:O	1:A:244:PHE:HD2	1.55	0.89
1:B:11:ARG:HA	1:B:142:THR:HG21	1.56	0.88
1:B:232:HIS:CD2	1:B:245:ILE:CB	2.56	0.88
1:B:235:ARG:HH12	1:B:237:ARG:HD3	0.74	0.88
1:B:234:LEU:H	1:B:234:LEU:HD12	1.35	0.88
1:B:79:GLU:HB2	1:B:147:VAL:HG21	0.92	0.88
1:A:62:TYR:HA	1:A:65:GLN:HE22	1.38	0.88
1:A:264:ALA:O	1:A:267:VAL:HB	1.74	0.87
1:B:286:PRO:CG	1:B:287:CYS:H	1.79	0.87
1:A:57:LEU:HD23	1:A:58:LEU:HG	1.55	0.87
1:B:125:LEU:C	1:B:127:CYS:H	1.83	0.87
1:B:139:VAL:HG13	1:B:140:ARG:N	1.89	0.87
1:A:252:GLU:HA	1:A:256:PRO:HD3	1.57	0.86
1:B:139:VAL:HG13	1:B:140:ARG:H	1.40	0.86
1:A:252:GLU:HB3	1:A:256:PRO:CG	2.04	0.86
1:A:144:SER:HB3	1:A:148:ARG:CG	2.04	0.86
1:B:144:SER:HB3	1:B:148:ARG:HG2	1.57	0.86
1:A:143:GLN:HB2	1:A:146:ALA:H	1.41	0.86
1:B:230:GLY:CA	1:B:249:LEU:HG	2.04	0.86
1:A:232:HIS:O	1:A:233:ASP:HB3	1.73	0.86
1:B:87:SER:HA	1:B:193:SER:HB3	1.56	0.86
1:B:232:HIS:O	1:B:233:ASP:HB3	1.76	0.86
1:B:143:GLN:HB2	1:B:146:ALA:H	1.40	0.85
1:B:242:THR:HB	1:B:280:VAL:HB	1.58	0.85
1:A:67:ALA:CB	1:A:69:ASP:HA	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:HB3	1:A:75:HIS:HD2	1.40	0.85
1:B:262:MET:HA	1:B:265:ASP:HB3	1.58	0.85
1:A:230:GLY:CA	1:A:249:LEU:HG	2.05	0.85
1:A:278:SER:H	1:A:280:VAL:HG13	1.41	0.85
1:B:63:SER:HA	1:B:76:GLY:HA2	1.56	0.85
1:B:248:HIS:HB2	1:B:252:GLU:O	1.75	0.85
1:B:232:HIS:CD2	1:B:245:ILE:HG21	2.07	0.85
1:B:245:ILE:HA	1:B:283:HIS:O	1.77	0.84
1:A:243:ARG:O	1:A:244:PHE:CD2	2.30	0.84
1:A:247:ILE:CG2	1:A:248:HIS:N	2.41	0.84
1:B:199:TYR:HA	1:B:202:VAL:HG22	1.58	0.84
1:B:206:LEU:HD22	1:B:237:ARG:NE	1.91	0.84
1:A:242:THR:H	1:A:280:VAL:CG1	1.90	0.84
1:A:67:ALA:HB3	1:A:69:ASP:CA	2.08	0.84
1:A:278:SER:OG	1:A:280:VAL:CG1	2.25	0.84
1:B:242:THR:H	1:B:280:VAL:HG12	1.42	0.84
1:B:252:GLU:CA	1:B:256:PRO:HD3	2.07	0.84
1:A:232:HIS:O	1:A:233:ASP:CB	2.25	0.83
1:B:209:ALA:HB1	1:B:236:THR:OG1	1.77	0.83
1:B:232:HIS:CD2	1:B:245:ILE:CG2	2.61	0.83
1:B:245:ILE:CG2	1:B:285:ASP:OD2	2.26	0.83
1:B:256:PRO:HA	1:B:257:LEU:HD23	1.61	0.83
1:B:6:GLY:C	1:B:12:ALA:HB3	2.03	0.83
1:A:73:PHE:CD2	1:A:73:PHE:O	2.32	0.83
1:B:247:ILE:HG12	1:B:248:HIS:CD2	2.14	0.83
1:A:139:VAL:CG1	1:A:140:ARG:N	2.40	0.82
1:A:244:PHE:O	1:A:282:ILE:HD13	1.79	0.82
1:A:67:ALA:HA	1:A:75:HIS:NE2	1.94	0.82
1:A:232:HIS:NE2	1:A:245:ILE:HG21	1.93	0.82
1:B:21:SER:HA	1:B:24:LEU:HB2	1.60	0.82
1:A:259:GLN:O	1:A:261:HIS:N	2.10	0.82
1:A:125:LEU:C	1:A:127:CYS:H	1.86	0.82
1:B:143:GLN:CD	1:B:143:GLN:H	1.88	0.82
1:A:14:ILE:HG12	1:A:142:THR:HG22	1.62	0.82
1:A:216:GLN:O	1:A:219:ILE:CG2	2.28	0.82
1:A:70:ASN:H	1:A:70:ASN:ND2	1.76	0.81
1:B:232:HIS:O	1:B:233:ASP:CB	2.27	0.81
1:A:242:THR:HB	1:A:280:VAL:HB	1.62	0.81
1:B:73:PHE:C	1:B:73:PHE:CD2	2.58	0.81
1:B:252:GLU:CB	1:B:256:PRO:CG	2.58	0.81
1:A:62:TYR:C	1:A:64:LEU:H	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HD11	1:B:154:TYR:OH	1.81	0.81
1:A:261:HIS:C	1:A:263:VAL:H	1.84	0.81
1:A:87:SER:HA	1:A:193:SER:HB3	1.63	0.80
1:A:91:SER:O	1:A:93:SER:OG	1.99	0.80
1:A:225:TRP:HZ3	1:A:266:GLN:HB3	1.20	0.80
1:A:208:ARG:O	1:A:210:LEU:CA	2.30	0.79
1:A:247:ILE:CG2	1:A:248:HIS:H	1.95	0.79
1:B:252:GLU:HA	1:B:255:LEU:HB3	1.62	0.79
1:B:272:LEU:HD13	1:B:273:ARG:CA	2.13	0.79
1:A:145:GLN:HE22	1:A:239:SER:H	1.29	0.79
1:A:262:MET:HA	1:A:265:ASP:HB3	1.64	0.79
1:A:9:VAL:HB	1:A:141:ARG:HH21	1.47	0.78
1:A:248:HIS:HB2	1:A:252:GLU:C	2.09	0.78
1:A:19:MET:HE3	1:A:135:GLN:HE22	1.49	0.78
1:B:64:LEU:C	1:B:65:GLN:HE21	1.91	0.78
1:B:247:ILE:HG23	1:B:248:HIS:CD2	2.18	0.78
1:A:203:GLN:HG3	1:A:205:LEU:HD12	1.65	0.78
1:B:218:ILE:O	1:B:222:VAL:HG23	1.84	0.78
1:B:245:ILE:HG23	1:B:285:ASP:OD2	1.83	0.78
1:A:245:ILE:HG22	1:A:285:ASP:HB2	1.66	0.77
1:A:278:SER:N	1:A:280:VAL:HG13	2.00	0.77
1:A:230:GLY:HA2	1:A:249:LEU:CD1	2.14	0.77
1:B:245:ILE:CA	1:B:245:ILE:HB	2.10	0.77
1:B:268:GLU:OE2	1:B:282:ILE:N	2.18	0.77
1:B:203:GLN:HG2	1:B:208:ARG:HG2	1.67	0.77
1:A:107:SER:HB3	1:A:108:PRO:HD3	1.65	0.76
1:A:203:GLN:HG2	1:A:208:ARG:HG2	1.67	0.76
1:A:248:HIS:HB2	1:A:252:GLU:O	1.85	0.76
1:A:208:ARG:O	1:A:210:LEU:N	2.18	0.76
1:A:250:GLU:O	1:A:251:MET:HB2	1.85	0.76
1:A:18:ALA:O	1:A:22:LEU:N	2.16	0.76
1:B:107:SER:HB3	1:B:108:PRO:HD3	1.68	0.76
1:B:203:GLN:HG3	1:B:205:LEU:HD12	1.66	0.76
1:B:228:VAL:O	1:B:229:SER:C	2.29	0.76
1:A:278:SER:OG	1:A:280:VAL:HG13	1.86	0.76
1:A:252:GLU:CB	1:A:256:PRO:HG3	2.10	0.76
1:B:247:ILE:CG2	1:B:248:HIS:N	2.49	0.76
1:B:18:ALA:O	1:B:22:LEU:N	2.14	0.75
1:A:14:ILE:HD13	1:A:141:ARG:HB3	1.67	0.75
1:A:207:ASP:C	1:A:209:ALA:N	2.44	0.75
1:A:228:VAL:H	1:A:248:HIS:HE1	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:HB3	1:B:69:ASP:CA	2.08	0.75
1:A:151:MET:O	1:A:154:TYR:N	2.19	0.75
1:B:222:VAL:HG13	1:B:267:VAL:HG11	1.69	0.75
1:B:67:ALA:CB	1:B:72:SER:O	2.27	0.75
1:B:144:SER:HB3	1:B:148:ARG:CG	2.17	0.75
1:B:232:HIS:NE2	1:B:245:ILE:CB	2.49	0.75
1:A:230:GLY:O	1:A:246:GLN:HA	1.86	0.74
1:B:91:SER:O	1:B:93:SER:OG	2.03	0.74
1:A:73:PHE:CE2	1:A:74:GLY:HA3	2.22	0.74
1:A:272:LEU:O	1:A:274:ARG:N	2.20	0.74
1:B:11:ARG:NH1	1:B:239:SER:OG	2.17	0.74
1:B:232:HIS:CD2	1:B:245:ILE:HB	2.21	0.74
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.67	0.74
1:A:197:MET:O	1:A:201:ALA:HB2	1.88	0.74
1:A:244:PHE:HD1	1:A:245:ILE:O	1.69	0.74
1:B:270:ALA:C	1:B:272:LEU:H	1.96	0.74
1:A:247:ILE:HG23	1:A:248:HIS:N	2.02	0.74
1:A:263:VAL:HG12	1:A:264:ALA:H	1.52	0.74
1:B:136:ARG:O	1:B:139:VAL:HG12	1.88	0.74
1:A:67:ALA:CB	1:A:72:SER:O	2.25	0.74
1:A:208:ARG:O	1:A:210:LEU:HA	1.88	0.74
1:B:153:HIS:O	1:B:157:ASP:HB2	1.88	0.73
1:A:22:LEU:HD23	1:A:131:LEU:CB	2.12	0.73
1:B:232:HIS:CD2	1:B:245:ILE:HD12	2.23	0.73
1:B:261:HIS:C	1:B:263:VAL:H	1.90	0.73
1:A:230:GLY:O	1:A:246:GLN:CB	2.36	0.73
1:A:278:SER:OG	1:A:280:VAL:HG12	1.87	0.73
1:B:242:THR:HG22	1:B:243:ARG:H	1.53	0.73
1:A:269:GLN:HG3	1:B:269:GLN:HE22	1.52	0.73
1:B:85:ALA:O	1:B:89:PHE:O	2.04	0.73
1:B:72:SER:HB3	1:B:75:HIS:CD2	2.21	0.73
1:A:138:VAL:HG11	1:A:148:ARG:HG3	1.70	0.73
1:A:230:GLY:O	1:A:246:GLN:CA	2.36	0.73
1:A:234:LEU:HD13	1:A:235:ARG:H	1.54	0.73
1:A:273:ARG:HB3	1:A:274:ARG:NH2	2.04	0.72
