



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:54 PM UTC

PDB ID : 1TIM / pdb_00001tim
Title : STRUCTURE OF TRIOSE PHOSPHATE ISOMERASE FROM CHICKEN MUSCLE
Authors : Banner, D.W.; Bloomer, A.C.; Petsko, G.A.; Phillips, D.C.; Wilson, I.A.
Deposited on : 1976-09-01
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

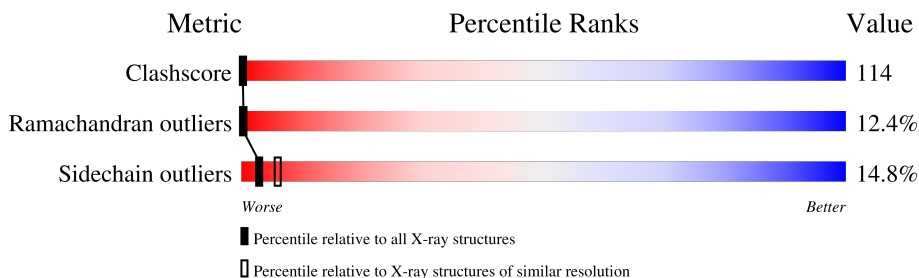
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3740 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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1870	1187	329	348	6			
1	B	247	Total	C	N	O	S	0	0	0
			1870	1187	329	348	6			

There are 16 discrepancies between the modelled and reference sequences:

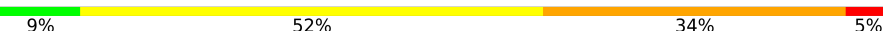
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	LYS	ASP	conflict	UNP P00940
A	18	ARG	LYS	conflict	UNP P00940
A	29	ASP	ASN	conflict	UNP P00940
A	145	GLN	GLU	conflict	UNP P00940
A	146	GLU	GLN	conflict	UNP P00940
A	194	THR	SER	conflict	UNP P00940
A	202	VAL	-	insertion	UNP P00940
A	?	-	THR	deletion	UNP P00940
B	17	LYS	ASP	conflict	UNP P00940
B	18	ARG	LYS	conflict	UNP P00940
B	29	ASP	ASN	conflict	UNP P00940
B	145	GLN	GLU	conflict	UNP P00940
B	146	GLU	GLN	conflict	UNP P00940
B	194	THR	SER	conflict	UNP P00940
B	202	VAL	-	insertion	UNP P00940
B	?	-	THR	deletion	UNP P00940

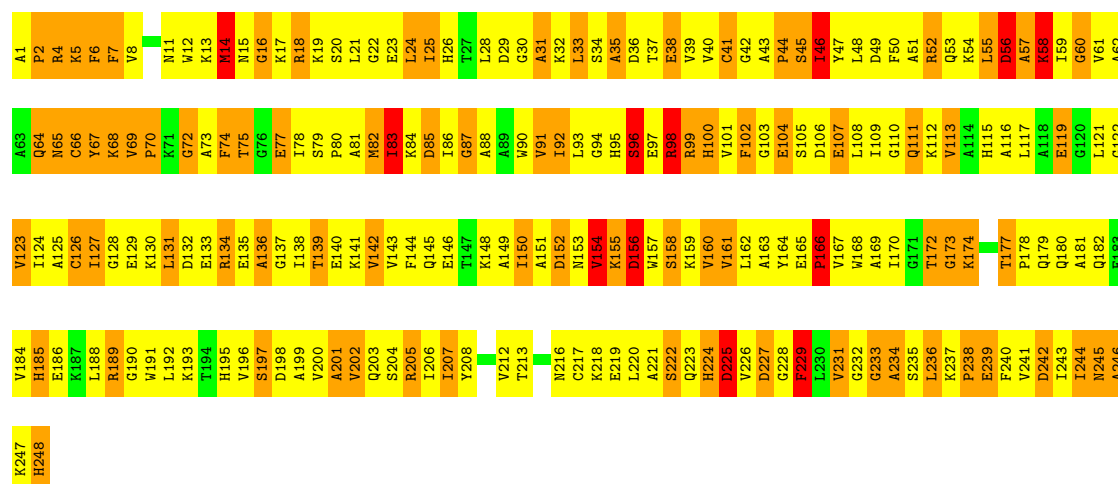
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

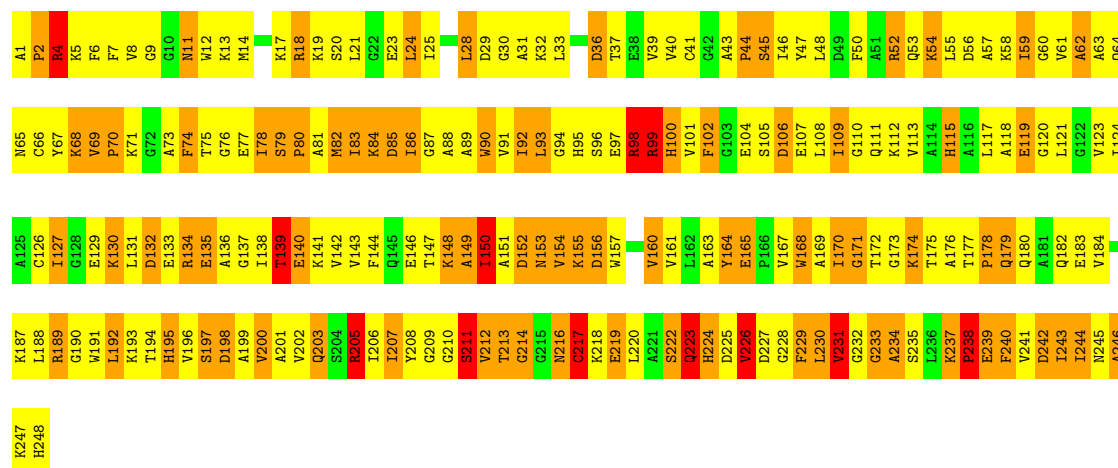
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.01Å 74.76Å 61.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3740	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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	1.25	10/1906 (0.5%)	1.92	54/2574 (2.1%)
1	B	1.33	9/1906 (0.5%)	2.21	100/2574 (3.9%)
All	All	1.29	19/3812 (0.5%)	2.07	154/5148 (3.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	ARG	NE-CZ	14.67	1.49	1.33
1	A	189	ARG	NE-CZ	13.06	1.47	1.33
1	A	52	ARG	NE-CZ	13.01	1.47	1.33
1	A	18	ARG	NE-CZ	12.99	1.47	1.33
1	B	99	ARG	NE-CZ	12.94	1.47	1.33
1	B	52	ARG	NE-CZ	12.92	1.47	1.33
1	A	4	ARG	NE-CZ	12.86	1.47	1.33
1	B	18	ARG	NE-CZ	12.79	1.47	1.33
1	A	99	ARG	NE-CZ	12.77	1.47	1.33
1	B	4	ARG	NE-CZ	12.76	1.47	1.33
1	B	98	ARG	NE-CZ	12.59	1.46	1.33
1	A	205	ARG	NE-CZ	12.53	1.46	1.33
1	B	189	ARG	NE-CZ	12.50	1.46	1.33
1	A	98	ARG	NE-CZ	12.38	1.46	1.33
1	B	205	ARG	NE-CZ	11.46	1.45	1.33
1	A	134	ARG	NE-CZ	10.53	1.44	1.33
1	B	98	ARG	C-N	-9.82	1.20	1.33
1	A	248	HIS	C-O	7.35	1.38	1.23
1	A	154	VAL	C-N	6.76	1.43	1.33

