



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:12 pm BST

PDB ID : 2ATC  
Title : CRYSTAL AND MOLECULAR STRUCTURES OF NATIVE AND CTP-LIGANDED ASPARTATE CARBAMOYLTRANSFERASE FROM ESCHERICHIA COLI  
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Deposited on : 1982-03-24  
Resolution : 3.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

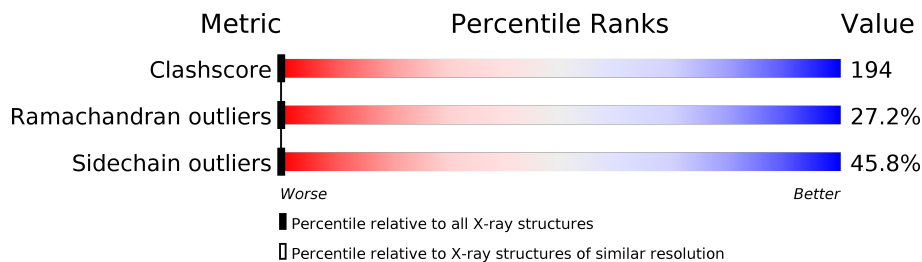
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	305	
2	B	152	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	B	153	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3511 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 ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	X			
1	A	305	2362	1491	420	441	8	2	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	LYS	CONFLICT	UNP P0A786
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	86	GLN	GLU	CONFLICT	UNP P0A786
A	90	ASN	ASP	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	153	ASN	ASP	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
A	?	-	MET	DELETION	UNP P0A786
A	?	-	ALA	DELETION	UNP P0A786
A	?	-	GLU	DELETION	UNP P0A786
A	?	-	VAL	DELETION	UNP P0A786
A	?	-	ASP	DELETION	UNP P0A786
A	?	-	ILE	DELETION	UNP P0A786
A	?	-	LEU	DELETION	UNP P0A786
A	?	-	TYR	DELETION	UNP P0A786
A	234	ASX	ASN	CONFLICT	UNP P0A786
A	240	LEU	VAL	CONFLICT	UNP P0A786
A	241	VAL	LEU	CONFLICT	UNP P0A786
A	244	ASN	-	INSERTION	UNP P0A786
A	246	LEU	-	INSERTION	UNP P0A786
A	247	GLY	-	INSERTION	UNP P0A786
A	248	GLY	ASP	CONFLICT	UNP P0A786
A	254	MET	ALA	CONFLICT	UNP P0A786
A	256	ALA	MET	CONFLICT	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	152	1148	714	202	227	5	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ASN	ASP	CONFLICT	UNP P0A7F3
B	5	ASP	ASN	CONFLICT	UNP P0A7F3
B	10	ALA	GLU	CONFLICT	UNP P0A7F3
B	11	GLU	ALA	CONFLICT	UNP P0A7F3
B	19	ASN	ASP	CONFLICT	UNP P0A7F3
B	24	GLU	GLN	CONFLICT	UNP P0A7F3
B	39	GLN	ASP	CONFLICT	UNP P0A7F3
B	40	ASP	GLN	CONFLICT	UNP P0A7F3
B	70	GLU	GLN	CONFLICT	UNP P0A7F3
B	73	GLU	GLN	CONFLICT	UNP P0A7F3
B	87	ASN	ASP	CONFLICT	UNP P0A7F3