1:B:230:GLY:HA3	1:B:247:ILE:O	1.89	0.72
1:A:145:GLN:HE22	1:A:239:SER:N	1.86	0.72
1:A:207:ASP:C	1:A:209:ALA:H	1.98	0.72
1:B:199:TYR:HA	1:B:202:VAL:HG23	1.70	0.72
1:A:216:GLN:O	1:A:217:GLU:C	2.32	0.72
1:B:222:VAL:HG13	1:B:267:VAL:CG1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:NE2	1:A:245:ILE:CD1	2.47	0.72
1:A:245:ILE:HD13	1:A:283:HIS:HD2	1.53	0.72
1:A:274:ARG:HH11	1:A:274:ARG:HB2	1.53	0.72
1:A:62:TYR:C	1:A:64:LEU:N	2.48	0.72
1:A:252:GLU:CA	1:A:256:PRO:HD3	2.19	0.72
1:B:14:ILE:O	1:B:148:ARG:NH2	2.21	0.72
1:A:286:PRO:HG2	1:A:287:CYS:N	2.02	0.72
1:A:11:ARG:NH1	1:A:239:SER:OG	2.15	0.72
1:A:209:ALA:C	1:A:236:THR:HB	2.15	0.72
1:B:138:VAL:O	1:B:139:VAL:O	2.08	0.72
1:B:259:GLN:O	1:B:261:HIS:N	2.23	0.72
1:A:18:ALA:C	1:A:20:ALA:H	1.98	0.71
1:A:144:SER:O	1:A:147:VAL:HB	1.90	0.71
1:A:283:HIS:CE1	1:A:285:ASP:OD1	2.44	0.71
1:B:233:ASP:O	1:B:244:PHE:HB3	1.89	0.71
1:A:240:GLY:CA	1:A:277:GLY:CA	2.67	0.71
1:A:148:ARG:O	1:A:150:ASP:N	2.23	0.71
1:B:244:PHE:O	1:B:282:ILE:HD13	1.90	0.71
1:B:22:LEU:HD23	1:B:131:LEU:CB	2.13	0.71
1:B:208:ARG:O	1:B:210:LEU:HA	1.91	0.71
1:A:189:TYR:HA	1:A:192:TYR:HB3	1.74	0.70
1:A:17:THR:H	1:A:148:ARG:NH2	1.83	0.70
1:A:144:SER:OG	1:A:148:ARG:N	2.18	0.70
1:B:268:GLU:HG2	1:B:282:ILE:HG13	1.72	0.70
1:A:247:ILE:HG22	1:A:248:HIS:H	1.53	0.70
1:B:22:LEU:O	1:B:22:LEU:HD22	1.92	0.70
1:B:248:HIS:O	1:B:253:ASP:CB	2.39	0.70
1:A:272:LEU:HD13	1:A:273:ARG:CA	2.20	0.70
1:B:230:GLY:O	1:B:246:GLN:CB	2.39	0.70
1:B:252:GLU:OE1	1:B:255:LEU:HD23	1.90	0.70
1:A:73:PHE:CG	1:A:74:GLY:N	2.55	0.70
1:A:245:ILE:CG2	1:A:285:ASP:OD2	2.40	0.70
1:A:144:SER:HG	1:A:148:ARG:H	1.39	0.70
1:B:84:LEU:HD12	1:B:201:ALA:HB1	1.71	0.70
1:B:76:GLY:O	1:B:79:GLU:HG2	1.92	0.70
1:B:87:SER:HA	1:B:193:SER:CB	2.22	0.69
1:B:234:LEU:CD1	1:B:234:LEU:N	2.50	0.69
1:B:256:PRO:CA	1:B:257:LEU:HD23	2.22	0.69
1:B:234:LEU:O	1:B:235:ARG:O	2.10	0.69
1:B:245:ILE:HG22	1:B:285:ASP:HB2	1.75	0.69
1:B:247:ILE:HG22	1:B:248:HIS:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:OE2	1:A:282:ILE:N	2.26	0.69
1:B:219:ILE:HG23	1:B:220:ASP:OD1	1.92	0.69
1:A:240:GLY:HA2	1:A:277:GLY:CA	2.22	0.69
1:A:139:VAL:CG1	1:A:140:ARG:H	1.92	0.69
1:B:14:ILE:HD13	1:B:141:ARG:HB3	1.75	0.69
1:B:86:GLN:O	1:B:91:SER:HB3	1.92	0.69
1:B:243:ARG:O	1:B:244:PHE:HB3	1.91	0.69
1:A:196:ARG:HG2	1:A:197:MET:N	2.06	0.69
1:B:144:SER:OG	1:B:148:ARG:HG2	1.93	0.69
1:A:10:SER:O	1:A:12:ALA:N	2.26	0.68
1:A:154:TYR:C	1:A:156:SER:H	2.01	0.68
1:B:216:GLN:O	1:B:217:GLU:C	2.34	0.68
1:B:9:VAL:HB	1:B:141:ARG:HH21	1.57	0.68
1:A:11:ARG:HA	1:A:142:THR:HG21	1.74	0.68
1:A:23:LEU:HB3	1:A:53:SER:HB2	1.76	0.68
1:A:67:ALA:HA	1:A:75:HIS:CE1	2.27	0.68
1:A:153:HIS:O	1:A:157:ASP:HB2	1.93	0.68
1:B:244:PHE:CE1	1:B:245:ILE:O	2.46	0.68
1:A:84:LEU:HD12	1:A:201:ALA:HB1	1.73	0.68
1:A:286:PRO:CG	1:A:287:CYS:H	1.99	0.68
1:B:57:LEU:HD23	1:B:58:LEU:HG	1.76	0.68
1:B:65:GLN:HB3	1:B:66:PRO:HD2	1.75	0.68
1:B:197:MET:O	1:B:201:ALA:HB2	1.94	0.68
1:A:232:HIS:HE1	1:A:285:ASP:OD2	1.77	0.68
1:B:14:ILE:HG12	1:B:142:THR:HG22	1.75	0.68
1:B:264:ALA:O	1:B:267:VAL:HB	1.94	0.67
1:A:145:GLN:NE2	1:A:239:SER:H	1.92	0.67
1:B:250:GLU:HG2	1:B:251:MET:N	2.08	0.67
1:B:278:SER:N	1:B:280:VAL:HG13	2.09	0.67
1:A:263:VAL:CG1	1:A:264:ALA:N	2.58	0.67
1:B:189:TYR:HA	1:B:192:TYR:HB3	1.77	0.67
1:B:244:PHE:O	1:B:282:ILE:HG23	1.93	0.67
1:A:218:ILE:O	1:A:222:VAL:HG23	1.94	0.67
1:A:228:VAL:H	1:A:248:HIS:CE1	2.12	0.67
1:A:247:ILE:CG1	1:A:248:HIS:HD2	2.05	0.67
1:A:216:GLN:O	1:A:217:GLU:O	2.12	0.67
1:A:23:LEU:HB2	1:A:53:SER:OG	1.94	0.67
1:B:133:SER:HA	1:B:136:ARG:HB2	1.77	0.67
1:B:262:MET:O	1:B:266:GLN:HG3	1.93	0.67
1:B:218:ILE:HD12	1:B:242:THR:HG21	1.77	0.67
1:B:154:TYR:C	1:B:156:SER:H	2.00	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLU:H	1:B:215:ARG:HB3	1.59	0.67
1:B:245:ILE:HD13	1:B:283:HIS:HD2	1.60	0.67
1:A:69:ASP:O	1:A:73:PHE:HA	1.95	0.67
1:B:159:MET:HB3	1:B:184:LEU:HD21	1.77	0.67
1:B:199:TYR:O	1:B:203:GLN:NE2	2.28	0.67
1:B:216:GLN:O	1:B:219:ILE:CG2	2.38	0.67
1:A:86:GLN:O	1:A:91:SER:HB3	1.94	0.67
1:A:259:GLN:C	1:A:261:HIS:H	2.03	0.67
1:B:261:HIS:CD2	1:B:265:ASP:HB2	2.29	0.67
1:A:6:GLY:HA2	1:A:10:SER:H	1.60	0.66
1:A:19:MET:CE	1:A:135:GLN:HE22	2.06	0.66
1:A:232:HIS:CD2	1:A:245:ILE:HD12	2.31	0.66
1:B:27:LYS:NZ	1:B:30:ALA:HB3	2.10	0.66
1:B:251:MET:C	1:B:253:ASP:N	2.52	0.66
1:B:73:PHE:CG	1:B:74:GLY:N	2.61	0.66
1:A:14:ILE:O	1:A:148:ARG:NH2	2.27	0.66
1:B:209:ALA:O	1:B:210:LEU:HG	1.96	0.66
1:A:67:ALA:C	1:A:69:ASP:H	2.01	0.66
1:B:251:MET:C	1:B:253:ASP:H	1.92	0.66
1:A:132:VAL:C	1:A:134:PHE:H	2.04	0.66
1:A:244:PHE:CE1	1:A:245:ILE:O	2.48	0.66
1:A:266:GLN:O	1:A:267:VAL:C	2.38	0.66
1:B:232:HIS:CD2	1:B:245:ILE:CG1	2.78	0.66
1:A:138:VAL:O	1:A:139:VAL:C	2.38	0.66
1:A:199:TYR:O	1:A:203:GLN:NE2	2.28	0.66
1:A:218:ILE:HD13	1:A:271:ILE:HG21	1.78	0.66
1:B:138:VAL:HG11	1:B:148:ARG:HG3	1.78	0.66
1:A:243:ARG:O	1:A:244:PHE:HB3	1.95	0.66
1:A:273:ARG:HB3	1:A:274:ARG:HH22	1.61	0.65
1:B:14:ILE:CD1	1:B:138:VAL:HA	2.22	0.65
1:B:19:MET:HE1	1:B:150:ASP:OD1	1.96	0.65
1:A:144:SER:OG	1:A:148:ARG:HG2	1.96	0.65
1:B:278:SER:OG	1:B:280:VAL:CG1	2.45	0.65
1:B:286:PRO:CG	1:B:287:CYS:N	2.40	0.65
1:A:252:GLU:CB	1:A:256:PRO:CG	2.71	0.65
1:A:228:VAL:N	1:A:248:HIS:CE1	2.64	0.65
1:A:276:PRO:CG	1:A:277:GLY:O	2.39	0.65
1:B:217:GLU:O	1:B:218:ILE:C	2.40	0.65
1:B:243:ARG:O	1:B:244:PHE:CD2	2.50	0.65
1:B:242:THR:H	1:B:280:VAL:CG1	2.09	0.65
1:A:27:LYS:NZ	1:A:30:ALA:HB3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLY:O	1:B:246:GLN:CA	2.44	0.65
1:A:73:PHE:CZ	1:A:74:GLY:O	2.50	0.65
1:A:209:ALA:O	1:A:210:LEU:HG	1.96	0.65
1:A:86:GLN:CD	1:A:86:GLN:H	2.05	0.65
1:B:245:ILE:HD13	1:B:283:HIS:CD2	2.31	0.65
1:B:208:ARG:O	1:B:210:LEU:CA	2.45	0.65
1:A:133:SER:HA	1:A:136:ARG:HB2	1.79	0.64
1:A:235:ARG:NH1	1:A:237:ARG:CD	2.41	0.64
1:B:151:MET:O	1:B:154:TYR:N	2.31	0.64
1:B:266:GLN:O	1:B:267:VAL:C	2.36	0.64
1:A:10:SER:C	1:A:12:ALA:H	2.06	0.64
1:A:145:GLN:O	1:A:200:GLU:OE1	2.15	0.64
1:A:245:ILE:HG21	1:A:285:ASP:OD2	1.97	0.64
1:A:270:ALA:C	1:A:272:LEU:H	2.05	0.64