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	ARG	CD-NE-CZ	-10.84	109.23	124.40
1	B	217	CYS	N-CA-CB	-10.51	92.73	110.49
1	A	202	VAL	N-CA-C	10.39	120.19	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	PHE	CA-CB-CG	-10.31	103.49	113.80
1	A	189	ARG	CD-NE-CZ	-10.05	110.33	124.40
1	A	52	ARG	CD-NE-CZ	-9.86	110.60	124.40
1	A	18	ARG	CD-NE-CZ	-9.78	110.71	124.40
1	B	160	VAL	CA-C-N	9.78	135.95	123.14
1	B	160	VAL	C-N-CA	9.78	135.95	123.14
1	B	99	ARG	CD-NE-CZ	-9.78	110.71	124.40
1	B	74	PHE	CA-CB-CG	-9.74	104.06	113.80
1	A	106	ASP	CA-CB-CG	-9.67	102.93	112.60
1	B	231	VAL	N-CA-C	9.65	123.54	108.87
1	A	4	ARG	CD-NE-CZ	-9.60	110.96	124.40
1	B	178	PRO	N-CA-C	-9.57	99.93	113.81
1	B	52	ARG	CD-NE-CZ	-9.56	111.02	124.40
1	B	195	HIS	N-CA-C	9.41	121.14	111.07
1	B	203	GLN	N-CA-C	9.27	121.38	111.28
1	B	174	LYS	N-CA-CB	-9.04	97.23	110.87
1	B	4	ARG	CD-NE-CZ	-8.97	111.85	124.40
1	B	223	GLN	CB-CA-C	-8.96	92.60	110.42
1	B	156	ASP	CA-CB-CG	-8.88	103.72	112.60
1	A	101	VAL	N-CA-C	8.82	120.62	111.00
1	B	18	ARG	CD-NE-CZ	-8.80	112.08	124.40
1	B	246	ALA	N-CA-C	-8.51	101.02	112.26
1	B	98	ARG	CD-NE-CZ	-8.35	112.71	124.40
1	B	153	ASN	N-CA-C	-8.34	102.15	111.07
1	A	99	ARG	CD-NE-CZ	-8.33	112.74	124.40
1	B	229	PHE	N-CA-C	8.13	122.89	109.06
1	B	238	PRO	N-CA-CB	7.99	111.64	103.25
1	B	239	GLU	N-CA-C	-7.86	101.68	111.11
1	A	107	GLU	O-C-N	7.85	130.44	122.12
1	B	11	ASN	CA-CB-CG	-7.77	104.83	112.60
1	B	59	ILE	CA-C-N	7.76	127.72	120.34
1	B	59	ILE	C-N-CA	7.76	127.72	120.34
1	B	195	HIS	CA-CB-CG	-7.73	106.07	113.80
1	A	160	VAL	N-CA-C	7.65	119.86	108.46
1	A	179	GLN	N-CA-C	7.64	119.30	110.97
1	B	192	LEU	CA-C-N	7.42	131.95	120.82
1	B	192	LEU	C-N-CA	7.42	131.95	120.82
1	B	127	ILE	N-CA-CB	7.35	121.24	111.25
1	A	7	PHE	N-CA-C	7.34	120.38	108.41
1	B	2	PRO	N-CA-C	-7.32	97.39	112.47
1	B	207	ILE	CA-CB-CG2	7.29	122.89	110.50
1	A	205	ARG	CD-NE-CZ	-7.05	114.53	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	GLN	CB-CG-CD	6.95	124.41	112.60
1	B	61	VAL	N-CA-C	6.94	118.72	108.45
1	A	100	HIS	N-CA-C	6.90	118.59	111.14
1	B	152	ASP	CA-C-O	6.88	127.78	120.70
1	B	54	LYS	N-CA-C	6.78	125.25	110.80
1	B	237	LYS	CA-C-N	6.73	128.25	119.84
1	B	237	LYS	C-N-CA	6.73	128.25	119.84
1	B	102	PHE	N-CA-C	-6.71	96.50	110.80
1	A	236	LEU	N-CA-C	6.71	120.56	112.38
1	A	98	ARG	CD-NE-CZ	-6.64	115.10	124.40
1	A	201	ALA	O-C-N	6.64	129.75	122.11
1	B	148	LYS	CB-CA-C	-6.58	100.45	110.92
1	A	72	GLY	CA-C-N	6.56	132.84	122.34
1	A	72	GLY	C-N-CA	6.56	132.84	122.34
1	A	100	HIS	CA-CB-CG	-6.48	107.32	113.80
1	A	46	ILE	N-CA-C	6.43	116.92	110.23
1	A	96	SER	CA-C-N	6.36	129.62	120.79
1	A	96	SER	C-N-CA	6.36	129.62	120.79
1	A	36	ASP	N-CA-C	-6.34	102.67	111.81
1	B	127	ILE	CA-C-N	-6.34	115.44	121.46
1	B	127	ILE	C-N-CA	-6.34	115.44	121.46
1	A	67	TYR	CA-CB-CG	-6.33	102.50	113.90
1	B	224	HIS	N-CA-C	6.30	124.22	110.80
1	B	62	ALA	N-CA-C	6.29	119.26	109.52
1	A	177	THR	N-CA-C	6.26	118.75	110.36
1	B	244	ILE	CA-C-N	-6.21	112.87	122.49
1	B	244	ILE	C-N-CA	-6.21	112.87	122.49
1	A	139	THR	O-C-N	6.20	128.71	122.08
1	B	90	TRP	N-CA-C	6.15	118.97	109.07
1	A	123	VAL	N-CA-CB	6.11	122.01	111.39
1	B	226	VAL	N-CA-C	6.10	116.71	108.17
1	A	68	LYS	N-CA-C	-6.09	102.92	110.41
1	B	216	ASN	N-CA-C	-6.09	106.49	114.04
1	A	15	ASN	CA-CB-CG	-6.09	106.51	112.60
1	A	122	GLY	CA-C-N	-6.04	114.72	123.06
1	A	122	GLY	C-N-CA	-6.04	114.72	123.06
1	B	139	THR	CB-CA-C	-6.04	100.82	110.84
1	B	153	ASN	CA-C-N	5.98	132.73	121.97
1	B	153	ASN	C-N-CA	5.98	132.73	121.97
1	B	149	ALA	N-CA-C	-5.97	101.57	111.37
1	A	136	ALA	N-CA-C	-5.93	104.63	112.34
1	A	213	THR	CB-CA-C	-5.92	100.20	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	LEU	N-CA-C	-5.91	97.09	107.73
1	B	214	GLY	N-CA-C	5.89	120.01	112.83
1	A	14	MET	N-CA-C	-5.87	100.78	109.11
1	B	179	GLN	CB-CA-C	-5.87	101.93	110.96
1	B	156	ASP	N-CA-CB	5.83	119.06	110.49
1	B	50	PHE	N-CA-C	-5.80	104.15	111.11
1	B	198	ASP	CA-CB-CG	-5.75	106.85	112.60
1	B	82	MET	N-CA-C	-5.73	104.03	111.02
1	A	166	PRO	CA-N-CD	-5.72	103.99	112.00
1	A	213	THR	O-C-N	5.69	130.29	122.72
1	B	80	PRO	CB-CA-C	-5.68	103.59	113.20
1	B	202	VAL	N-CA-C	5.67	115.80	110.30
1	B	242	ASP	N-CA-C	-5.67	102.07	111.37
1	B	160	VAL	O-C-N	5.67	128.86	123.03
1	B	127	ILE	CB-CA-C	5.64	119.24	110.83
1	B	100	HIS	CA-CB-CG	-5.64	108.16	113.80
1	B	150	ILE	CA-C-N	5.62	132.28	121.54
1	B	150	ILE	C-N-CA	5.62	132.28	121.54
1	A	134	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	B	134	ARG	O-C-N	5.56	128.51	122.11
1	B	30	GLY	N-CA-C	-5.55	107.45	114.16
1	B	39	VAL	N-CA-C	5.53	115.91	108.17
1	B	84	LYS	CB-CA-C	-5.52	102.22	110.88
1	B	189	ARG	CD-NE-CZ	-5.51	116.68	124.40
1	B	86	ILE	N-CA-C	-5.50	105.01	110.62
1	B	161	VAL	N-CA-C	5.50	115.80	108.11
1	A	165	GLU	N-CA-C	5.48	118.30	109.15
1	B	69	VAL	O-C-N	5.47	125.14	121.69
1	A	229	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	72	GLY	O-C-N	5.42	129.23	123.81
1	A	83	ILE	O-C-N	5.41	127.19	121.89
1	B	115	HIS	CB-CA-C	-5.41	101.48	110.68
1	B	173	GLY	N-CA-C	-5.39	106.60	114.90
1	A	56	ASP	N-CA-C	5.32	117.75	108.76
1	A	166	PRO	N-CA-C	-5.31	101.52	112.47
1	B	226	VAL	N-CA-CB	-5.29	104.06	111.25
1	B	161	VAL	CA-CB-CG1	5.27	119.36	110.40
1	B	137	GLY	N-CA-C	-5.26	107.38	116.01
1	A	102	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	164	TYR	CA-CB-CG	-5.25	104.45	113.90
1	A	126	CYS	CA-C-N	5.24	130.00	123.14
1	A	126	CYS	C-N-CA	5.24	130.00	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	VAL	N-CA-CB	-5.23	102.60	111.23
1	B	237	LYS	O-C-N	5.22	125.79	121.35
1	B	156	ASP	CB-CG-OD2	-5.21	106.42	118.40
1	A	83	ILE	CB-CA-C	-5.18	105.25	112.04
1	A	60	GLY	N-CA-C	-5.18	105.12	112.37
1	B	80	PRO	O-C-N	5.15	127.74	122.18
1	B	36	ASP	N-CA-C	-5.14	107.01	113.28
1	B	139	THR	N-CA-CB	-5.14	100.99	109.72
1	B	222	SER	N-CA-C	-5.12	105.70	111.28
1	B	235	SER	N-CA-C	5.11	120.42	113.37
1	B	205	ARG	N-CA-C	5.10	117.07	108.96
1	A	111	GLN	CB-CA-C	5.09	118.88	110.88
1	A	53	GLN	N-CA-C	5.09	117.49	111.33
1	B	2	PRO	O-C-N	5.09	129.51	122.64
1	A	207	ILE	N-CA-C	5.08	116.61	108.89
1	B	154	VAL	CB-CA-C	-5.06	102.99	111.29
1	B	231	VAL	N-CA-CB	-5.06	103.58	110.56
1	B	208	TYR	N-CA-CB	-5.03	102.15	109.95
1	B	93	LEU	CA-C-N	5.03	129.87	120.87
1	B	93	LEU	C-N-CA	5.03	129.87	120.87
1	B	124	ILE	CA-C-N	-5.03	116.07	123.00
1	B	124	ILE	C-N-CA	-5.03	116.07	123.00
1	A	119	GLU	N-CA-C	5.01	118.54	112.93
1	B	154	VAL	N-CA-CB	-5.01	102.97	111.23
1	B	165	GLU	N-CA-C	5.01	117.51	109.15

There are no chirality outliers.

There are no planarity outliers.

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	1870	0	1887	492	2
1	B	1870	0	1887	427	2
All	All	3740	0	3774	859	2

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 114.