B	88	ASP	ASN	CONFLICT	UNP P0A7F3
B	103	ASN	-	INSERTION	UNP P0A7F3
B	?	-	ASN	DELETION	UNP P0A7F3
B	111	ASP	ASN	CONFLICT	UNP P0A7F3
B	?	-	LYS	DELETION	UNP P0A7F3
B	131	ASP	ASN	CONFLICT	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

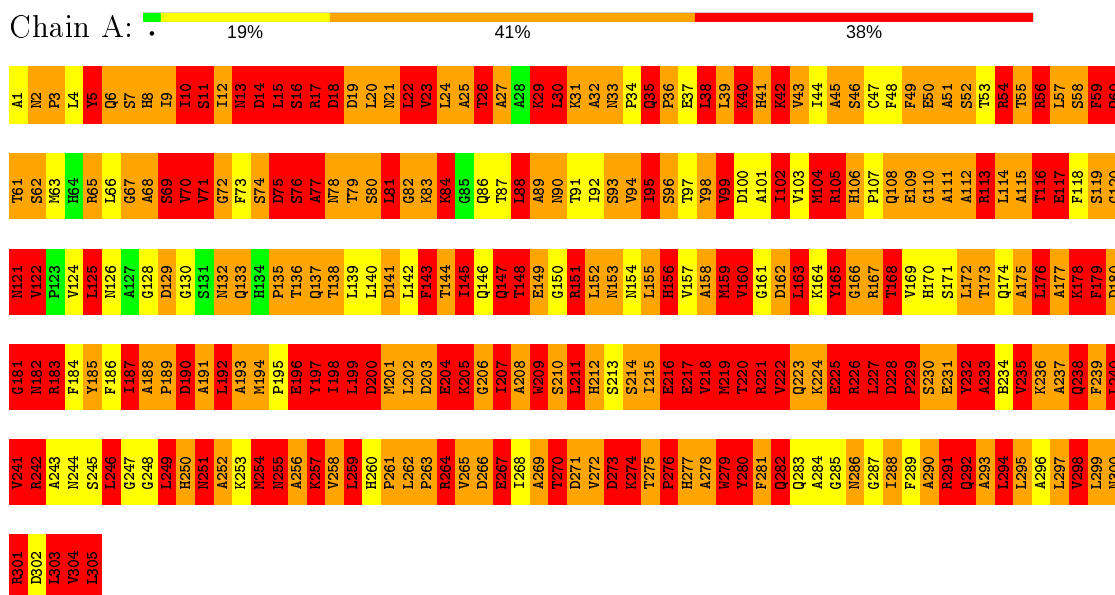
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0

### 3 Residue-property plots

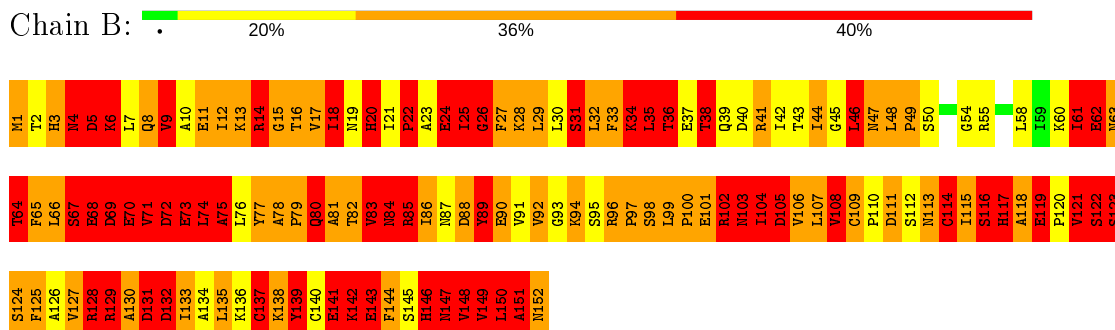
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN



- Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.70Å 131.70Å 199.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.270 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	1.67	28/2399 (1.2%)	3.68	435/3256 (13.4%)
2	B	1.80	14/1165 (1.2%)	3.50	210/1575 (13.3%)
All	All	1.71	42/3564 (1.2%)	3.62	645/4831 (13.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
2	B	0	4
All	All	0	19

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	GLY	N-CA	13.06	1.65	1.46
2	B	119	GLU	CD-OE1	-8.62	1.16	1.25
1	A	230	SER	C-O	8.43	1.39	1.23
1	A	230	SER	N-CA	7.88	1.62	1.46
2	B	143	GLU	CG-CD	-7.51	1.40	1.51
2	B	129	ARG	CZ-NH2	7.44	1.42	1.33
1	A	230	SER	CB-OG	7.32	1.51	1.42
1	A	225	GLU	CD-OE1	-7.08	1.17	1.25
1	A	204	GLU	CD-OE2	6.88	1.33	1.25
1	A	239	PHE	CA-CB	-6.32	1.40	1.53
2	B	114	CYS	CB-SG	-6.11	1.71	1.82
1	A	11	SER	CB-OG	-6.04	1.34	1.42
2	B	64	THR	C-O	6.02	1.34	1.23
1	A	301	ARG	CZ-NH2	5.94	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	ARG	CZ-NH1	5.92	1.40	1.33
1	A	214	SER	CA-CB	-5.81	1.44	1.52
2	B	68	GLU	CD-OE2	5.77	1.32	1.25
1	A	231	GLU	N-CA	5.76	1.57	1.46
2	B	124	SER	CB-OG	5.75	1.49	1.42
1	A	248	GLY	N-CA	-5.74	1.37	1.46
1	A	291	ARG	NE-CZ	-5.66	1.25	1.33
1	A	264	ARG	CD-NE	-5.60	1.36	1.46
1	A	242	ARG	CZ-NH2	5.59	1.40	1.33
1	A	210	SER	CA-CB	5.52	1.61	1.52
1	A	79	THR	CB-OG1	5.39	1.54	1.43
1	A	263	PRO	N-CD	-5.26	1.40	1.47
1	A	291	ARG	CD-NE	-5.25	1.37	1.46
1	A	16	SER	CA-CB	5.24	1.60	1.52
1	A	251	ASN	N-CA	5.24	1.56	1.46
2	B	81	ALA	N-CA	5.18	1.56	1.46
1	A	26	THR	N-CA	5.15	1.56	1.46
1	A	150	GLY	N-CA	-5.13	1.38	1.46
1	A	296	ALA	CA-CB	-5.13	1.41	1.52