1:A:274:ARG:H	1:A:274:ARG:NH1	1.95	0.64
1:A:67:ALA:C	1:A:69:ASP:N	2.56	0.64
1:B:149:ALA:CB	1:B:196:ARG:HH21	2.10	0.64
1:B:80:SER:O	1:B:83:ALA:HB3	1.97	0.64
1:A:14:ILE:CD1	1:A:138:VAL:HA	2.25	0.64
1:A:136:ARG:O	1:A:139:VAL:HG12	1.97	0.64
1:A:251:MET:C	1:A:253:ASP:N	2.48	0.64
1:A:199:TYR:HA	1:A:202:VAL:HG22	1.78	0.63
1:A:218:ILE:HD12	1:A:242:THR:HG21	1.78	0.63
1:A:203:GLN:HG3	1:A:205:LEU:CD1	2.28	0.63
1:A:107:SER:HB3	1:A:108:PRO:CD	2.28	0.63
1:B:86:GLN:H	1:B:86:GLN:CD	2.06	0.63
1:B:233:ASP:O	1:B:244:PHE:CB	2.46	0.63
1:B:232:HIS:CE1	1:B:285:ASP:OD2	2.50	0.63
1:B:143:GLN:HB2	1:B:146:ALA:N	2.11	0.63
1:B:268:GLU:CG	1:B:282:ILE:HG13	2.28	0.63
1:A:144:SER:O	1:A:144:SER:OG	2.15	0.63
1:A:263:VAL:HG12	1:A:264:ALA:N	2.14	0.63
1:B:244:PHE:N	1:B:281:ILE:O	2.32	0.63
1:B:276:PRO:CG	1:B:277:GLY:O	2.31	0.63
1:B:230:GLY:O	1:B:246:GLN:HA	1.99	0.63
1:A:22:LEU:CD2	1:A:131:LEU:HB3	2.14	0.63
1:A:143:GLN:HB2	1:A:146:ALA:N	2.12	0.63
1:B:248:HIS:CB	1:B:252:GLU:C	2.71	0.63
1:B:274:ARG:C	1:B:276:PRO:HA	2.24	0.62
1:A:203:GLN:HG2	1:A:208:ARG:CG	2.29	0.62
1:B:18:ALA:C	1:B:20:ALA:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD13	1:A:168:LEU:HB3	1.81	0.62
1:A:65:GLN:HB3	1:A:66:PRO:HD2	1.79	0.62
1:A:186:ILE:HG22	1:A:187:GLY:H	1.65	0.62
1:A:248:HIS:HB2	1:A:252:GLU:HB2	1.80	0.62
1:B:17:THR:H	1:B:148:ARG:NH2	1.93	0.62
1:B:247:ILE:HG23	1:B:248:HIS:HD2	1.65	0.62
1:B:259:GLN:C	1:B:261:HIS:H	2.07	0.62
1:B:268:GLU:HG2	1:B:282:ILE:CG1	2.29	0.62
1:B:243:ARG:O	1:B:244:PHE:HD2	1.81	0.62
1:A:9:VAL:HB	1:A:141:ARG:NH2	2.14	0.62
1:B:10:SER:O	1:B:12:ALA:N	2.32	0.62
1:B:70:ASN:ND2	1:B:70:ASN:H	1.95	0.62
1:A:79:GLU:HB2	1:A:147:VAL:HG21	0.81	0.62
1:A:213:GLU:O	1:A:216:GLN:N	2.33	0.61
1:B:11:ARG:CA	1:B:142:THR:HG21	2.28	0.61
1:B:22:LEU:CD2	1:B:131:LEU:HB3	2.15	0.61
1:A:212:ASP:O	1:A:213:GLU:HB2	1.99	0.61
1:B:23:LEU:HB3	1:B:53:SER:HB2	1.82	0.61
1:A:198:GLY:O	1:A:199:TYR:CD1	2.52	0.61
1:A:235:ARG:HG2	1:A:236:THR:H	1.64	0.61
1:B:6:GLY:HA2	1:B:10:SER:H	1.66	0.61
1:B:107:SER:HB3	1:B:108:PRO:CD	2.31	0.61
1:B:221:ILE:O	1:B:224:SER:OG	2.19	0.61
1:A:18:ALA:H	1:A:148:ARG:NH2	1.98	0.61
1:A:76:GLY:O	1:A:79:GLU:HG2	2.01	0.61
1:A:199:TYR:N	1:A:201:ALA:HB3	2.15	0.61
1:A:283:HIS:NE2	1:A:285:ASP:CG	2.59	0.61
1:B:252:GLU:HB3	1:B:256:PRO:CD	2.30	0.61
1:A:217:GLU:O	1:A:218:ILE:C	2.43	0.61
1:A:283:HIS:NE2	1:A:285:ASP:OD1	2.34	0.61
1:B:144:SER:O	1:B:147:VAL:HB	2.00	0.61
1:B:246:GLN:HE22	1:B:267:VAL:HG21	1.65	0.61
1:A:107:SER:HA	1:A:112:THR:HB	1.81	0.60
1:A:81:LEU:O	1:A:83:ALA:N	2.32	0.60
1:A:109:THR:CB	1:A:110:PRO:HD2	2.25	0.60
1:A:251:MET:O	1:A:253:ASP:N	2.29	0.60
1:B:87:SER:C	1:B:193:SER:HB2	2.27	0.60
1:B:107:SER:HA	1:B:112:THR:HB	1.82	0.60
1:A:80:SER:O	1:A:83:ALA:HB3	2.01	0.60
1:A:243:ARG:C	1:A:244:PHE:HD2	2.08	0.60
1:B:73:PHE:CE1	1:B:74:GLY:O	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:SER:OG	1:B:280:VAL:HG13	2.01	0.60
1:A:268:GLU:HG2	1:A:282:ILE:HG13	1.83	0.60
1:B:18:ALA:H	1:B:148:ARG:NH2	1.99	0.60
1:B:63:SER:O	1:B:64:LEU:HD22	2.02	0.60
1:A:87:SER:HA	1:A:193:SER:CB	2.32	0.60
1:B:69:ASP:O	1:B:73:PHE:HA	2.02	0.60
1:B:203:GLN:HG2	1:B:208:ARG:CG	2.31	0.60
1:A:23:LEU:HD11	1:A:154:TYR:HH	1.65	0.60
1:A:72:SER:HB3	1:A:75:HIS:CD2	2.31	0.60
1:A:192:TYR:CG	1:A:193:SER:N	2.66	0.60
1:A:252:GLU:HA	1:A:255:LEU:HB3	1.82	0.60
1:A:186:ILE:CG2	1:A:187:GLY:N	2.65	0.60
1:B:62:TYR:C	1:B:64:LEU:H	2.09	0.60
1:A:14:ILE:CD1	1:A:141:ARG:HB3	2.30	0.60
1:A:159:MET:CG	1:A:184:LEU:HD11	2.29	0.60
1:A:159:MET:HB3	1:A:184:LEU:HD21	1.82	0.60
1:B:109:THR:HB	1:B:110:PRO:CD	2.22	0.60
1:B:244:PHE:HD1	1:B:245:ILE:O	1.77	0.60
1:A:186:ILE:HG22	1:A:187:GLY:N	2.17	0.60
1:A:252:GLU:OE1	1:A:255:LEU:HD23	2.02	0.60
1:B:30:ALA:H	1:B:31:TRP:HE3	1.49	0.60
1:A:199:TYR:O	1:A:202:VAL:N	2.35	0.59
1:B:19:MET:HE3	1:B:135:GLN:HE22	1.66	0.59
1:B:230:GLY:HA2	1:B:249:LEU:CD1	2.32	0.59
1:A:202:VAL:O	1:A:205:LEU:CG	2.34	0.59
1:A:13:ALA:O	1:A:16:ALA:N	2.34	0.59
1:A:148:ARG:C	1:A:150:ASP:H	2.10	0.59
1:B:29:PHE:HA	1:B:31:TRP:HZ3	1.67	0.59
1:A:261:HIS:C	1:A:263:VAL:N	2.51	0.59
1:A:228:VAL:O	1:A:229:SER:C	2.45	0.59
1:B:166:LEU:HD13	1:B:168:LEU:HB3	1.83	0.59
1:B:240:GLY:HA3	1:B:277:GLY:HA2	1.83	0.59
1:B:262:MET:HA	1:B:265:ASP:CB	2.30	0.59
1:A:213:GLU:H	1:A:215:ARG:HB3	1.68	0.59
1:B:186:ILE:HG22	1:B:187:GLY:N	2.18	0.59
1:A:30:ALA:H	1:A:31:TRP:HE3	1.51	0.59
1:B:60:VAL:C	1:B:62:TYR:H	2.10	0.59
1:A:230:GLY:HA3	1:A:247:ILE:O	2.03	0.58
1:B:186:ILE:CG2	1:B:187:GLY:N	2.66	0.58
1:A:139:VAL:HG22	1:A:140:ARG:H	1.68	0.58
1:B:109:THR:O	1:B:111:MET:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ALA:O	1:A:20:ALA:N	2.29	0.58
1:A:242:THR:HG22	1:A:243:ARG:H	1.68	0.58
1:B:87:SER:HB2	1:B:197:MET:HB2	1.79	0.58
1:A:44:VAL:HG12	1:A:44:VAL:O	2.03	0.58
1:A:73:PHE:CD1	1:A:74:GLY:N	2.72	0.58
1:A:127:CYS:SG	1:A:128:THR:N	2.77	0.58
1:A:45:ASP:HA	1:A:48:VAL:HB	1.84	0.58
1:A:129:ILE:HG12	1:A:158:VAL:HG11	1.86	0.58
1:A:209:ALA:CB	1:A:236:THR:OG1	2.47	0.58
1:B:19:MET:CE	1:B:150:ASP:OD1	2.51	0.58
1:A:79:GLU:O	1:A:82:ALA:N	2.37	0.58
1:A:244:PHE:N	1:A:281:ILE:O	2.37	0.58
1:B:153:HIS:O	1:B:157:ASP:N	2.37	0.58
1:B:232:HIS:NE2	1:B:245:ILE:CG1	2.67	0.58
1:B:232:HIS:HE1	1:B:285:ASP:OD2	1.86	0.58
1:A:19:MET:HE1	1:A:150:ASP:OD1	2.03	0.58
1:A:85:ALA:O	1:A:87:SER:N	2.37	0.58
1:A:139:VAL:HG22	1:A:140:ARG:N	2.18	0.58
1:A:247:ILE:CG1	1:A:248:HIS:CD2	2.79	0.58
1:A:25:LEU:O	1:A:28:ILE:HG22	2.04	0.57
1:B:68:ASP:H	1:B:72:SER:HB2	1.68	0.57
1:B:188:ILE:HG23	1:B:188:ILE:O	2.04	0.57
1:B:199:TYR:O	1:B:202:VAL:HG23	2.04	0.57
1:A:261:HIS:CD2	1:A:265:ASP:HB2	2.39	0.57
1:A:125:LEU:C	1:A:127:CYS:N	2.56	0.57
1:B:77:LYS:HZ2	1:B:206:LEU:HD21	1.68	0.57
1:B:278:SER:H	1:B:280:VAL:HG13	1.68	0.57
1:A:227:GLY:HA2	1:A:248:HIS:NE2	2.19	0.57
1:B:235:ARG:NH1	1:B:237:ARG:CD	2.39	0.57
1:A:278:SER:H	1:A:280:VAL:CG1	2.16	0.57
1:B:248:HIS:O	1:B:253:ASP:N	2.38	0.57
1:A:6:GLY:C	1:A:12:ALA:CB	2.71	0.57
1:A:193:SER:C	1:A:195:LEU:H	2.12	0.57
1:A:274:ARG:N	1:A:274:ARG:NH1	2.51	0.57
1:B:212:ASP:HA	1:B:215:ARG:CB	2.34	0.57