All (859) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:C	1:B:46:ILE:HG22	1.44	1.42
1:A:46:ILE:CG2	1:B:45:SER:O	1.76	1.32
1:A:45:SER:O	1:A:48:LEU:HB2	1.16	1.28
1:B:129:GLU:OE1	1:B:134:ARG:HB2	1.32	1.27
1:A:189:ARG:NE	1:A:225:ASP:OD2	1.67	1.27
1:A:45:SER:O	1:B:46:ILE:HG22	1.36	1.23
1:A:45:SER:O	1:A:48:LEU:CB	1.89	1.19
1:A:14:MET:HE1	1:B:69:VAL:HG23	1.22	1.17
1:A:231:VAL:HG12	1:A:235:SER:HB3	1.16	1.15
1:A:45:SER:HB2	1:B:45:SER:HB2	1.17	1.15
1:B:67:TYR:HD2	1:B:69:VAL:HG22	0.99	1.14
1:B:237:LYS:HB3	1:B:238:PRO:HD2	1.20	1.14
1:B:164:TYR:CE1	1:B:184:VAL:HG11	1.83	1.13
1:B:67:TYR:CD2	1:B:69:VAL:HG22	1.85	1.10
1:A:47:TYR:CE1	1:B:82:MET:HE2	1.87	1.10
1:A:154:VAL:HG12	1:A:155:LYS:N	1.66	1.10
1:A:231:VAL:CG1	1:A:235:SER:HB3	1.82	1.09
1:A:151:ALA:O	1:A:154:VAL:HB	1.49	1.08
1:B:83:ILE:HG23	1:B:88:ALA:HB3	1.31	1.08
1:B:164:TYR:CD1	1:B:184:VAL:HG11	1.87	1.08
1:B:98:ARG:NH2	1:B:102:PHE:CE2	2.20	1.08
1:A:154:VAL:CG1	1:A:155:LYS:H	1.67	1.08
1:B:66:CYS:SG	1:B:91:VAL:HG21	1.94	1.08
1:B:220:LEU:O	1:B:223:GLN:HB2	1.52	1.07
1:A:66:CYS:HB2	1:A:91:VAL:HG11	1.31	1.07
1:A:83:ILE:O	1:A:86:ILE:HG22	1.52	1.06
1:B:5:LYS:HB2	1:B:36:ASP:O	1.51	1.06
1:A:12:TRP:CE3	1:A:43:ALA:HB2	1.91	1.06
1:A:138:ILE:CG2	1:A:141:LYS:HB2	1.86	1.05
1:A:150:ILE:O	1:A:154:VAL:HG23	1.53	1.05
1:B:25:ILE:HG12	1:B:55:LEU:HD21	1.36	1.05
1:B:43:ALA:HB1	1:B:44:PRO:HD2	1.40	1.04
1:B:196:VAL:HG12	1:B:200:VAL:HG21	1.36	1.03
1:A:46:ILE:HG23	1:B:45:SER:O	0.86	1.03
1:B:164:TYR:CE1	1:B:184:VAL:CG1	2.42	1.03
1:A:77:GLU:HG2	1:B:98:ARG:NH2	1.71	1.03
1:B:113:VAL:O	1:B:117:LEU:HG	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HG11	1:A:200:VAL:HG11	1.39	1.02
1:B:148:LYS:HA	1:B:191:TRP:HH2	1.23	1.02
1:B:222:SER:O	1:B:224:HIS:N	1.91	1.02
1:B:113:VAL:HG13	1:B:123:VAL:HG11	1.42	1.02
1:B:12:TRP:CZ2	1:B:41:CYS:HB2	1.95	1.01
1:A:92:ILE:HD12	1:A:93:LEU:N	1.74	1.01
1:B:167:VAL:C	1:B:169:ALA:H	1.60	1.01
1:B:164:TYR:CD1	1:B:184:VAL:CG1	2.44	1.01
1:A:66:CYS:CB	1:A:91:VAL:HG11	1.91	1.00
1:B:7:PHE:HD2	1:B:205:ARG:NH1	1.59	1.00
1:B:5:LYS:H	1:B:5:LYS:HD3	1.23	1.00
1:B:109:ILE:O	1:B:113:VAL:HG23	1.62	0.99
1:A:77:GLU:HG2	1:B:98:ARG:HH21	1.22	0.98
1:A:74:PHE:HD2	1:B:14:MET:HE3	1.27	0.98
1:A:129:GLU:OE1	1:A:139:THR:HG22	1.63	0.97
1:A:66:CYS:HB2	1:A:91:VAL:CG1	1.94	0.97
1:A:6:PHE:CZ	1:A:229:PHE:HE2	1.81	0.97
1:A:45:SER:C	1:B:46:ILE:CG2	2.36	0.97
1:A:46:ILE:HA	1:B:46:ILE:HA	1.45	0.97
1:B:196:VAL:CG1	1:B:200:VAL:HG21	1.95	0.96
1:A:64:GLN:OE1	1:B:76:GLY:N	1.97	0.96
1:A:46:ILE:HG23	1:B:45:SER:C	1.90	0.96
1:B:7:PHE:CD2	1:B:205:ARG:NH1	2.34	0.96
1:B:138:ILE:HD11	1:B:141:LYS:HD2	1.49	0.95
1:A:138:ILE:HG22	1:A:141:LYS:HB2	1.47	0.94
1:B:100:HIS:O	1:B:100:HIS:CD2	2.19	0.94
1:B:148:LYS:HA	1:B:191:TRP:CH2	2.00	0.94
1:A:49:ASP:CG	1:A:86:ILE:HD11	1.93	0.94
1:A:33:LEU:HB3	1:A:245:ASN:HD21	1.33	0.94
1:B:167:VAL:O	1:B:169:ALA:N	2.00	0.93
1:A:164:TYR:CE1	1:A:184:VAL:HG11	2.04	0.93
1:B:193:LYS:HE3	1:B:198:ASP:OD1	1.68	0.93
1:A:62:ALA:HB2	1:A:90:TRP:HB2	1.49	0.93
1:A:4:ARG:HD2	1:A:227:ASP:OD2	1.69	0.92
1:A:14:MET:HE1	1:B:69:VAL:CG2	2.00	0.92
1:A:115:HIS:NE2	1:A:119:GLU:OE1	2.03	0.92
1:A:12:TRP:HE3	1:A:43:ALA:HB2	1.33	0.92
1:A:33:LEU:HD22	1:A:33:LEU:H	1.32	0.92
1:A:154:VAL:HG12	1:A:155:LYS:H	1.25	0.92
1:B:150:ILE:O	1:B:154:VAL:HG23	1.69	0.92
1:A:151:ALA:HA	1:A:154:VAL:HG21	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HA	1:A:201:ALA:HB2	1.51	0.91
1:A:2:PRO:O	1:A:4:ARG:HB2	1.70	0.91
1:B:33:LEU:HD22	1:B:244:ILE:HG21	1.52	0.91
1:A:79:SER:O	1:A:82:MET:HG3	1.68	0.91
1:B:240:PHE:O	1:B:244:ILE:HG12	1.69	0.91
1:A:81:ALA:O	1:A:84:LYS:HB3	1.71	0.91
1:A:91:VAL:HG21	1:A:121:LEU:HD13	1.51	0.91
1:B:167:VAL:C	1:B:169:ALA:N	2.26	0.91
1:B:237:LYS:HB3	1:B:238:PRO:CD	2.00	0.91
1:A:32:LYS:O	1:A:33:LEU:C	2.14	0.90
1:A:92:ILE:HD12	1:A:92:ILE:C	1.95	0.90
1:A:154:VAL:CG1	1:A:155:LYS:N	2.27	0.90
1:A:62:ALA:HB2	1:A:90:TRP:CB	2.02	0.90
1:A:48:LEU:HD11	1:A:83:ILE:HG22	1.55	0.89
1:B:223:GLN:O	1:B:224:HIS:HB3	1.73	0.89
1:A:56:ASP:OD1	1:A:56:ASP:N	2.05	0.89
1:A:231:VAL:HG12	1:A:235:SER:CB	2.00	0.89
1:A:80:PRO:HB3	1:A:121:LEU:HD11	1.53	0.89
1:A:45:SER:CB	1:B:45:SER:HB2	2.03	0.89
1:B:148:LYS:HG2	1:B:149:ALA:N	1.86	0.89
1:B:5:LYS:HD3	1:B:5:LYS:N	1.85	0.88
1:B:237:LYS:CB	1:B:238:PRO:HD2	2.04	0.88
1:B:25:ILE:HG23	1:B:55:LEU:HD23	1.54	0.87
1:A:237:LYS:C	1:A:239:GLU:H	1.78	0.87
1:B:6:PHE:CE2	1:B:228:GLY:HA2	2.09	0.87
1:A:157:TRP:C	1:A:159:LYS:H	1.83	0.87
1:B:14:MET:CG	1:B:14:MET:O	2.21	0.86
1:B:216:ASN:O	1:B:219:GLU:HG2	1.75	0.86
1:A:66:CYS:H	1:A:93:LEU:CD2	1.87	0.86
1:A:151:ALA:HA	1:A:154:VAL:CG2	2.06	0.86
1:A:77:GLU:HG3	1:B:102:PHE:CZ	2.10	0.86
1:B:25:ILE:HG12	1:B:55:LEU:CD2	2.05	0.86
1:B:149:ALA:O	1:B:153:ASN:ND2	2.08	0.85
1:A:6:PHE:CZ	1:A:229:PHE:CE2	2.63	0.85
1:A:131:LEU:C	1:A:131:LEU:HD23	2.01	0.85
1:A:232:GLY:O	1:A:233:GLY:C	2.19	0.85
1:A:62:ALA:CB	1:A:90:TRP:HB2	2.05	0.85
1:A:217:CYS:SG	1:A:218:LYS:N	2.48	0.84
1:A:80:PRO:CB	1:A:121:LEU:HD11	2.06	0.84
1:A:157:TRP:HB2	1:A:203:GLN:NE2	1.92	0.84
1:A:182:GLN:OE1	1:A:186:GLU:OE2	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PHE:CD2	1:B:14:MET:HE3	2.13	0.83
1:A:172:THR:HG22	1:A:172:THR:O	1.78	0.83
1:A:82:MET:CE	1:B:14:MET:HB2	2.09	0.83
1:B:148:LYS:CA	1:B:191:TRP:CH2	2.62	0.83
1:B:167:VAL:O	1:B:170:ILE:N	2.12	0.83
1:A:109:ILE:O	1:A:113:VAL:HG23	1.79	0.82
1:B:1:ALA:HB1	1:B:2:PRO:CD	2.09	0.82
1:B:66:CYS:SG	1:B:91:VAL:CG2	2.66	0.82
1:B:196:VAL:O	1:B:197:SER:HB3	1.80	0.82
1:A:66:CYS:H	1:A:93:LEU:HD21	1.44	0.82
1:B:98:ARG:NH2	1:B:102:PHE:CD2	2.47	0.82
1:B:84:LYS:NZ	1:B:119:GLU:HB3	1.94	0.82
1:B:4:ARG:HD3	1:B:227:ASP:CG	2.06	0.81
1:A:164:TYR:CZ	1:A:184:VAL:HG11	2.14	0.81
1:B:177:THR:OG1	1:B:180:GLN:OE1	1.97	0.81
1:A:66:CYS:HB3	1:A:93:LEU:HD21	1.62	0.81
1:A:69:VAL:HG13	1:A:70:PRO:HD2	1.61	0.81
1:A:157:TRP:O	1:A:159:LYS:N	2.13	0.81
1:A:4:ARG:CD	1:A:227:ASP:OD2	2.28	0.81
1:A:45:SER:HB3	1:B:46:ILE:HG23	1.62	0.81
1:A:83:ILE:HB	1:A:88:ALA:HB3	1.61	0.81
1:B:83:ILE:HG23	1:B:88:ALA:CB	2.11	0.81
1:A:21:LEU:O	1:A:25:ILE:HG12	1.81	0.81
1:A:45:SER:O	1:B:46:ILE:CG2	2.25	0.81
1:A:191:TRP:CZ3	1:A:195:HIS:HB2	2.14	0.81
1:B:138:ILE:HD11	1:B:141:LYS:CD	2.11	0.80
1:B:110:GLY:CA	1:B:153:ASN:CG	2.55	0.80
1:B:129:GLU:OE1	1:B:134:ARG:CB	2.24	0.80
1:B:217:CYS:SG	1:B:243:ILE:HG23	2.22	0.79
1:B:138:ILE:HG13	1:B:141:LYS:HD3	1.62	0.79
1:A:237:LYS:O	1:A:239:GLU:N	2.16	0.79
1:B:17:LYS:HE3	1:B:19:LYS:HB2	1.64	0.79
1:A:49:ASP:CB	1:A:86:ILE:HD11	2.13	0.78
1:A:64:GLN:HB2	1:B:75:THR:HG23	1.64	0.78
1:B:164:TYR:CZ	1:B:184:VAL:HG11	2.16	0.78
1:A:32:LYS:O	1:A:33:LEU:O	2.02	0.78
1:A:79:SER:H	1:A:82:MET:HE3	1.49	0.78
1:A:48:LEU:HD11	1:A:83:ILE:CG2	2.13	0.78
1:A:131:LEU:HD23	1:A:132:ASP:N	1.99	0.78
1:A:247:LYS:O	1:A:248:HIS:O	2.02	0.78
1:A:134:ARG:O	1:A:137:GLY:HA2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE1	1:A:139:THR:CG2	2.31	0.77
1:A:221:ALA:C	1:A:223:GLN:H	1.90	0.77
1:A:212:VAL:HB	1:A:231:VAL:HG23	1.66	0.77
1:A:77:GLU:CG	1:B:98:ARG:NH2	2.47	0.77
1:B:85:ASP:C	1:B:85:ASP:OD1	2.27	0.77
1:B:110:GLY:HA3	1:B:153:ASN:CG	2.09	0.77
1:B:12:TRP:CZ2	1:B:41:CYS:CB	2.67	0.77
1:B:168:TRP:CH2	1:B:176:ALA:HA	2.19	0.77
1:B:190:GLY:O	1:B:193:LYS:HB3	1.84	0.77
1:A:75:THR:HG23	1:B:64:GLN:HB3	1.65	0.77
1:B:139:THR:O	1:B:142:VAL:HG22	1.83	0.77
1:A:151:ALA:O	1:A:154:VAL:CB	2.32	0.76
1:A:12:TRP:CZ2	1:A:41:CYS:SG	2.78	0.76
1:A:191:TRP:CD2	1:A:195:HIS:ND1	2.54	0.76
1:B:6:PHE:CZ	1:B:229:PHE:CE2	2.73	0.76
1:A:1:ALA:HB3	1:A:2:PRO:HD3	1.68	0.76
1:A:237:LYS:HB3	1:A:238:PRO:HD2	1.68	0.75
1:B:100:HIS:CD2	1:B:100:HIS:C	2.64	0.75
1:A:64:GLN:HB2	1:B:75:THR:CG2	2.15	0.75
1:A:29:ASP:OD1	1:A:56:ASP:OD1	2.04	0.75
1:A:52:ARG:HG2	1:A:87:GLY:HA3	1.69	0.75
1:A:62:ALA:CB	1:A:90:TRP:CB	2.64	0.75
1:B:36:ASP:O	1:B:36:ASP:OD2	2.04	0.75
1:B:117:LEU:HD23	1:B:123:VAL:HG23	1.68	0.75
1:A:47:TYR:CE1	1:B:82:MET:CE	2.68	0.75
1:A:203:GLN:HG3	1:A:204:SER:N	2.01	0.75
1:A:138:ILE:HG23	1:A:141:LYS:HB2	1.67	0.75
1:B:6:PHE:HB3	1:B:37:THR:HG23	1.67	0.75
1:B:14:MET:O	1:B:14:MET:HG2	1.87	0.75
1:A:42:GLY:CA	1:A:62:ALA:O	2.35	0.75
1:A:108:LEU:HG	1:A:112:LYS:HE2	1.69	0.75
1:B:119:GLU:HA	1:B:119:GLU:OE1	1.88	0.74
1:B:138:ILE:CG1	1:B:141:LYS:HD3	2.16	0.74
1:A:48:LEU:HD13	1:B:46:ILE:HG21	1.68	0.74
1:A:196:VAL:CG1	1:A:200:VAL:HG21	2.18	0.74
1:A:220:LEU:O	1:A:223:GLN:CB	2.35	0.74
1:A:80:PRO:HB3	1:A:121:LEU:CD1	2.17	0.74
1:A:45:SER:CA	1:B:46:ILE:HG22	2.16	0.74
1:A:115:HIS:CE1	1:A:119:GLU:OE1	2.41	0.74
1:B:139:THR:HG22	1:B:140:GLU:N	2.01	0.74
1:A:103:GLY:O	1:A:104:GLU:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:O	1:A:170:ILE:HG23	1.87	0.73
1:B:127:ILE:HG23	1:B:150:ILE:HD11	1.70	0.73
1:B:164:TYR:CE1	1:B:184:VAL:HG13	2.23	0.73
1:A:90:TRP:O	1:A:91:VAL:HG23	1.87	0.73
1:B:110:GLY:HA3	1:B:153:ASN:OD1	1.88	0.73
1:A:93:LEU:HD13	1:A:112:LYS:HB3	1.69	0.73
1:A:231:VAL:CG1	1:A:235:SER:CB	2.63	0.73
1:B:177:THR:HG1	1:B:180:GLN:CD	1.96	0.73
1:A:24:LEU:HD13	1:A:28:LEU:HD23	1.69	0.73
1:A:64:GLN:CB	1:B:75:THR:HG23	2.19	0.73
1:A:82:MET:HB3	1:B:46:ILE:HD11	1.71	0.73
1:A:237:LYS:C	1:A:239:GLU:N	2.41	0.73
1:B:93:LEU:HD22	1:B:112:LYS:HD2	1.69	0.72