1	A	54	ARG	CZ-NH2	5.13	1.39	1.33
2	B	54	GLY	N-CA	5.13	1.53	1.46
2	B	38	THR	CA-CB	5.11	1.66	1.53
1	A	82	GLY	CA-C	5.09	1.59	1.51
2	B	112	SER	CB-OG	5.09	1.48	1.42
1	A	181	GLY	C-O	5.08	1.31	1.23
1	A	242	ARG	CZ-NH1	5.06	1.39	1.33
2	B	93	GLY	C-O	5.04	1.31	1.23
2	B	116	SER	C-O	5.00	1.32	1.23

All (645) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ARG	CD-NE-CZ	26.04	160.05	123.60
1	A	242	ARG	NE-CZ-NH1	23.78	132.19	120.30
1	A	242	ARG	CD-NE-CZ	21.68	153.95	123.60
1	A	54	ARG	NE-CZ-NH2	-20.02	110.29	120.30
1	A	305	LEU	CA-CB-CG	19.93	161.14	115.30
1	A	197	TYR	CB-CG-CD1	-19.88	109.07	121.00
1	A	167	ARG	NE-CZ-NH2	18.97	129.79	120.30
1	A	197	TYR	CB-CG-CD2	18.89	132.34	121.00
1	A	147	GLN	CA-CB-CG	18.81	154.79	113.40
1	A	291	ARG	CD-NE-CZ	18.65	149.70	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	CD-NE-CZ	17.69	148.37	123.60
2	B	72	ASP	CB-CG-OD1	-17.45	102.59	118.30
1	A	105	ARG	NE-CZ-NH1	17.21	128.91	120.30
2	B	16	THR	N-CA-CB	17.12	142.82	110.30
1	A	54	ARG	NE-CZ-NH1	16.51	128.55	120.30
2	B	131	ASP	CA-CB-CG	16.16	148.96	113.40
1	A	292	GLN	CA-CB-CG	15.59	147.69	113.40
1	A	167	ARG	CD-NE-CZ	15.48	145.27	123.60
2	B	14	ARG	NE-CZ-NH2	15.22	127.91	120.30
1	A	221	ARG	NE-CZ-NH2	14.87	127.74	120.30
1	A	226	ARG	NE-CZ-NH1	14.81	127.71	120.30
1	A	149	GLU	C-N-CA	14.71	153.19	122.30
1	A	113	ARG	NE-CZ-NH1	-13.44	113.58	120.30
2	B	132	ASP	CB-CG-OD1	13.41	130.37	118.30
1	A	203	ASP	CB-CG-OD1	13.29	130.26	118.30
2	B	118	ALA	CB-CA-C	13.13	129.80	110.10
1	A	225	GLU	OE1-CD-OE2	13.10	139.02	123.30
2	B	128	ARG	NE-CZ-NH1	13.03	126.81	120.30
2	B	117	HIS	CA-CB-CG	13.02	135.73	113.60
1	A	204	GLU	CB-CG-CD	12.92	149.08	114.20
1	A	264	ARG	CD-NE-CZ	12.89	141.65	123.60
1	A	105	ARG	NE-CZ-NH2	-12.86	113.87	120.30
2	B	139	TYR	CB-CG-CD1	-12.80	113.32	121.00
1	A	212	HIS	CA-CB-CG	-12.80	91.84	113.60
1	A	250	HIS	CB-CA-C	12.72	135.84	110.40
1	A	292	GLN	CB-CG-CD	12.67	144.53	111.60
1	A	38	LEU	O-C-N	12.53	142.75	122.70
2	B	149	VAL	O-C-N	12.29	142.36	122.70
1	A	301	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	A	125	LEU	CB-CA-C	12.16	133.30	110.20