1:A:84:LEU:O	1:A:87:SER:OG	2.22	0.57
1:B:148:ARG:O	1:B:150:ASP:N	2.38	0.57
1:B:218:ILE:HD13	1:B:271:ILE:HG21	1.87	0.57
1:A:214:GLU:HB3	1:A:274:ARG:HE	1.70	0.56
1:A:248:HIS:O	1:A:253:ASP:HB2	2.05	0.56
1:B:192:TYR:CG	1:B:193:SER:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HB2	1:A:74:GLY:HA2	1.87	0.56
1:A:188:ILE:HG23	1:A:188:ILE:O	2.05	0.56
1:A:199:TYR:O	1:A:202:VAL:HG23	2.05	0.56
1:B:23:LEU:HB2	1:B:53:SER:OG	2.05	0.56
1:B:139:VAL:O	1:B:142:THR:C	2.48	0.56
1:B:256:PRO:C	1:B:257:LEU:CD2	2.72	0.56
1:B:186:ILE:HG22	1:B:187:GLY:H	1.70	0.56
1:A:156:SER:HB3	1:A:189:TYR:CE1	2.40	0.56
1:B:252:GLU:CA	1:B:256:PRO:CD	2.82	0.56
1:B:256:PRO:HA	1:B:257:LEU:CD2	2.34	0.56
1:A:142:THR:HG23	1:A:142:THR:O	2.06	0.56
1:A:232:HIS:CE1	1:A:285:ASP:OD2	2.58	0.56
1:B:27:LYS:HZ2	1:B:30:ALA:HB3	1.69	0.56
1:B:273:ARG:HB3	1:B:274:ARG:HH12	1.71	0.56
1:A:143:GLN:CD	1:A:143:GLN:N	2.49	0.56
1:B:136:ARG:O	1:B:139:VAL:CG1	2.54	0.56
1:A:109:THR:O	1:A:111:MET:N	2.38	0.56
1:B:109:THR:CB	1:B:110:PRO:HD2	2.20	0.56
1:A:29:PHE:HA	1:A:31:TRP:HZ3	1.71	0.55
1:B:85:ALA:O	1:B:87:SER:N	2.40	0.55
1:A:233:ASP:O	1:A:244:PHE:HB3	2.06	0.55
1:A:150:ASP:OD1	1:A:150:ASP:C	2.49	0.55
1:B:139:VAL:CG1	1:B:140:ARG:H	2.10	0.55
1:B:203:GLN:HG3	1:B:205:LEU:CD1	2.35	0.55
1:B:247:ILE:HG12	1:B:248:HIS:HD2	1.67	0.55
1:A:273:ARG:HB3	1:A:274:ARG:CZ	2.36	0.55
1:B:73:PHE:CD2	1:B:73:PHE:O	2.60	0.55
1:A:159:MET:HG3	1:A:161:ASN:HD22	1.72	0.55
1:B:154:TYR:C	1:B:156:SER:N	2.64	0.55
1:B:225:TRP:HZ3	1:B:266:GLN:HB2	1.62	0.55
1:A:19:MET:CE	1:A:150:ASP:OD1	2.55	0.55
1:A:225:TRP:HZ3	1:A:266:GLN:HB2	1.67	0.55
1:B:125:LEU:C	1:B:127:CYS:N	2.54	0.55
1:A:132:VAL:O	1:A:136:ARG:N	2.36	0.55
1:B:153:HIS:HD2	1:B:157:ASP:HB2	1.72	0.55
1:B:252:GLU:CB	1:B:256:PRO:CD	2.84	0.55
1:A:267:VAL:O	1:A:268:GLU:C	2.49	0.54
1:B:67:ALA:HB2	1:B:74:GLY:HA2	1.89	0.54
1:B:132:VAL:C	1:B:134:PHE:H	2.14	0.54
1:B:150:ASP:HB3	1:B:197:MET:HE2	1.88	0.54
1:B:207:ASP:C	1:B:209:ALA:N	2.64	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLY:HA2	1:B:248:HIS:NE2	2.22	0.54
1:B:245:ILE:CB	1:B:245:ILE:N	2.65	0.54
1:A:199:TYR:CA	1:A:202:VAL:HG23	2.27	0.54
1:A:154:TYR:C	1:A:156:SER:N	2.65	0.54
1:A:213:GLU:C	1:A:215:ARG:N	2.62	0.54
1:A:256:PRO:C	1:A:257:LEU:CD2	2.75	0.54
1:A:247:ILE:CG2	1:A:252:GLU:O	2.55	0.54
1:B:10:SER:C	1:B:12:ALA:H	2.14	0.54
1:B:20:ALA:HB1	1:B:57:LEU:HD12	1.89	0.54
1:B:270:ALA:C	1:B:272:LEU:N	2.59	0.54
1:A:262:MET:HA	1:A:265:ASP:CB	2.35	0.54
1:B:25:LEU:O	1:B:28:ILE:HG22	2.07	0.54
1:B:142:THR:O	1:B:142:THR:HG23	2.08	0.54
1:B:243:ARG:C	1:B:244:PHE:HD2	2.16	0.54
1:B:263:VAL:HG12	1:B:264:ALA:H	1.73	0.54
1:B:234:LEU:N	1:B:234:LEU:HD13	2.23	0.54
1:A:188:ILE:O	1:A:189:TYR:CD1	2.61	0.54
1:B:62:TYR:C	1:B:64:LEU:N	2.66	0.54
1:B:159:MET:CG	1:B:184:LEU:HD11	2.28	0.54
1:A:73:PHE:CD2	1:A:74:GLY:N	2.74	0.54
1:B:213:GLU:O	1:B:216:GLN:N	2.41	0.54
1:B:261:HIS:O	1:B:264:ALA:N	2.40	0.54
1:B:263:VAL:CG1	1:B:264:ALA:N	2.71	0.54
1:B:279:ASP:O	1:B:281:ILE:HA	2.08	0.54
1:B:85:ALA:HB3	1:B:86:GLN:NE2	2.24	0.53
1:A:87:SER:HB3	1:A:197:MET:HB3	1.86	0.53
1:A:205:LEU:HD12	1:A:205:LEU:O	2.09	0.53
1:B:243:ARG:O	1:B:244:PHE:CB	2.55	0.53
1:B:18:ALA:HB2	1:B:138:VAL:HG21	1.90	0.53
1:A:199:TYR:CA	1:A:202:VAL:CG2	2.74	0.53
1:A:243:ARG:CB	1:A:281:ILE:HD12	2.38	0.53
1:B:85:ALA:O	1:B:86:GLN:C	2.51	0.53
1:B:245:ILE:CA	1:B:245:ILE:CG2	2.78	0.53
1:A:143:GLN:N	1:A:143:GLN:OE1	2.33	0.53
1:B:152:LEU:HG	1:B:155:GLN:OE1	2.09	0.53
1:B:272:LEU:C	1:B:274:ARG:N	2.65	0.53
1:A:196:ARG:CG	1:A:197:MET:N	2.70	0.53
1:A:243:ARG:O	1:A:244:PHE:CB	2.56	0.53
1:B:212:ASP:HA	1:B:215:ARG:HB3	1.91	0.53
1:B:216:GLN:OE1	1:B:216:GLN:HA	2.06	0.53
1:B:252:GLU:CB	1:B:256:PRO:HD3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ALA:O	1:B:267:VAL:N	2.42	0.53
1:B:202:VAL:HG23	1:B:203:GLN:HE22	1.72	0.53
1:B:272:LEU:HD13	1:B:273:ARG:N	2.24	0.53
1:A:244:PHE:O	1:A:282:ILE:CD1	2.55	0.53
1:A:85:ALA:C	1:A:87:SER:N	2.67	0.52
1:A:156:SER:HB3	1:A:189:TYR:HE1	1.73	0.52
1:B:9:VAL:HB	1:B:141:ARG:NH2	2.23	0.52
1:B:197:MET:C	1:B:199:TYR:H	2.18	0.52
1:A:71:HIS:O	1:A:73:PHE:N	2.42	0.52
1:B:197:MET:O	1:B:201:ALA:CB	2.58	0.52
1:A:11:ARG:O	1:A:15:ALA:HB3	2.08	0.52
1:A:236:THR:C	1:A:237:ARG:HG2	2.34	0.52
1:A:247:ILE:HG23	1:A:252:GLU:O	2.09	0.52
1:A:60:VAL:C	1:A:62:TYR:H	2.17	0.52
1:A:245:ILE:CG2	1:A:283:HIS:CD2	2.80	0.52
1:B:143:GLN:C	1:B:145:GLN:N	2.67	0.52
1:B:154:TYR:O	1:B:156:SER:N	2.42	0.52
1:A:18:ALA:C	1:A:20:ALA:N	2.67	0.52
1:B:273:ARG:HB3	1:B:274:ARG:NH1	2.24	0.52
1:A:87:SER:O	1:A:91:SER:O	2.27	0.52
1:A:237:ARG:HG3	1:A:241:PRO:HB2	1.92	0.52
1:A:269:GLN:CG	1:B:269:GLN:HE22	2.20	0.52
1:A:66:PRO:O	1:A:69:ASP:OD1	2.27	0.52
1:A:145:GLN:O	1:A:147:VAL:N	2.43	0.52
1:A:286:PRO:CG	1:A:287:CYS:N	2.64	0.52
1:B:223:THR:HG22	1:B:223:THR:O	2.09	0.52
1:B:247:ILE:CG2	1:B:252:GLU:O	2.58	0.52
1:B:18:ALA:N	1:B:148:ARG:NH2	2.58	0.52
1:B:22:LEU:HA	1:B:131:LEU:HD23	1.91	0.52
1:B:219:ILE:HG23	1:B:220:ASP:H	1.73	0.52
1:A:65:GLN:HB2	1:A:75:HIS:HE1	1.75	0.51
1:A:85:ALA:O	1:A:86:GLN:C	2.52	0.51
1:A:209:ALA:HB1	1:A:236:THR:CB	2.40	0.51
1:B:91:SER:O	1:B:92:GLY:C	2.54	0.51
1:A:44:VAL:C	1:A:46:SER:H	2.19	0.51
1:A:154:TYR:O	1:A:156:SER:N	2.43	0.51
1:B:14:ILE:CD1	1:B:141:ARG:HB3	2.39	0.51
1:B:127:CYS:SG	1:B:128:THR:N	2.84	0.51
1:B:266:GLN:O	1:B:269:GLN:HB3	2.11	0.51
1:A:17:THR:O	1:A:21:SER:OG	2.27	0.51
1:A:18:ALA:N	1:A:148:ARG:NH2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:C	1:A:69:ASP:OD1	2.54	0.51
1:A:73:PHE:CZ	1:A:74:GLY:HA3	2.44	0.51
1:A:91:SER:HA	1:A:94:ALA:HB3	1.91	0.51
1:A:197:MET:O	1:A:201:ALA:CB	2.57	0.51
1:B:22:LEU:HD13	1:B:23:LEU:CD2	2.40	0.51
1:B:152:LEU:CB	1:B:192:TYR:CZ	2.94	0.51
1:B:245:ILE:HG23	1:B:283:HIS:CD2	2.46	0.51
1:A:109:THR:HB	1:A:110:PRO:CD	2.27	0.51
1:B:162:GLY:HA3	1:B:181:LEU:HD12	1.93	0.51
1:B:274:ARG:N	1:B:274:ARG:NH1	2.58	0.51
1:A:150:ASP:OD1	1:A:151:MET:N	2.43	0.51
1:A:273:ARG:HB3	1:A:274:ARG:NH1	2.25	0.51
1:B:79:GLU:O	1:B:80:SER:C	2.52	0.51
1:A:11:ARG:HH12	1:A:239:SER:HG	1.55	0.51
1:A:248:HIS:HB2	1:A:252:GLU:CB	2.41	0.51