1:A:42:GLY:HA2	1:A:62:ALA:O	1.88	0.72
1:B:28:LEU:O	1:B:31:ALA:HB3	1.88	0.72
1:B:67:TYR:HB2	1:B:77:GLU:OE2	1.89	0.72
1:A:172:THR:O	1:A:172:THR:CG2	2.36	0.72
1:A:221:ALA:C	1:A:223:GLN:N	2.45	0.72
1:A:41:CYS:O	1:A:61:VAL:HA	1.88	0.72
1:A:166:PRO:HD2	1:A:166:PRO:O	1.87	0.72
1:A:192:LEU:HD23	1:A:201:ALA:HA	1.70	0.72
1:A:221:ALA:O	1:A:223:GLN:N	2.22	0.72
1:A:196:VAL:HG12	1:A:200:VAL:HG21	1.72	0.71
1:B:115:HIS:O	1:B:118:ALA:HB3	1.90	0.71
1:B:222:SER:C	1:B:224:HIS:H	1.98	0.71
1:A:154:VAL:HG13	1:A:155:LYS:H	1.54	0.71
1:B:7:PHE:HB2	1:B:205:ARG:HD2	1.72	0.71
1:A:66:CYS:CB	1:A:91:VAL:CG1	2.61	0.71
1:A:66:CYS:N	1:A:93:LEU:HD21	2.06	0.71
1:B:134:ARG:HA	1:B:139:THR:OG1	1.89	0.71
1:A:45:SER:HB2	1:B:45:SER:CB	2.10	0.71
1:A:86:ILE:HG23	1:A:87:GLY:N	2.06	0.71
1:B:164:TYR:CG	1:B:184:VAL:HG11	2.25	0.71
1:B:98:ARG:CZ	1:B:102:PHE:CD2	2.74	0.71
1:A:157:TRP:N	1:A:157:TRP:CD1	2.58	0.71
1:A:196:VAL:HG11	1:A:200:VAL:CG1	2.20	0.71
1:A:45:SER:C	1:A:48:LEU:HB2	2.13	0.70
1:B:1:ALA:HB1	1:B:2:PRO:HD2	1.72	0.70
1:A:83:ILE:C	1:A:86:ILE:HG22	2.15	0.70
1:B:247:LYS:HD3	1:B:247:LYS:C	2.17	0.70
1:A:110:GLY:HA3	1:A:153:ASN:OD1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG12	1:A:124:ILE:N	2.06	0.70
1:B:211:SER:O	1:B:212:VAL:HB	1.91	0.70
1:A:150:ILE:C	1:A:154:VAL:HG23	2.16	0.70
1:B:12:TRP:CE3	1:B:43:ALA:HB2	2.27	0.70
1:A:78:ILE:HG12	1:A:82:MET:SD	2.32	0.70
1:A:103:GLY:O	1:A:104:GLU:C	2.35	0.69
1:B:101:VAL:O	1:B:101:VAL:HG22	1.92	0.69
1:A:193:LYS:CA	1:A:201:ALA:HB2	2.22	0.69
1:A:19:LYS:HG3	1:A:20:SER:H	1.55	0.69
1:B:6:PHE:HZ	1:B:229:PHE:CE2	2.10	0.69
1:B:43:ALA:HB1	1:B:44:PRO:CD	2.20	0.69
1:A:69:VAL:CG1	1:A:70:PRO:HD2	2.22	0.69
1:A:78:ILE:CD1	1:B:44:PRO:HB3	2.23	0.69
1:A:155:LYS:O	1:A:156:ASP:OD1	2.09	0.69
1:B:117:LEU:CD2	1:B:123:VAL:HG23	2.22	0.69
1:B:14:MET:O	1:B:14:MET:HG3	1.92	0.69
1:B:95:HIS:HA	1:B:126:CYS:SG	2.33	0.68
1:A:228:GLY:C	1:A:229:PHE:CD2	2.71	0.68
1:B:127:ILE:HG22	1:B:146:GLU:HB3	1.74	0.68
1:B:213:THR:O	1:B:217:CYS:HB2	1.93	0.68
1:A:189:ARG:O	1:A:192:LEU:HB3	1.94	0.68
1:A:1:ALA:HB3	1:A:2:PRO:CD	2.23	0.68
1:A:143:VAL:CG1	1:A:188:LEU:HD13	2.23	0.68
1:A:145:GLN:O	1:A:148:LYS:HB3	1.93	0.68
1:B:170:ILE:O	1:B:172:THR:OG1	2.10	0.68
1:A:14:MET:CE	1:B:69:VAL:HG23	2.14	0.68
1:B:33:LEU:HD22	1:B:244:ILE:CG2	2.24	0.68
1:B:105:SER:O	1:B:109:ILE:HD13	1.94	0.68
1:A:46:ILE:CD1	1:A:47:TYR:H	2.06	0.67
1:B:17:LYS:CE	1:B:19:LYS:HB2	2.23	0.67
1:A:5:LYS:HE3	1:A:205:ARG:CZ	2.24	0.67
1:B:84:LYS:HD3	1:B:119:GLU:O	1.94	0.67
1:A:157:TRP:HA	1:A:160:VAL:HG23	1.76	0.67
1:A:229:PHE:CD2	1:A:229:PHE:N	2.63	0.67
1:B:67:TYR:HB2	1:B:77:GLU:HG3	1.76	0.67
1:A:90:TRP:O	1:A:91:VAL:CG2	2.42	0.67
1:B:62:ALA:HB2	1:B:90:TRP:HB3	1.76	0.67
1:A:38:GLU:OE1	1:A:205:ARG:NH2	2.26	0.67
1:A:24:LEU:HD13	1:A:28:LEU:CD2	2.23	0.67
1:B:62:ALA:HB2	1:B:90:TRP:CB	2.25	0.67
1:A:40:VAL:HG11	1:A:90:TRP:CD1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TRP:C	1:A:91:VAL:HG23	2.20	0.67
1:A:129:GLU:OE1	1:A:139:THR:CB	2.43	0.67
1:B:194:THR:HB	1:B:195:HIS:ND1	2.09	0.67
1:B:211:SER:O	1:B:212:VAL:CB	2.42	0.67
1:A:157:TRP:C	1:A:159:LYS:N	2.52	0.66
1:A:12:TRP:HE3	1:A:43:ALA:CB	2.07	0.66
1:A:49:ASP:OD1	1:A:86:ILE:HD11	1.95	0.66
1:B:130:LYS:HA	1:B:167:VAL:HB	1.76	0.66
1:A:135:GLU:C	1:A:137:GLY:N	2.49	0.66
1:B:84:LYS:HZ3	1:B:119:GLU:HB3	1.61	0.66
1:B:117:LEU:HD21	1:B:123:VAL:CG2	2.25	0.66
1:A:13:LYS:HA	1:A:64:GLN:NE2	2.10	0.66
1:A:13:LYS:HA	1:A:64:GLN:HE22	1.59	0.66
1:A:46:ILE:HD12	1:A:47:TYR:H	1.60	0.66
1:A:47:TYR:HE1	1:B:82:MET:HE2	1.56	0.66
1:B:143:VAL:CG1	1:B:188:LEU:HD21	2.25	0.65
1:A:82:MET:HE1	1:B:14:MET:HB2	1.77	0.65
1:A:32:LYS:HD3	1:A:32:LYS:C	2.21	0.65
1:B:117:LEU:CD2	1:B:123:VAL:CG2	2.74	0.65
1:A:123:VAL:CG1	1:A:124:ILE:N	2.60	0.65
1:A:48:LEU:CD1	1:A:83:ILE:HG22	2.27	0.65
1:A:64:GLN:O	1:A:65:ASN:HB3	1.97	0.65
1:A:231:VAL:HG21	1:A:243:ILE:HD13	1.78	0.65
1:A:49:ASP:CG	1:A:86:ILE:CD1	2.70	0.64
1:B:118:ALA:C	1:B:120:GLY:H	2.04	0.64
1:B:148:LYS:CA	1:B:191:TRP:HH2	1.99	0.64
1:B:154:VAL:HG12	1:B:155:LYS:N	2.12	0.64
1:A:45:SER:O	1:A:48:LEU:HB3	1.91	0.64
1:B:142:VAL:HG23	1:B:143:VAL:N	2.13	0.64
1:B:43:ALA:HA	1:B:64:GLN:NE2	2.13	0.64
1:A:45:SER:CA	1:B:46:ILE:CG2	2.74	0.64
1:A:93:LEU:HD13	1:A:112:LYS:CB	2.28	0.64
1:B:67:TYR:CD2	1:B:69:VAL:CG2	2.75	0.63
1:A:2:PRO:O	1:A:4:ARG:CB	2.44	0.63
1:A:49:ASP:HB2	1:A:86:ILE:HD11	1.79	0.63
1:A:131:LEU:CD2	1:A:132:ASP:N	2.62	0.63
1:A:4:ARG:CG	1:A:227:ASP:OD2	2.46	0.63
1:A:56:ASP:O	1:A:57:ALA:C	2.40	0.63
1:A:77:GLU:CG	1:B:98:ARG:HH21	2.06	0.63
1:A:173:GLY:O	1:A:174:LYS:HB2	1.98	0.63
1:B:68:LYS:HG3	1:B:69:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:THR:HG22	1:B:191:TRP:CZ3	2.33	0.63
1:B:229:PHE:HB2	1:B:231:VAL:CG2	2.29	0.63
1:A:153:ASN:O	1:A:154:VAL:O	2.16	0.63
1:B:67:TYR:HB2	1:B:77:GLU:CG	2.28	0.63
1:B:199:ALA:O	1:B:203:GLN:HG2	1.98	0.63
1:A:5:LYS:HE3	1:A:205:ARG:NH1	2.13	0.63
1:A:47:TYR:HE2	1:B:86:ILE:HD11	1.63	0.63
1:B:25:ILE:HG21	1:B:54:LYS:HG3	1.80	0.63
1:B:193:LYS:HA	1:B:201:ALA:HB2	1.80	0.63
1:B:219:GLU:CD	1:B:219:GLU:H	2.07	0.63
1:B:148:LYS:O	1:B:151:ALA:HB3	1.98	0.62
1:A:86:ILE:CG2	1:A:87:GLY:N	2.61	0.62
1:B:7:PHE:HD2	1:B:205:ARG:HH12	1.45	0.62
1:A:191:TRP:CE2	1:A:195:HIS:CE1	2.87	0.62
1:A:47:TYR:O	1:A:50:PHE:HB3	1.99	0.62
1:A:6:PHE:HE2	1:A:246:ALA:HB3	1.64	0.62
1:B:80:PRO:HG2	1:B:115:HIS:CE1	2.35	0.62
1:B:74:PHE:O	1:B:77:GLU:HB2	1.99	0.62
1:A:42:GLY:HA3	1:A:62:ALA:O	1.99	0.62
1:A:191:TRP:CZ3	1:A:195:HIS:CB	2.82	0.62
1:A:220:LEU:O	1:A:223:GLN:HB3	1.99	0.62
1:B:12:TRP:N	1:B:12:TRP:CD1	2.58	0.62
1:A:34:SER:O	1:A:35:ALA:HB3	1.98	0.61
1:B:110:GLY:CA	1:B:153:ASN:OD1	2.48	0.61
1:A:162:LEU:HD11	1:A:192:LEU:HD11	1.82	0.61
1:A:62:ALA:CA	1:A:90:TRP:HB2	2.30	0.61
1:A:232:GLY:O	1:A:233:GLY:O	2.17	0.61
1:B:99:ARG:NH1	1:B:126:CYS:O	2.34	0.61
1:A:22:GLY:O	1:A:25:ILE:HG13	2.01	0.61
1:A:30:GLY:O	1:A:32:LYS:N	2.33	0.61
1:A:243:ILE:O	1:A:244:ILE:C	2.42	0.61
1:B:25:ILE:HG23	1:B:55:LEU:CD2	2.29	0.61
1:A:80:PRO:CB	1:A:121:LEU:CD1	2.77	0.61
1:B:164:TYR:CZ	1:B:184:VAL:HG21	2.36	0.61
1:B:189:ARG:NH1	1:B:206:ILE:HD12	2.15	0.61
1:A:83:ILE:O	1:A:86:ILE:CG2	2.40	0.60
1:A:212:VAL:HG11	1:A:229:PHE:CD1	2.35	0.60
1:A:135:GLU:C	1:A:137:GLY:H	2.08	0.60
1:A:245:ASN:O	1:A:246:ALA:O	2.19	0.60
1:A:73:ALA:O	1:A:74:PHE:CD1	2.55	0.60
1:B:79:SER:OG	1:B:81:ALA:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ALA:O	1:A:182:GLN:C	2.44	0.60
1:B:97:GLU:O	1:B:98:ARG:C	2.43	0.60
1:B:211:SER:C	1:B:212:VAL:HG23	2.27	0.60
1:A:6:PHE:HZ	1:A:229:PHE:CE2	2.18	0.60
1:A:95:HIS:O	1:A:96:SER:C	2.44	0.60
1:A:245:ASN:O	1:A:246:ALA:C	2.44	0.60
1:A:31:ALA:O	1:A:32:LYS:C	2.45	0.60
1:A:130:LYS:O	1:A:131:LEU:C	2.44	0.60
1:B:12:TRP:HZ2	1:B:41:CYS:CB	2.13	0.60
1:B:220:LEU:O	1:B:223:GLN:CB	2.40	0.60
1:A:26:HIS:CE1	1:A:54:LYS:HD3	2.36	0.59
1:A:152:ASP:OD2	1:A:152:ASP:C	2.45	0.59
1:A:39:VAL:CG2	1:A:244:ILE:HD13	2.32	0.59
1:A:45:SER:CB	1:B:46:ILE:HG23	2.31	0.59
1:B:151:ALA:O	1:B:154:VAL:HB	2.01	0.59
1:B:229:PHE:CB	1:B:231:VAL:HG22	2.32	0.59
1:A:22:GLY:HA2	1:A:25:ILE:HD11	1.84	0.59
1:A:212:VAL:HB	1:A:231:VAL:CG2	2.31	0.59
1:B:174:LYS:HG3	1:B:175:THR:N	2.17	0.59
1:B:79:SER:O	1:B:83:ILE:HD12	2.03	0.59
1:B:6:PHE:HZ	1:B:229:PHE:CZ	2.21	0.59
1:B:12:TRP:CE2	1:B:41:CYS:HB2	2.37	0.59
1:B:148:LYS:HB2	1:B:191:TRP:CZ2	2.37	0.58
1:A:66:CYS:CB	1:A:93:LEU:HD21	2.33	0.58
1:A:144:PHE:N	1:A:144:PHE:CD2	2.70	0.58
1:A:166:PRO:O	1:A:166:PRO:CD	2.51	0.58
1:A:91:VAL:CG2	1:A:121:LEU:HD13	2.30	0.58
1:A:196:VAL:O	1:A:197:SER:CB	2.52	0.58
1:B:13:LYS:NZ	1:B:97:GLU:OE2	2.33	0.58
1:A:139:THR:OG1	1:A:140:GLU:N	2.35	0.58
1:A:229:PHE:N	1:A:229:PHE:HD2	2.01	0.58
1:A:240:PHE:O	1:A:244:ILE:HG13	2.04	0.58
1:A:80:PRO:HB2	1:A:121:LEU:HD11	1.84	0.58
1:A:105:SER:O	1:A:109:ILE:HD13	2.02	0.58
1:A:173:GLY:O	1:A:174:LYS:CB	2.51	0.58
1:B:167:VAL:O	1:B:169:ALA:C	2.47	0.58
1:A:33:LEU:HD22	1:A:33:LEU:N	2.10	0.58
1:A:108:LEU:CG	1:A:112:LYS:HE2	2.33	0.58
1:A:191:TRP:CE3	1:A:195:HIS:ND1	2.72	0.58
1:B:232:GLY:O	1:B:233:GLY:C	2.46	0.58
1:B:196:VAL:HG11	1:B:200:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:C	1:A:104:GLU:O	2.46	0.57
1:B:170:ILE:O	1:B:171:GLY:C	2.47	0.57
1:A:220:LEU:O	1:A:223:GLN:HB2	2.03	0.57
1:A:24:LEU:HD21	1:A:236:LEU:O	2.04	0.57
1:A:39:VAL:HG21	1:A:244:ILE:HD13	1.87	0.57
1:A:78:ILE:HD11	1:B:44:PRO:HB3	1.85	0.57
1:A:82:MET:CB	1:B:46:ILE:HD11	2.35	0.57
1:A:161:VAL:HG13	1:A:205:ARG:HB2	1.85	0.57
1:B:170:ILE:O	1:B:170:ILE:CG2	2.52	0.57
1:B:191:TRP:CD1	1:B:195:HIS:CE1	2.92	0.57
1:B:6:PHE:CZ	1:B:228:GLY:HA2	2.39	0.57
1:B:168:TRP:CZ2	1:B:176:ALA:HA	2.40	0.57
1:A:163:ALA:HA	1:A:207:ILE:HG12	1.87	0.57
1:A:29:ASP:O	1:A:30:GLY:C	2.48	0.57
1:A:48:LEU:O	1:A:51:ALA:HB3	2.04	0.57
1:A:157:TRP:HB2	1:A:203:GLN:HE21	1.69	0.57
1:A:196:VAL:O	1:A:197:SER:HB3	2.04	0.57
1:A:239:GLU:O	1:A:242:ASP:HB2	2.05	0.57
1:B:210:GLY:O	1:B:211:SER:O	2.23	0.57
1:B:89:ALA:O	1:B:121:LEU:HG	2.05	0.56
1:A:131:LEU:HB2	1:A:168:TRP:HA	1.87	0.56
1:B:66:CYS:SG	1:B:93:LEU:HD21	2.45	0.56
1:B:130:LYS:NZ	1:B:133:GLU:OE1	2.23	0.56
1:B:138:ILE:CD1	1:B:141:LYS:CD	2.83	0.56
1:A:127:ILE:HD13	1:A:163:ALA:O	2.06	0.56