2	B	129	ARG	NE-CZ-NH1	12.13	126.36	120.30
1	A	226	ARG	N-CA-CB	-12.06	88.89	110.60
1	A	267	GLU	OE1-CD-OE2	11.73	137.38	123.30
1	A	43	VAL	CA-C-N	11.62	142.77	117.20
1	A	204	GLU	CA-CB-CG	11.54	138.79	113.40
1	A	249	LEU	N-CA-CB	11.41	133.23	110.40
1	A	162	ASP	CB-CG-OD2	-11.27	108.15	118.30
1	A	56	ARG	CD-NE-CZ	-11.25	107.85	123.60
2	B	81	ALA	CB-CA-C	11.15	126.82	110.10
1	A	152	LEU	C-N-CA	11.14	149.56	121.70
1	A	225	GLU	CG-CD-OE2	-11.11	96.08	118.30
1	A	296	ALA	CB-CA-C	11.11	126.76	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ASN	N-CA-CB	-10.69	91.35	110.60
1	A	220	THR	O-C-N	10.65	139.74	122.70
1	A	271	ASP	CA-CB-CG	10.64	136.81	113.40
2	B	143	GLU	CB-CG-CD	10.59	142.78	114.20
1	A	243	ALA	N-CA-CB	-10.58	95.29	110.10
1	A	232	TYR	CB-CG-CD1	10.56	127.33	121.00
1	A	270	THR	CA-CB-CG2	10.50	127.10	112.40
1	A	226	ARG	CB-CA-C	10.47	131.34	110.40
1	A	220	THR	N-CA-CB	10.42	130.11	110.30
1	A	242	ARG	N-CA-CB	10.40	129.33	110.60
2	B	103	ASN	CA-CB-CG	-10.40	90.51	113.40
1	A	227	LEU	CA-C-N	10.40	140.08	117.20
1	A	217	GLU	N-CA-CB	10.34	129.22	110.60
1	A	247	GLY	C-N-CA	10.28	143.89	122.30
1	A	196	GLU	O-C-N	10.25	139.10	122.70
1	A	112	ALA	N-CA-CB	10.14	124.29	110.10
1	A	67	GLY	CA-C-N	10.09	139.39	117.20
1	A	210	SER	N-CA-CB	-10.08	95.37	110.50
1	A	144	THR	OG1-CB-CG2	10.06	133.15	110.00
2	B	72	ASP	CB-CG-OD2	10.06	127.35	118.30
1	A	273	ASP	CB-CG-OD1	10.04	127.34	118.30
1	A	102	ILE	CA-C-O	-10.02	99.06	120.10
1	A	116	THR	N-CA-CB	9.91	129.12	110.30
2	B	6	LYS	CA-C-N	-9.90	95.41	117.20
2	B	139	TYR	CB-CG-CD2	9.89	126.93	121.00
1	A	143	PHE	CA-C-O	9.88	140.84	120.10
1	A	109	GLU	OE1-CD-OE2	-9.86	111.47	123.30
1	A	57	LEU	CB-CA-C	9.82	128.85	110.20
1	A	200	ASP	CB-CG-OD2	-9.82	109.47	118.30
2	B	48	LEU	CA-CB-CG	9.81	137.86	115.30
2	B	61	ILE	C-N-CA	9.78	146.16	121.70
1	A	26	THR	CA-CB-OG1	-9.78	88.47	109.00
1	A	204	GLU	OE1-CD-OE2	-9.72	111.64	123.30
1	A	205	LYS	CA-CB-CG	9.68	134.69	113.40
1	A	1	ALA	N-CA-CB	-9.67	96.57	110.10
2	B	81	ALA	N-CA-CB	-9.66	96.58	110.10
2	B	103	ASN	CA-C-N	-9.63	96.01	117.20
1	A	25	ALA	N-CA-CB	9.57	123.50	110.10