1:B:132:VAL:O	1:B:136:ARG:N	2.41	0.51
1:B:274:ARG:HH11	1:B:274:ARG:HB2	1.75	0.51
1:A:20:ALA:O	1:A:21:SER:CB	2.58	0.51
1:A:22:LEU:HA	1:A:131:LEU:HD23	1.92	0.51
1:A:65:GLN:HE21	1:A:65:GLN:N	2.06	0.51
1:A:93:SER:C	1:A:95:LEU:N	2.67	0.51
1:B:93:SER:C	1:B:95:LEU:N	2.68	0.51
1:A:139:VAL:CG2	1:A:140:ARG:H	2.23	0.51
1:A:189:TYR:CA	1:A:192:TYR:HB3	2.39	0.50
1:A:234:LEU:HD12	1:A:234:LEU:N	2.26	0.50
1:B:219:ILE:HG23	1:B:220:ASP:N	2.26	0.50
1:B:105:LEU:O	1:B:107:SER:N	2.43	0.50
1:A:156:SER:HB2	1:A:189:TYR:OH	2.11	0.50
1:A:269:GLN:CG	1:B:269:GLN:NE2	2.74	0.50
1:B:87:SER:O	1:B:88:MET:C	2.54	0.50
1:B:234:LEU:HD13	1:B:235:ARG:H	1.76	0.50
1:B:248:HIS:HB3	1:B:252:GLU:H	1.76	0.50
1:B:252:GLU:CB	1:B:256:PRO:HG3	2.19	0.50
1:B:268:GLU:OE2	1:B:282:ILE:CB	2.59	0.50
1:B:278:SER:OG	1:B:280:VAL:HG12	2.09	0.50
1:A:64:LEU:O	1:A:65:GLN:NE2	2.44	0.50
1:A:139:VAL:O	1:A:142:THR:C	2.54	0.50
1:A:65:GLN:HB3	1:A:66:PRO:CD	2.41	0.50
1:A:105:LEU:O	1:A:107:SER:N	2.45	0.50
1:A:143:GLN:CB	1:A:146:ALA:H	2.20	0.50
1:A:162:GLY:HA3	1:A:181:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD13	1:A:235:ARG:N	2.24	0.50
1:B:17:THR:O	1:B:21:SER:OG	2.29	0.50
1:B:281:ILE:HG22	1:B:282:ILE:N	2.27	0.50
1:B:65:GLN:HB3	1:B:66:PRO:CD	2.41	0.50
1:B:229:SER:O	1:B:247:ILE:O	2.28	0.50
1:B:247:ILE:HG23	1:B:248:HIS:CG	2.46	0.50
1:B:261:HIS:C	1:B:261:HIS:CD2	2.90	0.50
1:A:20:ALA:HB1	1:A:57:LEU:HD12	1.93	0.50
1:A:149:ALA:O	1:A:197:MET:SD	2.70	0.50
1:B:67:ALA:HA	1:B:75:HIS:NE2	2.26	0.50
1:B:248:HIS:HB2	1:B:252:GLU:HB2	1.94	0.50
1:A:283:HIS:NE2	1:A:285:ASP:OD2	2.45	0.50
1:B:270:ALA:O	1:B:272:LEU:N	2.44	0.50
1:B:45:ASP:HA	1:B:48:VAL:HB	1.93	0.49
1:B:91:SER:C	1:B:93:SER:N	2.69	0.49
1:A:259:GLN:C	1:A:261:HIS:N	2.68	0.49
1:B:150:ASP:O	1:B:151:MET:C	2.55	0.49
1:A:93:SER:C	1:A:95:LEU:H	2.19	0.49
1:B:17:THR:N	1:B:148:ARG:NH2	2.38	0.49
1:B:213:GLU:C	1:B:215:ARG:N	2.69	0.49
1:B:252:GLU:OE1	1:B:255:LEU:CD2	2.60	0.49
1:B:44:VAL:HG12	1:B:44:VAL:O	2.13	0.49
1:B:87:SER:CA	1:B:193:SER:CB	2.91	0.49
1:B:143:GLN:CD	1:B:143:GLN:N	2.66	0.49
1:B:189:TYR:CA	1:B:192:TYR:HB3	2.42	0.49
1:B:248:HIS:O	1:B:253:ASP:CA	2.60	0.49
1:A:63:SER:HA	1:A:76:GLY:CA	2.33	0.49
1:A:77:LYS:HZ2	1:A:206:LEU:HD21	1.77	0.49
1:A:203:GLN:HA	1:A:205:LEU:O	2.12	0.49
1:B:18:ALA:O	1:B:20:ALA:N	2.42	0.49
1:B:156:SER:HA	1:B:159:MET:HB2	1.95	0.49
1:B:156:SER:HB2	1:B:189:TYR:OH	2.12	0.49
1:B:156:SER:HB3	1:B:189:TYR:HE1	1.78	0.49
1:B:205:LEU:HD12	1:B:205:LEU:O	2.12	0.49
1:A:22:LEU:HD13	1:A:23:LEU:CD2	2.43	0.49
1:A:54:LEU:O	1:A:55:THR:C	2.56	0.49
1:A:85:ALA:HB3	1:A:86:GLN:NE2	2.27	0.49
1:B:22:LEU:HD13	1:B:23:LEU:HG	1.93	0.49
1:B:77:LYS:HZ1	1:B:206:LEU:HG	1.78	0.49
1:B:209:ALA:HA	1:B:236:THR:O	2.13	0.49
1:A:144:SER:HG	1:A:148:ARG:N	2.05	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:OG	1:B:144:SER:O	2.29	0.48
1:B:150:ASP:OD1	1:B:150:ASP:C	2.56	0.48
1:B:208:ARG:O	1:B:210:LEU:N	2.46	0.48
1:A:219:ILE:HG23	1:A:220:ASP:N	2.28	0.48
1:A:256:PRO:HA	1:A:257:LEU:HD23	1.94	0.48
1:B:138:VAL:O	1:B:139:VAL:C	2.55	0.48
1:A:11:ARG:HD3	1:A:145:GLN:H	1.79	0.48
1:A:268:GLU:O	1:A:269:GLN:C	2.56	0.48
1:B:23:LEU:CB	1:B:53:SER:HB2	2.41	0.48
1:B:44:VAL:C	1:B:46:SER:H	2.21	0.48
1:B:67:ALA:C	1:B:69:ASP:N	2.70	0.48
1:A:57:LEU:O	1:A:60:VAL:HG22	2.14	0.48
1:A:73:PHE:CE1	1:A:74:GLY:O	2.66	0.48
1:B:68:ASP:O	1:B:70:ASN:N	2.46	0.48
1:B:214:GLU:HB3	1:B:274:ARG:HE	1.78	0.48
1:B:245:ILE:CB	1:B:245:ILE:C	2.76	0.48
1:A:68:ASP:HB2	1:A:72:SER:HB2	1.95	0.48
1:A:270:ALA:C	1:A:272:LEU:N	2.66	0.48
1:B:247:ILE:HG23	1:B:248:HIS:CB	2.43	0.48
1:A:274:ARG:C	1:A:276:PRO:HA	2.39	0.48
1:B:143:GLN:CB	1:B:146:ALA:H	2.20	0.48
1:B:153:HIS:C	1:B:153:HIS:CD2	2.91	0.48
1:B:263:VAL:O	1:B:266:GLN:HB2	2.13	0.48
1:A:198:GLY:O	1:A:199:TYR:HD1	1.95	0.48
1:B:81:LEU:O	1:B:83:ALA:N	2.43	0.48
1:A:217:GLU:C	1:A:221:ILE:HD12	2.38	0.48
1:A:49:ASP:O	1:A:52:ALA:HB3	2.14	0.48
1:A:152:LEU:HG	1:A:155:GLN:OE1	2.13	0.48
1:B:45:ASP:CG	1:B:45:ASP:O	2.57	0.48
1:B:79:GLU:CA	1:B:147:VAL:HG21	2.40	0.48
1:B:139:VAL:HG22	1:B:140:ARG:H	1.78	0.48
1:B:145:GLN:O	1:B:200:GLU:OE1	2.30	0.48
1:B:152:LEU:HB2	1:B:192:TYR:CE1	2.48	0.48
1:B:250:GLU:O	1:B:251:MET:HB2	2.14	0.48
1:A:195:LEU:O	1:A:199:TYR:HB2	2.13	0.47
1:A:6:GLY:HA3	1:A:12:ALA:HB2	1.96	0.47
1:A:87:SER:HB2	1:A:197:MET:HB2	1.87	0.47
1:A:150:ASP:O	1:A:151:MET:C	2.57	0.47
1:B:247:ILE:HG23	1:B:248:HIS:N	2.27	0.47
1:A:238:GLN:O	1:A:239:SER:HB2	2.14	0.47
1:A:258:VAL:O	1:A:259:GLN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:HG22	1:A:101:GLY:N	2.30	0.47
1:A:235:ARG:HG2	1:A:236:THR:N	2.28	0.47
1:A:249:LEU:HA	1:A:253:ASP:OD2	2.15	0.47
1:A:274:ARG:HH11	1:A:274:ARG:CB	2.23	0.47
1:B:136:ARG:HD3	1:B:151:MET:HE1	1.95	0.47
1:A:11:ARG:CA	1:A:142:THR:HG21	2.44	0.47
1:A:73:PHE:O	1:A:73:PHE:HD2	1.94	0.47
1:B:92:GLY:C	1:B:95:LEU:HD23	2.40	0.47
1:B:129:ILE:HG12	1:B:158:VAL:HG11	1.95	0.47
1:B:225:TRP:CG	1:B:226:PRO:HD2	2.50	0.47
1:A:125:LEU:O	1:A:127:CYS:N	2.47	0.47
1:A:156:SER:CB	1:A:189:TYR:OH	2.63	0.47
1:A:267:VAL:O	1:A:270:ALA:N	2.47	0.47
1:B:66:PRO:O	1:B:74:GLY:HA2	2.15	0.47
1:A:113:ASP:N	1:A:114:PRO:CD	2.78	0.47
1:A:193:SER:C	1:A:195:LEU:N	2.72	0.47
1:A:77:LYS:O	1:A:78:ALA:C	2.58	0.46
1:A:229:SER:O	1:A:247:ILE:O	2.33	0.46
1:A:256:PRO:CA	1:A:257:LEU:HD23	2.45	0.46
1:A:262:MET:CA	1:A:265:ASP:HB3	2.41	0.46
1:A:60:VAL:O	1:A:64:LEU:HB2	2.15	0.46
1:A:67:ALA:HB3	1:A:69:ASP:OD1	2.15	0.46
1:A:78:ALA:O	1:A:79:GLU:C	2.56	0.46
1:A:234:LEU:O	1:A:235:ARG:O	2.33	0.46
1:A:76:GLY:HA2	1:A:78:ALA:HB3	1.97	0.46
1:B:177:ARG:HB2	1:B:181:LEU:HD22	1.98	0.46
1:A:16:ALA:C	1:A:148:ARG:HH22	2.13	0.46
1:A:243:ARG:C	1:A:244:PHE:CD2	2.88	0.46
1:B:139:VAL:HG22	1:B:140:ARG:N	2.30	0.46
1:B:154:TYR:HA	1:B:157:ASP:HB3	1.98	0.46
1:B:275:PHE:N	1:B:276:PRO:HA	2.31	0.46
1:A:18:ALA:HB2	1:A:138:VAL:HG21	1.97	0.46
1:B:11:ARG:NH2	1:B:239:SER:HA	2.16	0.46
1:B:139:VAL:CG1	1:B:140:ARG:N	2.60	0.46
1:B:209:ALA:C	1:B:236:THR:HB	2.34	0.46
1:B:245:ILE:CA	1:B:245:ILE:CG1	2.82	0.46
1:B:252:GLU:HB3	1:B:256:PRO:HD3	1.96	0.46