1:B:198:ASP:O	1:B:199:ALA:C	2.48	0.56
1:B:240:PHE:O	1:B:243:ILE:HB	2.05	0.56
1:A:113:VAL:O	1:A:117:LEU:HG	2.05	0.56
1:A:98:ARG:NH2	1:A:102:PHE:CE2	2.74	0.56
1:A:108:LEU:CD2	1:A:112:LYS:HE2	2.36	0.56
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.71	0.56
1:B:154:VAL:HG11	1:B:157:TRP:CZ2	2.41	0.56
1:B:12:TRP:CZ2	1:B:41:CYS:SG	2.99	0.55
1:A:41:CYS:HB2	1:A:59:ILE:CG2	2.36	0.55
1:A:129:GLU:CD	1:A:134:ARG:HB2	2.32	0.55
1:A:18:ARG:HG2	1:B:85:ASP:OD1	2.06	0.55
1:A:170:ILE:O	1:A:170:ILE:CG2	2.55	0.55
1:A:157:TRP:HA	1:A:160:VAL:CG2	2.36	0.55
1:A:191:TRP:CE3	1:A:191:TRP:C	2.85	0.55
1:B:117:LEU:CD1	1:B:154:VAL:HA	2.36	0.55
1:B:127:ILE:HD12	1:B:164:TYR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:O	1:A:137:GLY:CA	2.54	0.55
1:A:185:HIS:NE2	1:A:206:ILE:HG22	2.22	0.54
1:A:208:TYR:CD2	1:A:220:LEU:CD1	2.90	0.54
1:B:163:ALA:HB2	1:B:207:ILE:HD11	1.87	0.54
1:A:93:LEU:CD1	1:A:112:LYS:HB3	2.34	0.54
1:A:151:ALA:CA	1:A:154:VAL:CG2	2.82	0.54
1:A:168:TRP:CZ3	1:A:174:LYS:HB3	2.43	0.54
1:A:4:ARG:HG2	1:A:227:ASP:OD2	2.06	0.54
1:A:65:ASN:HD22	1:A:98:ARG:HD2	1.71	0.54
1:B:101:VAL:O	1:B:101:VAL:CG2	2.55	0.54
1:B:237:LYS:O	1:B:239:GLU:N	2.40	0.54
1:A:128:GLY:O	1:A:142:VAL:HG11	2.08	0.54
1:A:131:LEU:C	1:A:131:LEU:CD2	2.74	0.54
1:A:138:ILE:HG22	1:A:138:ILE:O	2.08	0.54
1:B:66:CYS:HB2	1:B:80:PRO:HD3	1.90	0.54
1:B:209:GLY:HA2	1:B:230:LEU:HB3	1.90	0.54
1:A:33:LEU:HG	1:A:245:ASN:OD1	2.08	0.54
1:A:172:THR:O	1:A:173:GLY:O	2.24	0.54
1:B:70:PRO:HD3	1:B:115:HIS:CE1	2.43	0.54
1:A:52:ARG:HD3	1:A:87:GLY:O	2.08	0.54
1:A:141:LYS:O	1:A:145:GLN:HG3	2.09	0.53
1:A:128:GLY:O	1:A:142:VAL:CG1	2.56	0.53
1:B:231:VAL:HG12	1:B:234:ALA:HB3	1.90	0.53
1:A:43:ALA:O	1:A:44:PRO:C	2.52	0.53
1:A:189:ARG:O	1:A:192:LEU:CB	2.55	0.53
1:A:66:CYS:H	1:A:93:LEU:HD23	1.70	0.53
1:A:157:TRP:HB2	1:A:203:GLN:HE22	1.73	0.53
1:B:68:LYS:NZ	1:B:111:GLN:OE1	2.27	0.53
1:A:8:VAL:HG11	1:A:244:ILE:HG12	1.89	0.53
1:A:47:TYR:HE1	1:B:82:MET:CE	2.15	0.53
1:A:57:ALA:O	1:A:59:ILE:N	2.42	0.53
1:B:2:PRO:O	1:B:4:ARG:HB2	2.08	0.53
1:B:95:HIS:HA	1:B:126:CYS:CB	2.38	0.53
1:A:62:ALA:CB	1:A:90:TRP:HB3	2.37	0.53
1:B:238:PRO:O	1:B:239:GLU:C	2.50	0.53
1:B:143:VAL:HG13	1:B:188:LEU:HD21	1.90	0.53
1:B:149:ALA:C	1:B:153:ASN:HD22	2.17	0.53
1:A:143:VAL:HG12	1:A:188:LEU:HD13	1.91	0.53
1:B:4:ARG:HD3	1:B:227:ASP:OD2	2.08	0.53
1:B:84:LYS:O	1:B:87:GLY:N	2.41	0.53
1:A:98:ARG:CZ	1:A:102:PHE:CD2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HG3	1:A:167:VAL:HG12	1.90	0.52
1:B:216:ASN:C	1:B:219:GLU:HG2	2.34	0.52
1:A:8:VAL:HG12	1:A:240:PHE:HE1	1.75	0.52
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.24	0.52
1:A:93:LEU:HD22	1:A:112:LYS:HD3	1.91	0.52
1:A:85:ASP:OD1	1:B:47:TYR:OH	2.21	0.52
1:A:151:ALA:HB2	1:A:157:TRP:HH2	1.74	0.52
1:B:9:GLY:HA2	1:B:40:VAL:O	2.09	0.52
1:B:68:LYS:CE	1:B:108:LEU:HD12	2.39	0.52
1:B:218:LYS:HE2	1:B:248:HIS:O	2.09	0.52
1:A:37:THR:HG21	1:A:244:ILE:HG23	1.92	0.52
1:A:92:ILE:C	1:A:92:ILE:CD1	2.62	0.52
1:A:177:THR:HB	1:A:178:PRO:HD2	1.90	0.52
1:B:157:TRP:HA	1:B:160:VAL:HB	1.90	0.52
1:B:167:VAL:O	1:B:170:ILE:HB	2.08	0.52
1:A:1:ALA:N	1:A:2:PRO:HD2	2.25	0.52
1:A:20:SER:O	1:A:23:GLU:HB2	2.09	0.52
1:A:135:GLU:O	1:A:136:ALA:C	2.52	0.52
1:B:211:SER:O	1:B:212:VAL:HG23	2.09	0.52
1:B:94:GLY:HA3	1:B:109:ILE:HG13	1.90	0.52
1:B:150:ILE:HG22	1:B:154:VAL:HG21	1.91	0.52
1:B:135:GLU:O	1:B:136:ALA:C	2.53	0.52
1:A:55:LEU:CD2	1:A:59:ILE:HD12	2.40	0.52
1:A:216:ASN:O	1:A:217:CYS:C	2.53	0.52
1:A:32:LYS:O	1:A:32:LYS:HD3	2.10	0.51
1:B:93:LEU:HD13	1:B:112:LYS:HB3	1.92	0.51
1:B:142:VAL:HG23	1:B:143:VAL:H	1.74	0.51
1:B:144:PHE:CE2	1:B:191:TRP:HB2	2.45	0.51
1:B:67:TYR:CB	1:B:77:GLU:HG3	2.40	0.51
1:A:41:CYS:N	1:A:60:GLY:O	2.39	0.51
1:B:25:ILE:HG22	1:B:29:ASP:OD2	2.10	0.51
1:B:118:ALA:O	1:B:120:GLY:N	2.40	0.51
1:B:127:ILE:HG23	1:B:150:ILE:CD1	2.38	0.51
1:A:79:SER:O	1:A:82:MET:CG	2.51	0.51
1:B:4:ARG:CD	1:B:227:ASP:OD2	2.59	0.51
1:B:25:ILE:CG1	1:B:55:LEU:HD21	2.26	0.51
1:B:8:VAL:HG12	1:B:240:PHE:CZ	2.46	0.51
1:A:74:PHE:N	1:B:97:GLU:OE1	2.44	0.51
1:A:98:ARG:HD3	1:A:104:GLU:OE2	2.09	0.51
1:B:56:ASP:O	1:B:58:LYS:N	2.43	0.51
1:B:193:LYS:CA	1:B:201:ALA:HB2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:O	1:A:134:ARG:C	2.53	0.51
1:B:1:ALA:CB	1:B:2:PRO:CD	2.82	0.51
1:B:62:ALA:HA	1:B:90:TRP:O	2.10	0.51
1:B:80:PRO:O	1:B:83:ILE:HB	2.10	0.51
1:B:98:ARG:HD3	1:B:104:GLU:OE1	2.10	0.51
1:A:28:LEU:O	1:A:31:ALA:HB3	2.11	0.51
1:B:229:PHE:HB2	1:B:231:VAL:HG22	1.91	0.51
1:A:49:ASP:CG	1:A:86:ILE:CG1	2.84	0.51
1:A:163:ALA:HB2	1:A:207:ILE:HD11	1.92	0.51
1:B:213:THR:OG1	1:B:214:GLY:N	2.44	0.51
1:B:129:GLU:OE1	1:B:134:ARG:NE	2.44	0.50
1:A:135:GLU:O	1:A:137:GLY:N	2.43	0.50
1:B:96:SER:OG	1:B:97:GLU:N	2.43	0.50
1:B:106:ASP:O	1:B:107:GLU:C	2.52	0.50
1:B:67:TYR:CE2	1:B:68:LYS:HG2	2.46	0.50
1:B:163:ALA:HB2	1:B:207:ILE:CG1	2.42	0.50
1:B:241:VAL:O	1:B:242:ASP:C	2.53	0.50
1:B:154:VAL:CG1	1:B:155:LYS:N	2.74	0.50
1:A:78:ILE:CG1	1:A:82:MET:SD	3.00	0.50
1:A:191:TRP:CE2	1:A:195:HIS:ND1	2.79	0.50
1:B:54:LYS:HD2	1:B:54:LYS:C	2.36	0.50
1:B:79:SER:O	1:B:83:ILE:CD1	2.60	0.50
1:B:84:LYS:HZ2	1:B:119:GLU:HB3	1.71	0.50
1:A:245:ASN:C	1:A:246:ALA:O	2.55	0.50
1:B:6:PHE:CE1	1:B:229:PHE:CE2	3.00	0.50
1:A:92:ILE:HD13	1:A:126:CYS:SG	2.52	0.50
1:B:96:SER:HB3	1:B:165:GLU:CD	2.37	0.50
1:A:241:VAL:O	1:A:242:ASP:C	2.54	0.49
1:B:133:GLU:O	1:B:134:ARG:C	2.55	0.49
1:B:149:ALA:C	1:B:153:ASN:ND2	2.70	0.49
1:A:78:ILE:HG13	1:B:44:PRO:HB3	1.94	0.49
1:A:138:ILE:O	1:A:142:VAL:HG23	2.11	0.49
1:B:12:TRP:HZ2	1:B:41:CYS:SG	2.36	0.49
1:A:67:TYR:O	1:A:80:PRO:CD	2.60	0.49
1:A:198:ASP:O	1:A:199:ALA:C	2.55	0.49
1:B:63:ALA:O	1:B:92:ILE:HG13	2.13	0.49
1:A:40:VAL:CG1	1:A:90:TRP:CD1	2.94	0.49
1:B:194:THR:HB	1:B:195:HIS:HD1	1.78	0.49
1:B:229:PHE:HB3	1:B:231:VAL:HG22	1.93	0.49
1:A:144:PHE:N	1:A:144:PHE:HD2	2.10	0.49
1:A:216:ASN:O	1:A:219:GLU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:VAL:HG13	1:B:160:VAL:HG21	1.93	0.49
1:B:223:GLN:O	1:B:223:GLN:CG	2.60	0.49
1:A:198:ASP:O	1:A:202:VAL:HG23	2.13	0.49
1:B:54:LYS:HG3	1:B:55:LEU:N	2.28	0.49
1:A:64:GLN:CB	1:B:75:THR:CG2	2.85	0.49
1:A:72:GLY:HA3	1:A:74:PHE:CE2	2.47	0.49
1:A:90:TRP:C	1:A:91:VAL:CG2	2.84	0.49
1:B:63:ALA:C	1:B:65:ASN:H	2.21	0.49
1:B:144:PHE:CD2	1:B:191:TRP:HB2	2.46	0.49
1:A:221:ALA:O	1:A:222:SER:C	2.56	0.49
1:A:46:ILE:HG13	1:B:45:SER:HB3	1.95	0.48
1:A:62:ALA:HB2	1:A:90:TRP:HB3	1.91	0.48
1:B:93:LEU:HD13	1:B:112:LYS:CB	2.43	0.48
1:A:66:CYS:HB3	1:A:91:VAL:HG11	1.88	0.48
1:B:110:GLY:C	1:B:153:ASN:OD1	2.56	0.48
1:A:11:ASN:C	1:A:11:ASN:OD1	2.55	0.48
1:A:44:PRO:HB3	1:B:78:ILE:HD12	1.96	0.48
1:A:224:HIS:C	1:A:226:VAL:H	2.21	0.48
1:B:67:TYR:CG	1:B:77:GLU:HG3	2.48	0.48
1:B:96:SER:HB3	1:B:165:GLU:OE1	2.12	0.48
1:B:177:THR:CB	1:B:180:GLN:OE1	2.61	0.48
1:A:6:PHE:CE2	1:A:246:ALA:HB3	2.48	0.48
1:A:146:GLU:O	1:A:149:ALA:HB3	2.14	0.48
1:B:223:GLN:HB3	1:B:226:VAL:HG23	1.96	0.48
1:B:64:GLN:O	1:B:65:ASN:HB2	2.13	0.48
1:B:211:SER:O	1:B:212:VAL:CG2	2.61	0.48
1:A:62:ALA:HA	1:A:90:TRP:HB2	1.94	0.48
1:B:62:ALA:HB2	1:B:90:TRP:HB2	1.94	0.48
1:B:107:GLU:HG3	1:B:111:GLN:NE2	2.29	0.48
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.44	0.48
1:A:73:ALA:C	1:B:97:GLU:OE1	2.56	0.48
1:A:80:PRO:O	1:A:81:ALA:C	2.57	0.48
1:A:64:GLN:O	1:A:65:ASN:CB	2.62	0.48
1:A:73:ALA:C	1:A:74:PHE:CG	2.92	0.48
1:B:54:LYS:C	1:B:54:LYS:CD	2.85	0.48
1:B:132:ASP:C	1:B:132:ASP:OD2	2.55	0.48
1:B:223:GLN:O	1:B:223:GLN:HG3	2.12	0.48
1:A:45:SER:CB	1:B:46:ILE:CG2	2.92	0.48
1:A:158:SER:C	1:A:159:LYS:HG3	2.39	0.48
1:B:44:PRO:O	1:B:48:LEU:HG	2.14	0.48
1:B:139:THR:O	1:B:142:VAL:CG2	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:O	1:A:58:LYS:C	2.57	0.47
1:A:162:LEU:CD1	1:A:192:LEU:HD11	2.43	0.47
1:A:18:ARG:NH1	1:A:18:ARG:HG3	2.28	0.47
1:A:24:LEU:O	1:A:28:LEU:HD23	2.14	0.47
1:A:33:LEU:H	1:A:33:LEU:CD2	2.16	0.47
1:A:46:ILE:C	1:A:48:LEU:N	2.64	0.47
1:A:64:GLN:HB2	1:B:75:THR:HG22	1.95	0.47
1:A:138:ILE:HG23	1:A:141:LYS:CB	2.40	0.47
1:B:243:ILE:O	1:B:246:ALA:N	2.42	0.47
1:A:80:PRO:O	1:A:83:ILE:HG13	2.14	0.47
1:A:95:HIS:O	1:A:97:GLU:N	2.47	0.47
1:A:110:GLY:HA3	1:A:153:ASN:CG	2.40	0.47
1:B:36:ASP:OD2	1:B:36:ASP:C	2.55	0.47
1:B:154:VAL:HG11	1:B:157:TRP:CE2	2.50	0.47
1:B:180:GLN:O	1:B:184:VAL:HG23	2.14	0.47
1:B:223:GLN:HB3	1:B:226:VAL:CG2	2.45	0.47
1:A:37:THR:HG21	1:A:244:ILE:CG2	2.44	0.47
1:B:148:LYS:N	1:B:191:TRP:CH2	2.83	0.47
1:B:247:LYS:C	1:B:247:LYS:CD	2.86	0.47
1:B:6:PHE:CE2	1:B:228:GLY:CA	2.89	0.47
1:A:66:CYS:HB3	1:A:91:VAL:CG1	2.44	0.47
1:B:82:MET:O	1:B:83:ILE:C	2.58	0.47
1:A:29:ASP:CG	1:A:56:ASP:OD1	2.58	0.47
1:A:185:HIS:CD2	1:A:206:ILE:HG22	2.50	0.47
1:A:196:VAL:HG12	1:A:200:VAL:CG2	2.43	0.47
1:B:43:ALA:O	1:B:44:PRO:C	2.58	0.47
1:B:237:LYS:C	1:B:239:GLU:N	2.73	0.47
1:B:247:LYS:HD3	1:B:247:LYS:O	2.15	0.47
1:A:100:HIS:N	1:A:100:HIS:CD2	2.79	0.46
1:A:4:ARG:HD2	1:A:4:ARG:HH21	1.52	0.46
1:B:138:ILE:CD1	1:B:141:LYS:HB3	2.45	0.46
1:A:33:LEU:CB	1:A:245:ASN:HD21	2.18	0.46
1:A:167:VAL:HG13	1:A:170:ILE:CG2	2.45	0.46
1:B:25:ILE:HG12	1:B:55:LEU:CG	2.46	0.46
1:B:164:TYR:CE2	1:B:184:VAL:HG11	2.49	0.46
1:A:178:PRO:HD3	1:A:219:GLU:OE1	2.16	0.46