2	B	14	ARG	NH1-CZ-NH2	-9.53	108.92	119.40
1	A	288	ILE	N-CA-CB	9.52	132.69	110.80
2	B	149	VAL	CA-C-N	-9.48	96.35	117.20
1	A	180	ASP	CB-CG-OD1	-9.47	109.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	SER	CA-C-N	9.46	138.01	117.20
2	B	16	THR	O-C-N	9.44	137.81	122.70
1	A	251	ASN	CA-C-O	-9.43	100.29	120.10
2	B	68	GLU	N-CA-CB	9.29	127.31	110.60
1	A	100	ASP	CB-CG-OD1	9.26	126.64	118.30
1	A	18	ASP	N-CA-CB	-9.26	93.93	110.60
2	B	32	LEU	CB-CA-C	9.24	127.75	110.20
1	A	204	GLU	C-N-CA	9.23	144.78	121.70
1	A	246	LEU	C-N-CA	9.19	141.59	122.30
1	A	269	ALA	N-CA-CB	-9.17	97.26	110.10
1	A	235	VAL	N-CA-CB	9.17	131.67	111.50
2	B	36	THR	N-CA-CB	9.17	127.72	110.30
2	B	141	GLU	CG-CD-OE2	-9.10	100.09	118.30
2	B	33	PHE	CB-CG-CD1	-9.09	114.44	120.80
2	B	68	GLU	CG-CD-OE1	9.09	136.47	118.30
2	B	150	LEU	CB-CA-C	9.08	127.45	110.20
1	A	292	GLN	OE1-CD-NE2	-9.06	101.07	121.90
1	A	108	GLN	O-C-N	9.04	137.17	122.70
1	A	227	LEU	CA-C-O	-9.04	101.11	120.10
1	A	197	TYR	CB-CA-C	9.03	128.46	110.40
1	A	35	GLN	CA-CB-CG	9.00	133.21	113.40
1	A	180	ASP	CB-CG-OD2	8.97	126.37	118.30
1	A	238	GLN	CA-CB-CG	8.96	133.11	113.40
2	B	119	GLU	CG-CD-OE2	-8.96	100.38	118.30
1	A	256	ALA	CB-CA-C	-8.89	96.76	110.10
1	A	302	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	A	269	ALA	CB-CA-C	-8.87	96.79	110.10
1	A	43	VAL	CA-CB-CG2	8.86	124.19	110.90
1	A	5	TYR	CA-CB-CG	-8.85	96.58	113.40
1	A	212	HIS	CB-CA-C	-8.85	92.69	110.40
2	B	14	ARG	C-N-CA	-8.83	103.77	122.30
2	B	117	HIS	O-C-N	8.79	136.77	122.70
1	A	221	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	A	144	THR	N-CA-CB	-8.72	93.72	110.30
2	B	137	CYS	O-C-N	8.72	136.65	122.70
1	A	8	HIS	CA-CB-CG	-8.67	98.86	113.60
1	A	43	VAL	CA-C-O	-8.67	101.90	120.10
2	B	15	GLY	CA-C-O	-8.67	105.00	120.60
1	A	301	ARG	CG-CD-NE	8.64	129.95	111.80
1	A	89	ALA	O-C-N	8.64	136.52	122.70
1	A	239	PHE	C-N-CA	8.62	143.26	121.70
1	A	40	LYS	CB-CA-C	-8.61	93.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	PHE	CB-CG-CD2	-8.60	114.78	120.80
2	B	141	GLU	OE1-CD-OE2	8.60	133.61	123.30
1	A	17	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	A	226	ARG	NE-CZ-NH2	-8.51	116.05	120.30