1:A:248:HIS:C	1:A:250:GLU:H	2.24	0.46
1:A:150:ASP:HB3	1:A:197:MET:HE2	1.98	0.46
1:A:23:LEU:CB	1:A:53:SER:CB	2.94	0.46
1:A:78:ALA:O	1:A:81:LEU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:CA	1:A:283:HIS:O	2.49	0.46
1:B:225:TRP:O	1:B:228:VAL:HG22	2.16	0.46
1:A:144:SER:O	1:A:145:GLN:C	2.59	0.46
1:A:208:ARG:C	1:A:210:LEU:N	2.74	0.46
1:B:213:GLU:H	1:B:215:ARG:CB	2.26	0.46
1:B:279:ASP:O	1:B:280:VAL:C	2.57	0.46
1:A:91:SER:HA	1:A:94:ALA:CB	2.44	0.46
1:A:243:ARG:HA	1:A:281:ILE:H	1.81	0.46
1:A:244:PHE:O	1:A:282:ILE:CG2	2.42	0.46
1:A:267:VAL:HG12	1:A:268:GLU:N	2.30	0.46
1:B:201:ALA:O	1:B:204:SER:HB2	2.16	0.46
1:A:23:LEU:HB3	1:A:53:SER:CB	2.46	0.45
1:A:230:GLY:O	1:A:246:GLN:HB3	2.13	0.45
1:B:154:TYR:O	1:B:158:VAL:N	2.47	0.45
1:B:236:THR:HA	1:B:241:PRO:O	2.16	0.45
1:A:66:PRO:O	1:A:67:ALA:CB	2.64	0.45
1:A:132:VAL:HG13	1:A:151:MET:HE3	1.98	0.45
1:A:136:ARG:O	1:A:139:VAL:CG1	2.63	0.45
1:A:248:HIS:O	1:A:253:ASP:CB	2.63	0.45
1:B:18:ALA:HB1	1:B:135:GLN:HG2	1.97	0.45
1:B:149:ALA:HB3	1:B:196:ARG:HH21	1.79	0.45
1:B:150:ASP:O	1:B:153:HIS:HB3	2.16	0.45
1:A:55:THR:O	1:A:59:VAL:HG23	2.16	0.45
1:A:219:ILE:HG23	1:A:220:ASP:H	1.81	0.45
1:A:245:ILE:HD13	1:A:283:HIS:CD2	2.42	0.45
1:B:156:SER:HB3	1:B:189:TYR:CE1	2.51	0.45
1:B:233:ASP:HB2	1:B:234:LEU:HD12	1.98	0.45
1:B:238:GLN:O	1:B:239:SER:HB2	2.16	0.45
1:A:142:THR:O	1:A:142:THR:CG2	2.63	0.45
1:A:152:LEU:CB	1:A:192:TYR:CZ	3.00	0.45
1:A:222:VAL:HG13	1:A:267:VAL:CG1	2.46	0.45
1:A:185:GLY:O	1:A:186:ILE:C	2.60	0.45
1:A:223:THR:O	1:A:223:THR:HG22	2.16	0.45
1:A:103:GLN:CA	1:A:108:PRO:HG3	2.47	0.45
1:A:153:HIS:HD2	1:A:157:ASP:HB2	1.81	0.45
1:A:233:ASP:HB2	1:A:234:LEU:HD12	1.98	0.45
1:B:152:LEU:HA	1:B:155:GLN:HB2	1.99	0.45
1:B:203:GLN:HA	1:B:205:LEU:O	2.16	0.45
1:A:73:PHE:CZ	1:A:74:GLY:CA	3.00	0.45
1:A:132:VAL:C	1:A:134:PHE:N	2.69	0.45
1:A:136:ARG:HD3	1:A:151:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HD2	1:A:234:LEU:HD23	1.98	0.45
1:A:272:LEU:C	1:A:274:ARG:N	2.74	0.45
1:B:23:LEU:HB2	1:B:53:SER:CB	2.46	0.45
1:B:59:VAL:HG11	1:B:82:ALA:CB	2.46	0.45
1:B:87:SER:HB3	1:B:197:MET:HB3	1.83	0.45
1:B:235:ARG:HG2	1:B:236:THR:H	1.81	0.45
1:B:261:HIS:C	1:B:263:VAL:N	2.52	0.45
1:B:268:GLU:OE2	1:B:282:ILE:HB	2.16	0.45
1:A:77:LYS:HZ2	1:A:206:LEU:CD2	2.30	0.45
1:A:253:ASP:HA	1:A:286:PRO:O	2.16	0.45
1:B:148:ARG:C	1:B:150:ASP:H	2.25	0.45
1:B:195:LEU:O	1:B:199:TYR:HB2	2.17	0.45
1:B:11:ARG:HG2	1:B:144:SER:HA	1.99	0.45
1:B:233:ASP:N	1:B:244:PHE:CD1	2.85	0.45
1:A:23:LEU:CB	1:A:53:SER:OG	2.62	0.45
1:A:68:ASP:O	1:A:70:ASN:N	2.49	0.45
1:A:185:GLY:O	1:A:189:TYR:HB2	2.17	0.45
1:A:238:GLN:O	1:A:238:GLN:HG3	2.17	0.45
1:B:55:THR:O	1:B:59:VAL:HG23	2.16	0.45
1:B:243:ARG:C	1:B:244:PHE:CD2	2.95	0.45
1:A:184:LEU:O	1:A:188:ILE:HG22	2.17	0.44
1:B:125:LEU:O	1:B:127:CYS:N	2.47	0.44
1:B:152:LEU:HB3	1:B:192:TYR:CZ	2.52	0.44
1:B:154:TYR:HA	1:B:157:ASP:CB	2.46	0.44
1:A:263:VAL:O	1:A:267:VAL:HG23	2.17	0.44
1:B:143:GLN:O	1:B:145:GLN:N	2.51	0.44
1:B:244:PHE:O	1:B:282:ILE:CD1	2.62	0.44
1:A:27:LYS:HZ2	1:A:30:ALA:HB3	1.80	0.44
1:A:149:ALA:CB	1:A:196:ARG:HH21	2.29	0.44
1:A:154:TYR:O	1:A:158:VAL:N	2.49	0.44
1:B:8:LEU:O	1:B:14:ILE:HG21	2.17	0.44
1:B:29:PHE:HA	1:B:31:TRP:CZ3	2.51	0.44
1:B:132:VAL:HG13	1:B:151:MET:HE3	1.99	0.44
1:B:258:VAL:HG12	1:B:258:VAL:O	2.17	0.44
1:A:55:THR:O	1:A:56:ASN:C	2.60	0.44
1:A:87:SER:C	1:A:193:SER:HB2	2.42	0.44
1:A:247:ILE:HG23	1:A:248:HIS:CD2	2.53	0.44
1:A:253:ASP:OD1	1:A:287:CYS:SG	2.66	0.44
1:B:64:LEU:HD13	1:B:64:LEU:HA	1.79	0.44
1:B:222:VAL:HG13	1:B:267:VAL:HG13	1.94	0.44
1:B:86:GLN:H	1:B:86:GLN:NE2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLN:CA	1:B:108:PRO:HG3	2.47	0.44
1:B:237:ARG:HG3	1:B:241:PRO:HB2	1.99	0.44
1:A:152:LEU:HA	1:A:155:GLN:HB2	2.00	0.44
1:A:188:ILE:O	1:A:188:ILE:CG2	2.66	0.44
1:A:197:MET:C	1:A:199:TYR:H	2.25	0.44
1:B:193:SER:C	1:B:195:LEU:H	2.26	0.44
1:A:54:LEU:O	1:A:55:THR:O	2.36	0.44
1:A:81:LEU:O	1:A:84:LEU:N	2.50	0.44
1:B:113:ASP:N	1:B:114:PRO:CD	2.80	0.44
1:B:144:SER:HG	1:B:148:ARG:H	1.61	0.44
1:B:236:THR:CG2	1:B:242:THR:HG23	2.47	0.44
1:B:18:ALA:C	1:B:20:ALA:N	2.75	0.44
1:A:66:PRO:O	1:A:67:ALA:HB2	2.18	0.44
1:A:128:THR:C	1:A:130:ILE:N	2.75	0.44
1:A:146:ALA:HB1	1:A:196:ARG:NH2	2.33	0.44
1:B:142:THR:O	1:B:142:THR:CG2	2.66	0.44
1:B:263:VAL:HG12	1:B:264:ALA:N	2.31	0.44
1:A:102:ILE:O	1:A:102:ILE:HG22	2.18	0.43
1:A:266:GLN:O	1:A:270:ALA:N	2.29	0.43
1:B:73:PHE:CZ	1:B:74:GLY:O	2.71	0.43
1:B:232:HIS:CD2	1:B:245:ILE:CD1	2.89	0.43
1:B:269:GLN:O	1:B:272:LEU:N	2.51	0.43
1:A:127:CYS:O	1:A:130:ILE:HG22	2.18	0.43
1:B:235:ARG:O	1:B:236:THR:HG23	2.17	0.43
1:B:263:VAL:O	1:B:267:VAL:HG23	2.17	0.43
1:A:13:ALA:C	1:A:16:ALA:H	2.25	0.43
1:A:23:LEU:CB	1:A:53:SER:HB2	2.45	0.43
1:A:213:GLU:O	1:A:217:GLU:N	2.51	0.43
1:A:156:SER:CB	1:A:189:TYR:CE1	3.01	0.43
1:A:216:GLN:HA	1:A:216:GLN:OE1	2.18	0.43
1:A:226:PRO:O	1:A:228:VAL:HG23	2.18	0.43
1:B:103:GLN:HA	1:B:108:PRO:HG3	2.00	0.43
1:B:245:ILE:HG23	1:B:285:ASP:CG	2.42	0.43
1:B:247:ILE:HG23	1:B:248:HIS:HB2	2.00	0.43
1:A:18:ALA:HB3	1:A:148:ARG:NE	2.34	0.43
1:A:193:SER:O	1:A:195:LEU:N	2.52	0.43
1:A:234:LEU:N	1:A:234:LEU:CD1	2.81	0.43
1:B:20:ALA:O	1:B:21:SER:CB	2.66	0.43
1:B:267:VAL:O	1:B:270:ALA:N	2.52	0.43
1:A:213:GLU:O	1:A:216:GLN:CA	2.66	0.43
1:A:268:GLU:O	1:A:271:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:SER:O	1:B:91:SER:O	2.36	0.43
1:B:248:HIS:HB2	1:B:252:GLU:CA	2.49	0.43
1:A:17:THR:O	1:A:18:ALA:O	2.37	0.43
1:A:103:GLN:HA	1:A:108:PRO:HG3	1.99	0.43
1:A:183:ALA:O	1:A:184:LEU:C	2.62	0.43
1:B:65:GLN:CB	1:B:66:PRO:HD2	2.41	0.43
1:B:188:ILE:O	1:B:188:ILE:CG2	2.66	0.43
1:A:79:GLU:O	1:A:80:SER:C	2.61	0.43
1:A:27:LYS:HZ3	1:A:30:ALA:HB3	1.84	0.43
1:A:44:VAL:C	1:A:46:SER:N	2.76	0.43
1:A:216:GLN:C	1:A:219:ILE:HG22	2.41	0.43
1:B:98:PHE:HD2	1:B:98:PHE:HA	1.71	0.43
1:B:184:LEU:O	1:B:188:ILE:HG22	2.19	0.43
1:B:245:ILE:CA	1:B:283:HIS:O	2.56	0.43
1:B:248:HIS:HB2	1:B:252:GLU:CB	2.49	0.43
1:A:137:TRP:CH2	1:A:141:ARG:CD	3.02	0.42
1:A:153:HIS:O	1:A:157:ASP:N	2.51	0.42