1:A:188:LEU:O	1:A:189:ARG:C	2.59	0.46
1:B:25:ILE:HG21	1:B:54:LYS:CG	2.46	0.46
1:B:143:VAL:CG1	1:B:188:LEU:CD2	2.94	0.46
1:A:49:ASP:OD1	1:A:86:ILE:CD1	2.64	0.46
1:B:138:ILE:O	1:B:139:THR:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HG11	1:B:200:VAL:HG21	1.89	0.46
1:B:149:ALA:O	1:B:150:ILE:C	2.59	0.46
1:B:164:TYR:CD2	1:B:164:TYR:C	2.93	0.46
1:A:78:ILE:CG1	1:B:44:PRO:HB3	2.45	0.46
1:A:172:THR:C	1:A:173:GLY:O	2.58	0.46
1:B:33:LEU:HD21	1:B:241:VAL:HG22	1.98	0.46
1:B:67:TYR:C	1:B:69:VAL:H	2.24	0.46
1:B:131:LEU:HD22	1:B:172:THR:HG23	1.97	0.46
1:A:64:GLN:H	1:A:64:GLN:HG3	1.55	0.46
1:A:237:LYS:CB	1:A:238:PRO:HD2	2.37	0.46
1:B:237:LYS:C	1:B:239:GLU:H	2.24	0.46
1:A:145:GLN:O	1:A:148:LYS:CB	2.62	0.46
1:A:191:TRP:CD2	1:A:195:HIS:CE1	3.04	0.46
1:B:33:LEU:HA	1:B:245:ASN:HD21	1.81	0.46
1:A:77:GLU:HG3	1:B:102:PHE:CE2	2.49	0.45
1:A:107:GLU:O	1:A:111:GLN:HG3	2.16	0.45
1:A:154:VAL:HG12	1:A:156:ASP:H	1.81	0.45
1:B:148:LYS:O	1:B:149:ALA:C	2.59	0.45
1:B:152:ASP:O	1:B:153:ASN:C	2.58	0.45
1:B:40:VAL:HA	1:B:60:GLY:O	2.16	0.45
1:B:52:ARG:O	1:B:53:GLN:C	2.60	0.45
1:B:182:GLN:OE1	1:B:223:GLN:HG3	2.17	0.45
1:A:22:GLY:O	1:A:25:ILE:CG1	2.64	0.45
1:A:116:ALA:O	1:A:121:LEU:HB2	2.16	0.45
1:A:231:VAL:HG13	1:A:235:SER:H	1.82	0.45
1:B:94:GLY:O	1:B:99:ARG:NE	2.40	0.45
1:A:13:LYS:O	1:A:44:PRO:HG3	2.17	0.45
1:A:167:VAL:C	1:A:169:ALA:H	2.24	0.45
1:B:11:ASN:ND2	1:B:64:GLN:HG2	2.32	0.45
1:B:142:VAL:CG2	1:B:143:VAL:N	2.77	0.45
1:A:7:PHE:CD2	1:A:38:GLU:HB3	2.50	0.45
1:A:45:SER:HB3	1:B:46:ILE:CG2	2.42	0.45
1:A:92:ILE:HD12	1:A:93:LEU:CA	2.45	0.45
1:A:208:TYR:CD2	1:A:220:LEU:HD11	2.51	0.45
1:B:5:LYS:N	1:B:5:LYS:CD	2.63	0.45
1:B:138:ILE:HD12	1:B:141:LYS:HB3	1.98	0.45
1:B:205:ARG:HE	1:B:205:ARG:HB2	1.26	0.45
1:A:143:VAL:HG11	1:A:188:LEU:HD13	1.98	0.45
1:B:148:LYS:HB2	1:B:191:TRP:HZ2	1.80	0.45
1:B:110:GLY:HA2	1:B:153:ASN:CG	2.38	0.45
1:A:24:LEU:CD1	1:A:28:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TYR:CE2	1:B:86:ILE:HD11	2.48	0.45
1:A:191:TRP:C	1:A:191:TRP:HE3	2.25	0.45
1:B:164:TYR:CD1	1:B:184:VAL:HG13	2.45	0.45
1:B:164:TYR:CD2	1:B:184:VAL:HG11	2.51	0.45
1:A:7:PHE:HD2	1:A:38:GLU:HB3	1.82	0.45
1:A:208:TYR:CD2	1:A:220:LEU:HD13	2.51	0.45
1:B:64:GLN:HA	1:B:92:ILE:HB	1.99	0.45
1:A:66:CYS:N	1:A:93:LEU:CD2	2.66	0.45
1:A:138:ILE:N	1:A:138:ILE:HD13	2.32	0.45
1:A:6:PHE:HZ	1:A:229:PHE:CZ	2.34	0.44
1:A:34:SER:O	1:A:35:ALA:CB	2.65	0.44
1:B:177:THR:HG23	1:B:180:GLN:OE1	2.18	0.44
1:B:223:GLN:HG2	1:B:226:VAL:HG21	1.99	0.44
1:A:134:ARG:HD2	1:A:168:TRP:CG	2.52	0.44
1:A:170:ILE:C	1:A:172:THR:N	2.73	0.44
1:A:185:HIS:O	1:A:186:GLU:C	2.60	0.44
1:B:54:LYS:HD2	1:B:54:LYS:O	2.17	0.44
1:B:71:LYS:O	1:B:71:LYS:HG3	2.17	0.44
1:B:105:SER:O	1:B:108:LEU:HB3	2.18	0.44
1:B:94:GLY:CA	1:B:109:ILE:HG13	2.47	0.44
1:B:100:HIS:O	1:B:100:HIS:HD2	1.93	0.44
1:B:147:THR:O	1:B:150:ILE:HB	2.17	0.44
1:A:203:GLN:HG3	1:A:204:SER:H	1.77	0.44
1:A:17:LYS:O	1:A:18:ARG:C	2.60	0.44
1:A:25:ILE:HD12	1:A:54:LYS:HB3	2.00	0.44
1:A:72:GLY:H	1:B:14:MET:HG2	1.83	0.44
1:A:157:TRP:O	1:A:160:VAL:N	2.46	0.44
1:B:7:PHE:CB	1:B:205:ARG:HD2	2.45	0.44
1:A:17:LYS:H	1:A:20:SER:HG	1.64	0.44
1:A:66:CYS:CA	1:A:93:LEU:HD21	2.47	0.44
1:B:69:VAL:HG21	1:B:74:PHE:CE2	2.53	0.44
1:A:25:ILE:HG12	1:A:25:ILE:H	1.60	0.44
1:B:66:CYS:HG	1:B:91:VAL:HG21	1.75	0.44
1:A:44:PRO:O	1:A:45:SER:C	2.61	0.44
1:A:92:ILE:O	1:A:92:ILE:HG13	2.18	0.44
1:A:142:VAL:O	1:A:146:GLU:HG3	2.18	0.44
1:B:7:PHE:HB2	1:B:205:ARG:CD	2.46	0.43
1:B:138:ILE:CG1	1:B:141:LYS:CD	2.94	0.43
1:B:194:THR:HB	1:B:195:HIS:CE1	2.52	0.43
1:A:231:VAL:HG13	1:A:235:SER:HB3	1.86	0.43
1:B:151:ALA:HA	1:B:157:TRP:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:CZ3	1:A:174:LYS:HD3	2.53	0.43
1:B:195:HIS:ND1	1:B:195:HIS:N	2.66	0.43
1:A:39:VAL:HG22	1:A:244:ILE:HD13	1.99	0.43
1:A:46:ILE:C	1:A:48:LEU:H	2.26	0.43
1:A:80:PRO:O	1:A:83:ILE:CG1	2.67	0.43
1:A:155:LYS:O	1:A:156:ASP:CB	2.66	0.43
1:A:233:GLY:O	1:A:234:ALA:C	2.60	0.43
1:B:212:VAL:HB	1:B:231:VAL:HG13	2.00	0.43
1:A:24:LEU:HD22	1:A:24:LEU:HA	1.68	0.43
1:B:67:TYR:HB2	1:B:77:GLU:CD	2.43	0.43
1:B:242:ASP:O	1:B:246:ALA:N	2.51	0.43
1:A:151:ALA:CA	1:A:154:VAL:HG23	2.48	0.43
1:A:231:VAL:CG1	1:A:235:SER:CA	2.96	0.43
1:B:134:ARG:HD2	1:B:168:TRP:CD2	2.53	0.43
1:A:92:ILE:HA	1:A:124:ILE:HB	2.00	0.43
1:A:125:ALA:HB1	1:A:150:ILE:HD13	2.01	0.43
1:A:130:LYS:HG3	1:A:167:VAL:CG1	2.49	0.43
1:B:189:ARG:CZ	1:B:206:ILE:HD12	2.49	0.43
1:B:154:VAL:HG12	1:B:155:LYS:H	1.84	0.43
1:B:170:ILE:O	1:B:170:ILE:HG22	2.19	0.43
1:B:177:THR:O	1:B:178:PRO:C	2.62	0.43
1:A:94:GLY:C	1:A:126:CYS:HB2	2.43	0.43
1:A:167:VAL:C	1:A:169:ALA:N	2.76	0.43
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.83	0.43
1:A:33:LEU:N	1:A:33:LEU:CD2	2.81	0.43
1:A:86:ILE:CG2	1:A:87:GLY:H	2.32	0.43
1:A:182:GLN:HG3	1:A:223:GLN:NE2	2.33	0.43
1:B:67:TYR:CE2	1:B:69:VAL:HG13	2.54	0.43
1:B:131:LEU:HD22	1:B:172:THR:CG2	2.49	0.43
1:A:217:CYS:HB3	1:A:243:ILE:HG23	1.99	0.42
1:B:21:LEU:HD23	1:B:21:LEU:HA	1.74	0.42
1:B:109:ILE:CD1	1:B:109:ILE:N	2.82	0.42
1:B:142:VAL:CG2	1:B:143:VAL:H	2.32	0.42
1:B:223:GLN:CG	1:B:226:VAL:HG21	2.48	0.42
1:A:98:ARG:HB3	1:A:104:GLU:HG3	2.01	0.42
1:B:73:ALA:C	1:B:74:PHE:CD2	2.97	0.42
1:A:24:LEU:CD1	1:A:28:LEU:CD2	2.93	0.42
1:A:131:LEU:HD23	1:A:132:ASP:CA	2.50	0.42
1:A:237:LYS:HB3	1:A:238:PRO:CD	2.45	0.42
1:B:134:ARG:HH11	1:B:134:ARG:HD3	1.48	0.42
1:B:174:LYS:CG	1:B:175:THR:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:CA	1:A:64:GLN:HE22	2.29	0.42
1:A:67:TYR:CB	1:A:78:ILE:O	2.68	0.42
1:A:73:ALA:HA	1:B:13:LYS:HD2	2.02	0.42
1:A:191:TRP:O	1:A:195:HIS:ND1	2.51	0.42
1:B:11:ASN:HD21	1:B:64:GLN:HG2	1.85	0.42
1:B:58:LYS:HD2	1:B:58:LYS:HA	1.62	0.42
1:B:84:LYS:O	1:B:85:ASP:C	2.63	0.42
1:B:85:ASP:OD1	1:B:85:ASP:O	2.36	0.42
1:B:86:ILE:HD13	1:B:86:ILE:HA	1.84	0.42
1:B:100:HIS:O	1:B:100:HIS:CG	2.66	0.42
1:A:232:GLY:O	1:A:235:SER:N	2.48	0.42
1:B:177:THR:C	1:B:179:GLN:N	2.74	0.42
1:B:219:GLU:O	1:B:222:SER:OG	2.19	0.42
1:A:25:ILE:O	1:A:26:HIS:C	2.62	0.42
1:A:77:GLU:HG3	1:B:102:PHE:HZ	1.71	0.42
1:B:138:ILE:CD1	1:B:141:LYS:HD3	2.48	0.42
1:B:180:GLN:O	1:B:183:GLU:HB3	2.19	0.42
1:B:17:LYS:NZ	1:B:19:LYS:HB2	2.33	0.42
1:A:67:TYR:O	1:A:80:PRO:HD2	2.20	0.42
1:A:138:ILE:O	1:A:139:THR:C	2.62	0.42
1:A:196:VAL:CG1	1:A:200:VAL:CG2	2.95	0.42
1:A:224:HIS:O	1:A:226:VAL:N	2.47	0.42
1:B:32:LYS:O	1:B:32:LYS:HG2	2.17	0.42
1:A:129:GLU:OE1	1:A:139:THR:CA	2.68	0.41
1:A:221:ALA:O	1:A:223:GLN:O	2.38	0.41
1:B:28:LEU:HG	1:B:241:VAL:HG23	2.01	0.41
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.68	0.41
1:A:95:HIS:O	1:A:98:ARG:N	2.53	0.41
1:A:150:ILE:O	1:A:151:ALA:C	2.62	0.41
1:B:4:ARG:HD3	1:B:227:ASP:OD1	2.21	0.41
1:B:163:ALA:HB2	1:B:207:ILE:CD1	2.50	0.41
1:A:46:ILE:HD12	1:A:46:ILE:N	2.35	0.41
1:A:73:ALA:O	1:A:74:PHE:CG	2.73	0.41
1:A:127:ILE:CD1	1:A:163:ALA:O	2.68	0.41
1:A:99:ARG:NH1	1:A:146:GLU:OE1	2.54	0.41
1:A:207:ILE:HB	1:A:228:GLY:C	2.45	0.41
1:B:244:ILE:HG12	1:B:244:ILE:H	1.59	0.41
1:A:28:LEU:HB3	1:A:59:ILE:HD11	2.03	0.41
1:A:35:ALA:C	1:A:37:THR:H	2.27	0.41
1:A:48:LEU:CD2	1:A:86:ILE:HG21	2.51	0.41
1:A:167:VAL:HG13	1:A:170:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:HD3	1:B:187:LYS:HA	1.52	0.41
1:B:216:ASN:O	1:B:219:GLU:CG	2.59	0.41
1:A:5:LYS:HG3	1:A:205:ARG:HD3	2.02	0.41
1:A:130:LYS:O	1:A:133:GLU:N	2.51	0.41
1:B:12:TRP:HE3	1:B:43:ALA:HB2	1.80	0.41
1:B:96:SER:O	1:B:97:GLU:C	2.64	0.41
1:B:110:GLY:HA3	1:B:153:ASN:ND2	2.34	0.41
1:B:192:LEU:HD12	1:B:192:LEU:HA	1.86	0.41
1:B:81:ALA:O	1:B:84:LYS:HB2	2.21	0.41
1:A:12:TRP:CE3	1:A:43:ALA:CB	2.80	0.41
1:A:16:GLY:O	1:B:82:MET:HE3	2.20	0.41
1:A:28:LEU:HD13	1:A:28:LEU:HA	1.78	0.41
1:A:67:TYR:CD2	1:A:68:LYS:O	2.73	0.41
1:A:190:GLY:O	1:A:191:TRP:C	2.63	0.41
1:A:191:TRP:CH2	1:A:195:HIS:CG	3.08	0.41
1:B:17:LYS:HE2	1:B:20:SER:OG	2.21	0.41
1:B:127:ILE:CG2	1:B:150:ILE:HD11	2.47	0.41
1:B:217:CYS:HB3	1:B:218:LYS:H	1.72	0.41
1:B:80:PRO:HG2	1:B:115:HIS:ND1	2.36	0.41
1:A:13:LYS:CA	1:A:64:GLN:NE2	2.81	0.40
1:A:18:ARG:HH11	1:A:18:ARG:CG	2.33	0.40
1:A:66:CYS:SG	1:A:67:TYR:N	2.94	0.40
1:A:75:THR:O	1:A:75:THR:HG22	2.20	0.40
1:A:221:ALA:HB2	1:A:229:PHE:HZ	1.87	0.40
1:B:97:GLU:O	1:B:98:ARG:O	2.38	0.40
1:B:117:LEU:HD21	1:B:123:VAL:HG21	1.99	0.40
1:B:222:SER:C	1:B:224:HIS:N	2.60	0.40
1:A:50:PHE:O	1:A:51:ALA:C	2.65	0.40
1:A:54:LYS:HE3	1:A:54:LYS:HB2	1.77	0.40
1:A:192:LEU:HB3	1:A:193:LYS:H	1.54	0.40
1:B:23:GLU:O	1:B:24:LEU:C	2.64	0.40
1:B:147:THR:HG22	1:B:191:TRP:HZ3	1.85	0.40
1:A:40:VAL:HA	1:A:60:GLY:O	2.22	0.40
1:A:115:HIS:O	1:A:119:GLU:HG3	2.21	0.40
1:A:96:SER:O	1:A:99:ARG:HB2	2.21	0.40
1:A:107:GLU:C	1:A:111:GLN:HE21	2.29	0.40
1:A:177:THR:O	1:A:178:PRO:C	2.64	0.40
1:B:148:LYS:CB	1:B:191:TRP:CH2	3.05	0.40
1:B:156:ASP:O	1:B:160:VAL:HG23	2.22	0.40
1:A:109:ILE:HD12	1:A:109:ILE:N	2.36	0.40
1:A:129:GLU:OE1	1:A:139:THR:HB	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TYR:CD1	1:A:184:VAL:HG11	2.53	0.40
1:B:243:ILE:HD13	1:B:243:ILE:HG21	1.91	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLN:NE2	1:B:171:GLY:O[2_565]	1.08	1.12
1:A:180:GLN:NE2	1:B:171:GLY:C[2_565]	1.90	0.30