1:A:232:HIS:CE1	1:A:245:ILE:HG22	2.43	0.42
1:B:11:ARG:HD3	1:B:145:GLN:H	1.84	0.42
1:B:85:ALA:C	1:B:87:SER:N	2.77	0.42
1:B:152:LEU:HB2	1:B:192:TYR:CZ	2.53	0.42
1:B:161:ASN:O	1:B:165:LEU:HB3	2.19	0.42
1:B:202:VAL:HG23	1:B:203:GLN:NE2	2.34	0.42
1:A:18:ALA:N	1:A:148:ARG:CZ	2.82	0.42
1:A:279:ASP:O	1:A:281:ILE:HA	2.19	0.42
1:B:185:GLY:O	1:B:189:TYR:HB2	2.20	0.42
1:B:246:GLN:O	1:B:284:GLN:HA	2.18	0.42
1:A:125:LEU:HG	1:A:128:THR:HB	2.01	0.42
1:A:210:LEU:HA	1:A:211:PRO:HD2	1.63	0.42
1:A:242:THR:N	1:A:280:VAL:CG1	2.70	0.42
1:B:27:LYS:HD2	1:B:27:LYS:HA	1.66	0.42
1:B:73:PHE:CD1	1:B:74:GLY:N	2.87	0.42
1:B:245:ILE:HG12	1:B:245:ILE:H	1.83	0.42
1:A:60:VAL:C	1:A:62:TYR:N	2.78	0.42
1:B:259:GLN:C	1:B:261:HIS:N	2.76	0.42
1:A:137:TRP:CH2	1:A:141:ARG:HD2	2.54	0.42
1:A:156:SER:HA	1:A:159:MET:HB2	2.01	0.42
1:A:193:SER:HA	1:A:197:MET:HG2	2.02	0.42
1:A:243:ARG:HB3	1:A:281:ILE:HD12	2.01	0.42
1:B:196:ARG:HG2	1:B:197:MET:N	2.33	0.42
1:B:207:ASP:C	1:B:209:ALA:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:SER:C	1:B:280:VAL:H	2.24	0.42
1:A:15:ALA:C	1:A:148:ARG:NH2	2.78	0.42
1:A:77:LYS:O	1:A:80:SER:N	2.52	0.42
1:A:161:ASN:O	1:A:165:LEU:HB3	2.20	0.42
1:A:261:HIS:O	1:A:264:ALA:N	2.53	0.42
1:B:11:ARG:O	1:B:15:ALA:HB3	2.19	0.42
1:B:145:GLN:OE1	1:B:238:GLN:OE1	2.38	0.42
1:A:87:SER:O	1:A:88:MET:C	2.63	0.42
1:A:264:ALA:O	1:A:268:GLU:N	2.42	0.42
1:B:60:VAL:C	1:B:62:TYR:N	2.77	0.42
1:B:252:GLU:HB2	1:B:256:PRO:HG2	2.02	0.42
1:B:93:SER:C	1:B:95:LEU:H	2.26	0.42
1:B:130:ILE:HG13	1:B:131:LEU:HD12	2.02	0.42
1:B:252:GLU:CB	1:B:256:PRO:HG2	2.47	0.42
1:A:159:MET:HG3	1:A:161:ASN:ND2	2.33	0.41
1:A:216:GLN:O	1:A:219:ILE:HG23	2.17	0.41
1:B:11:ARG:N	1:B:142:THR:HG21	2.35	0.41
1:B:268:GLU:O	1:B:269:GLN:C	2.63	0.41
1:A:229:SER:O	1:A:248:HIS:HA	2.20	0.41
1:A:269:GLN:HG2	1:B:269:GLN:NE2	2.34	0.41
1:B:102:ILE:HG23	1:B:108:PRO:HD3	2.01	0.41
1:A:160:MET:HB3	1:A:163:ALA:HB3	2.00	0.41
1:A:222:VAL:HG13	1:A:267:VAL:HG11	2.02	0.41
1:A:272:LEU:HD13	1:A:273:ARG:N	2.35	0.41
1:B:209:ALA:HA	1:B:236:THR:C	2.46	0.41
1:B:285:ASP:HA	1:B:286:PRO:HD2	1.74	0.41
1:A:237:ARG:N	1:A:241:PRO:O	2.53	0.41
1:B:242:THR:O	1:B:280:VAL:HA	2.20	0.41
1:A:79:GLU:CA	1:A:147:VAL:HG21	2.46	0.41
1:A:129:ILE:HD13	1:A:129:ILE:HA	1.91	0.41
1:B:13:ALA:O	1:B:16:ALA:N	2.49	0.41
1:A:95:LEU:C	1:A:95:LEU:HD12	2.46	0.41
1:A:284:GLN:CG	1:A:284:GLN:O	2.68	0.41
1:B:84:LEU:HB2	1:B:201:ALA:HB1	2.01	0.41
1:B:144:SER:OG	1:B:148:ARG:N	2.31	0.41
1:A:64:LEU:HD13	1:A:64:LEU:HA	1.81	0.41
1:B:213:GLU:O	1:B:217:GLU:N	2.54	0.41
1:A:214:GLU:HA	1:A:217:GLU:HB2	2.03	0.41
1:A:218:ILE:O	1:A:219:ILE:C	2.61	0.41
1:A:250:GLU:HG2	1:A:251:MET:N	2.35	0.41
1:B:144:SER:HB3	1:B:148:ARG:HG3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLY:HA2	1:A:10:SER:N	2.32	0.41
1:A:55:THR:HG22	1:A:56:ASN:N	2.35	0.41
1:A:56:ASN:O	1:A:57:LEU:C	2.62	0.41
1:A:67:ALA:HA	1:A:75:HIS:CD2	2.55	0.41
1:A:83:ALA:CA	1:A:86:GLN:HG2	2.50	0.41
1:A:91:SER:O	1:A:92:GLY:C	2.62	0.41
1:A:102:ILE:HG23	1:A:108:PRO:HD3	2.03	0.41
1:A:153:HIS:CD2	1:A:153:HIS:C	2.98	0.41
1:A:248:HIS:HB2	1:A:252:GLU:CA	2.51	0.41
1:A:285:ASP:HA	1:A:286:PRO:HD2	1.69	0.41
1:B:23:LEU:CB	1:B:53:SER:CB	2.99	0.41
1:B:64:LEU:O	1:B:65:GLN:NE2	2.52	0.41
1:B:67:ALA:HB2	1:B:74:GLY:CA	2.51	0.41
1:B:245:ILE:HG21	1:B:285:ASP:OD2	2.17	0.41
1:A:177:ARG:HB2	1:A:181:LEU:HD22	2.03	0.41
1:A:212:ASP:HA	1:A:215:ARG:HB3	2.03	0.41
1:B:66:PRO:O	1:B:67:ALA:HB2	2.21	0.41
1:B:87:SER:CA	1:B:193:SER:HB2	2.51	0.41
1:B:128:THR:C	1:B:130:ILE:N	2.76	0.41
1:B:233:ASP:OD2	1:B:234:LEU:HD13	2.21	0.41
1:B:235:ARG:HH22	1:B:237:ARG:HD2	1.85	0.41
1:A:10:SER:C	1:A:12:ALA:N	2.71	0.40
1:A:45:ASP:O	1:A:45:ASP:CG	2.64	0.40
1:A:98:PHE:HD2	1:A:98:PHE:HA	1.72	0.40
1:A:229:SER:O	1:A:249:LEU:N	2.37	0.40
1:B:63:SER:C	1:B:64:LEU:HD22	2.47	0.40
1:B:127:CYS:O	1:B:130:ILE:HG22	2.21	0.40
1:B:215:ARG:O	1:B:216:GLN:C	2.64	0.40
1:A:120:VAL:O	1:A:120:VAL:HG12	2.21	0.40
1:A:120:VAL:HG13	1:A:122:ILE:HG12	2.04	0.40
1:B:68:ASP:O	1:B:71:HIS:N	2.54	0.40
1:B:159:MET:HG3	1:B:161:ASN:HD22	1.86	0.40
1:A:215:ARG:HB3	1:A:216:GLN:H	1.75	0.40
1:A:8:LEU:O	1:A:14:ILE:HG21	2.22	0.40
1:B:18:ALA:HB3	1:B:148:ARG:NE	2.37	0.40
1:A:212:ASP:O	1:A:213:GLU:CB	2.62	0.40
1:A:212:ASP:HA	1:A:215:ARG:CB	2.51	0.40
1:B:152:LEU:CB	1:B:192:TYR:CE1	3.05	0.40
1:B:217:GLU:C	1:B:221:ILE:HD12	2.46	0.40
1:B:243:ARG:HA	1:B:281:ILE:N	2.37	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:NE2	2:A:306:ZN:ZN[4_556]	1.49	0.71
1:A:68:ASP:N	2:A:303:ZN:ZN[4_556]	1.54	0.66
1:A:261:HIS:CE1	1:A:285:ASP:OD1[4_556]	1.56	0.64
1:A:261:HIS:ND1	1:A:285:ASP:OD1[4_556]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/300 (95%)	133 (47%)	76 (27%)	75 (26%)	0	0
1	B	284/300 (95%)	129 (45%)	76 (27%)	79 (28%)	0	0
All	All	568/600 (95%)	262 (46%)	152 (27%)	154 (27%)	0	0

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	21	SER
1	A	55	THR
1	A	67	ALA
1	A	69	ASP
1	A	78	ALA
1	A	86	GLN
1	A	93	SER
1	A	102	ILE
1	A	110	PRO
1	A	126	ILE
1	A	139	VAL
1	A	151	MET
1	A	207	ASP
1	A	209	ALA

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Mol	Chain	Res	Type
1	A	213	GLU
1	A	228	VAL
1	A	235	ARG
1	A	244	PHE
1	A	247	ILE
1	A	254	SER
1	A	260	ALA
1	A	273	ARG
1	A	276	PRO
1	B	18	ALA
1	B	21	SER
1	B	55	THR
1	B	67	ALA
1	B	69	ASP
1	B	78	ALA
1	B	86	GLN
1	B	102	ILE
1	B	110	PRO
1	B	126	ILE
1	B	139	VAL
1	B	149	ALA
1	B	151	MET
1	B	209	ALA
1	B	213	GLU
1	B	235	ARG
1	B	241	PRO
1	B	247	ILE
1	B	253	ASP
1	B	254	SER
1	B	255	LEU
1	B	260	ALA
1	B	273	ARG
1	B	276	PRO
1	B	278	SER
1	B	280	VAL
1	A	11	ARG
1	A	19	MET
1	A	34	THR
1	A	61	ARG
1	A	87	SER
1	A	90	ILE
1	A	106	ILE

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Mol	Chain	Res	Type
1	A	129	ILE
1	A	145	GLN
1	A	149	ALA
1	A	181	LEU
1	A	186	ILE
1	A	194	ALA
1	A	201	ALA
1	A	217	GLU
1	A	218	ILE
1	A	225	TRP
1	A	241	PRO
1	A	251	MET
1	A	259	GLN
1	A	262	MET
1	A	267	VAL
1	A	271	ILE
1	A	286	PRO
1	B	11	ARG
1	B	19	MET
1	B	34	THR
1	B	61	ARG
1	B	87	SER
1	B	90	ILE
1	B	93	SER
1	B	106	ILE
1	B	128	THR
1	B	155	GLN
1	B	181	LEU
1	B	186	ILE
1	B	194	ALA
1	B	207	ASP
1	B	216	GLN
1	B	217	GLU
1	B	225	TRP
1	B	228	VAL
1	B	230	GLY
1	B	244	PHE
1	B	245	ILE
1	B	251	MET
1	B	256	PRO
1	B	259	GLN
1	B	262	MET

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Mol	Chain	Res	Type
1	B	271	ILE
1	B	286	PRO
1	A	72	SER
1	A	77	LYS
1	A	82	ALA
1	A	107	SER
1	A	128	THR
1	A	146	ALA
1	A	155	GLN
1	A	216	GLN
1	A	230	GLY
1	A	278	SER
1	B	82	ALA
1	B	88	MET
1	B	107	SER
1	B	115	GLY
1	B	145	GLN
1	B	211	PRO
1	A	30	ALA
1	A	71	HIS
1	A	88	MET
1	A	115	GLY
1	A	133	SER
1	A	211	PRO
1	A	215	ARG
1	B	30	ALA
1	B	77	LYS
1	B	144	SER
1	B	212	ASP
1	B	215	ARG
1	B	261	HIS
1	A	62	TYR
1	A	74	GLY
1	A	272	LEU
1	A	275	PHE
1	B	63	SER
1	B	83	ALA
1	B	98	PHE
1	B	129	ILE
1	B	133	SER
1	B	146	ALA
1	B	249	LEU

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Mol	Chain	Res	Type
1	A	37	VAL
1	A	252	GLU
1	B	37	VAL
1	B	218	ILE
1	B	275	PHE
1	A	35	GLY
1	A	188	ILE
1	B	35	GLY
1	A	164	ILE
1	A	256	PRO
1	B	74	GLY
1	B	164	ILE
1	B	267	VAL

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	236/249 (95%)	156 (66%)	80 (34%)	0	1
1	B	236/249 (95%)	156 (66%)	80 (34%)	0	1
All	All	472/498 (95%)	312 (66%)	160 (34%)	0	1

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	LEU
1	A	9	VAL
1	A	14	ILE
1	A	17	THR
1	A	22	LEU
1	A	26	ILE
1	A	27	LYS
1	A	46	SER
1	A	48	VAL

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Mol	Chain	Res	Type
1	A	50	ILE
1	A	57	LEU
1	A	64	LEU
1	A	65	GLN
1	A	70	ASN
1	A	73	PHE
1	A	86	GLN
1	A	89	PHE
1	A	90	ILE
1	A	95	LEU
1	A	98	PHE
1	A	99	LEU
1	A	121	THR
1	A	123	VAL
1	A	128	THR
1	A	129	ILE
1	A	132	VAL
1	A	143	GLN
1	A	147	VAL
1	A	151	MET
1	A	153	HIS
1	A	159	MET
1	A	164	ILE
1	A	165	LEU
1	A	166	LEU
1	A	170	LEU
1	A	182	PHE
1	A	186	ILE
1	A	188	ILE
1	A	190	ILE
1	A	191	LEU
1	A	193	SER
1	A	199	TYR
1	A	202	VAL
1	A	203	GLN
1	A	206	LEU
1	A	210	LEU
1	A	212	ASP
1	A	216	GLN
1	A	218	ILE
1	A	219	ILE
1	A	220	ASP

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Mol	Chain	Res	Type
1	A	222	VAL
1	A	228	VAL
1	A	232	HIS
1	A	233	ASP
1	A	234	LEU
1	A	236	THR
1	A	238	GLN
1	A	241	PRO
1	A	245	ILE
1	A	246	GLN
1	A	247	ILE
1	A	252	GLU
1	A	257	LEU
1	A	258	VAL
1	A	262	MET
1	A	263	VAL
1	A	271	ILE
1	A	272	LEU
1	A	274	ARG
1	A	275	PHE
1	A	278	SER
1	A	280	VAL
1	A	281	ILE
1	A	282	ILE
1	A	283	HIS
1	A	284	GLN
1	A	288	SER
1	A	290	VAL
1	B	7	ARG
1	B	8	LEU
1	B	9	VAL
1	B	14	ILE
1	B	17	THR
1	B	22	LEU
1	B	26	ILE
1	B	27	LYS
1	B	31	TRP
1	B	46	SER
1	B	48	VAL
1	B	50	ILE
1	B	57	LEU
1	B	64	LEU

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Mol	Chain	Res	Type
1	B	65	GLN
1	B	70	ASN
1	B	73	PHE
1	B	86	GLN
1	B	89	PHE
1	B	90	ILE
1	B	95	LEU
1	B	98	PHE
1	B	99	LEU
1	B	121	THR
1	B	123	VAL
1	B	128	THR
1	B	129	ILE
1	B	132	VAL
1	B	143	GLN
1	B	147	VAL
1	B	151	MET
1	B	152	LEU
1	B	153	HIS
1	B	159	MET
1	B	164	ILE
1	B	165	LEU
1	B	166	LEU
1	B	170	LEU
1	B	182	PHE
1	B	186	ILE
1	B	188	ILE
1	B	190	ILE
1	B	191	LEU
1	B	193	SER
1	B	199	TYR
1	B	202	VAL
1	B	206	LEU
1	B	210	LEU
1	B	212	ASP
1	B	218	ILE
1	B	220	ASP
1	B	222	VAL
1	B	225	TRP
1	B	228	VAL
1	B	229	SER
1	B	232	HIS

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Mol	Chain	Res	Type
1	B	233	ASP
1	B	234	LEU
1	B	236	THR
1	B	237	ARG
1	B	241	PRO
1	B	242	THR
1	B	245	ILE
1	B	246	GLN
1	B	247	ILE
1	B	252	GLU
1	B	257	LEU
1	B	258	VAL
1	B	262	MET
1	B	263	VAL
1	B	271	ILE
1	B	272	LEU
1	B	274	ARG
1	B	275	PHE
1	B	278	SER
1	B	281	ILE
1	B	284	GLN
1	B	287	CYS
1	B	288	SER
1	B	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	70	ASN
1	A	75	HIS
1	A	86	GLN
1	A	135	GLN
1	A	145	GLN
1	A	153	HIS
1	A	161	ASN
1	A	203	GLN
1	A	232	HIS
1	A	248	HIS
1	A	261	HIS
1	A	266	GLN
1	A	283	HIS

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Mol	Chain	Res	Type
1	A	284	GLN
1	B	65	GLN
1	B	70	ASN
1	B	135	GLN
1	B	145	GLN
1	B	153	HIS
1	B	161	ASN
1	B	203	GLN
1	B	246	GLN
1	B	261	HIS
1	B	266	GLN
1	B	269	GLN
1	B	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	286/300 (95%)	1.08	49 (17%) 4 7	34, 112, 307, 364	0
1	B	286/300 (95%)	0.91	40 (13%) 6 9	48, 212, 575, 683	0
All	All	572/600 (95%)	1.00	89 (15%) 5 8	34, 151, 522, 683	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	GLY	10.5
1	A	249	LEU	7.3
1	A	250	GLU	6.5
1	B	184	LEU	6.4
1	A	10	SER	6.1
1	B	200	GLU	6.0
1	A	189	TYR	5.6
1	A	109	THR	5.5
1	B	249	LEU	5.0
1	B	194	ALA	4.9
1	A	175	TRP	4.4
1	A	106	ILE	4.3
1	B	252	GLU	4.1
1	A	279	ASP	4.0
1	A	135	GLN	3.9
1	A	140	ARG	3.7
1	B	250	GLU	3.5
1	A	252	GLU	3.5
1	A	30	ALA	3.5
1	A	33	TYR	3.4
1	A	178	ALA	3.3
1	B	279	ASP	3.2
1	B	117	GLY	3.2
1	B	142	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	23	LEU	3.1
1	B	251	MET	3.1
1	A	170	LEU	3.0
1	A	173	TYR	3.0
1	A	265	ASP	2.9
1	B	102	ILE	2.9
1	B	106	ILE	2.9
1	A	65	GLN	2.8
1	A	71	HIS	2.8
1	A	96	PHE	2.8
1	B	10	SER	2.8
1	A	22	LEU	2.7
1	B	233	ASP	2.7
1	B	158	VAL	2.7
1	A	176	HIS	2.6
1	B	135	GLN	2.6
1	B	123	VAL	2.6
1	A	67	ALA	2.6
1	A	161	ASN	2.6
1	A	9	VAL	2.6
1	A	123	VAL	2.6
1	B	71	HIS	2.6
1	B	118	VAL	2.5
1	B	34	THR	2.5
1	B	215	ARG	2.5
1	A	200	GLU	2.5
1	A	259	GLN	2.5
1	B	122	ILE	2.5
1	B	111	MET	2.5
1	B	41	ALA	2.5
1	A	28	ILE	2.4
1	A	276	PRO	2.4
1	B	17	THR	2.4
1	A	145	GLN	2.4
1	A	27	LYS	2.4
1	B	68	ASP	2.4
1	B	166	LEU	2.4
1	A	164	ILE	2.4
1	A	275	PHE	2.3
1	A	181	LEU	2.3
1	A	289	VAL	2.3
1	B	167	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	198	GLY	2.3
1	B	247	ILE	2.3
1	B	67	ALA	2.3
1	A	44	VAL	2.3
1	B	176	HIS	2.3
1	B	21	SER	2.3
1	B	138	VAL	2.3
1	A	6	GLY	2.2
1	B	168	LEU	2.2
1	A	88	MET	2.2
1	B	33	TYR	2.2
1	A	182	PHE	2.2
1	B	189	TYR	2.2
1	A	256	PRO	2.1
1	A	166	LEU	2.1
1	A	230	GLY	2.1
1	A	180	ALA	2.1
1	A	172	TRP	2.1
1	A	269	GLN	2.1
1	A	136	ARG	2.0
1	A	253	ASP	2.0
1	B	46	SER	2.0
1	B	163	ALA	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	307	1/1	0.94	0.08	109,109,109,109	0
2	ZN	B	305	1/1	0.95	0.04	77,77,77,77	0
2	ZN	B	301	1/1	0.96	0.04	25,25,25,25	0
2	ZN	A	303	1/1	0.96	0.03	26,26,26,26	0
2	ZN	A	306	1/1	0.97	0.04	28,28,28,28	0
2	ZN	A	302	1/1	0.97	0.05	28,28,28,28	0
2	ZN	B	304	1/1	0.99	0.06	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.