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	245/247 (99%)	144 (59%)	63 (26%)	38 (16%)	0	0
1	B	245/247 (99%)	162 (66%)	60 (24%)	23 (9%)	0	0
All	All	490/494 (99%)	306 (62%)	123 (25%)	61 (12%)	0	0

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ALA
1	A	57	ALA
1	A	58	LYS
1	A	77	GLU
1	A	104	GLU
1	A	131	LEU
1	A	154	VAL
1	A	155	LYS
1	A	156	ASP
1	A	158	SER

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Mol	Chain	Res	Type
1	A	174	LYS
1	A	197	SER
1	A	224	HIS
1	A	233	GLY
1	B	4	ARG
1	B	57	ALA
1	B	70	PRO
1	B	119	GLU
1	B	168	TRP
1	B	197	SER
1	B	211	SER
1	B	223	GLN
1	A	33	LEU
1	A	142	VAL
1	A	173	GLY
1	A	222	SER
1	A	225	ASP
1	A	234	ALA
1	A	238	PRO
1	A	245	ASN
1	A	246	ALA
1	B	68	LYS
1	B	150	ILE
1	B	155	LYS
1	B	212	VAL
1	B	217	CYS
1	B	233	GLY
1	A	35	ALA
1	A	44	PRO
1	A	166	PRO
1	B	44	PRO
1	B	238	PRO
1	A	2	PRO
1	A	5	LYS
1	A	16	GLY
1	A	45	SER
1	A	70	PRO
1	A	96	SER
1	B	98	ARG
1	B	106	ASP
1	A	65	ASN
1	A	150	ILE

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Mol	Chain	Res	Type
1	B	234	ALA
1	A	91	VAL
1	B	200	VAL
1	A	244	ILE
1	B	83	ILE
1	A	69	VAL
1	B	243	ILE
1	A	87	GLY
1	B	171	GLY

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	192/192 (100%)	161 (84%)	31 (16%)	2	4
1	B	192/192 (100%)	166 (86%)	26 (14%)	4	8
All	All	384/384 (100%)	327 (85%)	57 (15%)	3	6

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	14	MET
1	A	24	LEU
1	A	25	ILE
1	A	38	GLU
1	A	41	CYS
1	A	46	ILE
1	A	55	LEU
1	A	56	ASP
1	A	58	LYS
1	A	64	GLN
1	A	66	CYS
1	A	74	PHE
1	A	75	THR

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Mol	Chain	Res	Type
1	A	82	MET
1	A	83	ILE
1	A	85	ASP
1	A	92	ILE
1	A	98	ARG
1	A	127	ILE
1	A	152	ASP
1	A	156	ASP
1	A	161	VAL
1	A	172	THR
1	A	185	HIS
1	A	225	ASP
1	A	227	ASP
1	A	229	PHE
1	A	231	VAL
1	A	239	GLU
1	A	242	ASP
1	B	18	ARG
1	B	24	LEU
1	B	28	LEU
1	B	45	SER
1	B	59	ILE
1	B	78	ILE
1	B	79	SER
1	B	85	ASP
1	B	92	ILE
1	B	98	ARG
1	B	99	ARG
1	B	109	ILE
1	B	130	LYS
1	B	132	ASP
1	B	135	GLU
1	B	139	THR
1	B	140	GLU
1	B	170	ILE
1	B	205	ARG
1	B	211	SER
1	B	213	THR
1	B	219	GLU
1	B	225	ASP
1	B	226	VAL
1	B	231	VAL

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Mol	Chain	Res	Type
1	B	240	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	65	ASN
1	A	100	HIS
1	A	115	HIS
1	A	145	GLN
1	A	203	GLN
1	A	223	GLN
1	A	245	ASN
1	B	100	HIS
1	B	245	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	98:ARG	C	99:ARG	N	1.19

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.