2	B	72	ASP	C-N-CA	8.46	142.86	121.70
1	A	143	PHE	CA-C-N	-8.43	98.64	117.20
2	B	151	ALA	N-CA-CB	-8.43	98.30	110.10
1	A	168	THR	CA-CB-OG1	-8.41	91.33	109.00
1	A	98	TYR	CB-CG-CD2	8.40	126.04	121.00
1	A	15	LEU	C-N-CA	8.39	142.69	121.70
1	A	129	ASP	CB-CG-OD2	8.32	125.79	118.30
2	B	24	GLU	N-CA-CB	-8.25	95.75	110.60
1	A	149	GLU	CG-CD-OE1	8.24	134.79	118.30
2	B	22	PRO	N-CA-C	-8.23	90.69	112.10
1	A	230	SER	CA-C-O	-8.23	102.81	120.10
1	A	278	ALA	CA-C-N	8.20	135.25	117.20
1	A	32	ALA	N-CA-CB	-8.18	98.65	110.10
1	A	106	HIS	N-CA-CB	-8.17	95.90	110.60
2	B	71	VAL	CG1-CB-CG2	8.16	123.95	110.90
2	B	103	ASN	C-N-CA	-8.14	101.34	121.70
2	B	62	GLU	CB-CA-C	-8.14	94.13	110.40
2	B	103	ASN	CB-CG-OD1	-8.13	105.34	121.60
2	B	131	ASP	N-CA-CB	8.13	125.24	110.60
2	B	70	GLU	OE1-CD-OE2	8.12	133.05	123.30
1	A	93	SER	N-CA-CB	8.12	122.68	110.50
1	A	228	ASP	CB-CG-OD1	-8.11	111.00	118.30
1	A	71	VAL	N-CA-CB	-8.07	93.74	111.50
1	A	240	LEU	CA-CB-CG	8.07	133.87	115.30
2	B	47	ASN	O-C-N	8.04	135.57	122.70
2	B	24	GLU	CA-CB-CG	8.04	131.09	113.40
1	A	27	ALA	CB-CA-C	8.03	122.14	110.10
1	A	8	HIS	O-C-N	8.02	135.54	122.70
1	A	21	ASN	CA-CB-CG	8.02	131.05	113.40
1	A	77	ALA	CB-CA-C	8.02	122.13	110.10
2	B	80	GLN	CA-CB-CG	8.00	131.00	113.40
1	A	8	HIS	N-CA-CB	7.98	124.96	110.60
1	A	288	ILE	O-C-N	7.97	135.46	122.70
1	A	197	TYR	N-CA-CB	-7.97	96.26	110.60
2	B	70	GLU	C-N-CA	7.96	141.59	121.70
2	B	15	GLY	N-CA-C	-7.95	93.23	113.10
2	B	126	ALA	CB-CA-C	7.94	122.01	110.10
1	A	50	GLU	OE1-CD-OE2	-7.93	113.78	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ALA	O-C-N	7.91	135.36	122.70
2	B	68	GLU	N-CA-C	-7.89	89.68	111.00
2	B	117	HIS	N-CA-CB	7.87	124.76	110.60
1	A	242	ARG	NH1-CZ-NH2	-7.86	110.76	119.40
1	A	167	ARG	NH1-CZ-NH2	-7.84	110.78	119.40
2	B	141	GLU	N-CA-CB	-7.83	96.51	110.60
1	A	197	TYR	O-C-N	-7.78	110.25	122.70
1	A	52	SER	CB-CA-C	7.78	124.87	110.10
1	A	242	ARG	NE-CZ-NH2	-7.73	116.43	120.30
2	B	124	SER	CB-CA-C	7.72	124.77	110.10
1	A	129	ASP	N-CA-CB	7.72	124.49	110.60
1	A	270	THR	CA-CB-OG1	-7.72	92.79	109.00
1	A	237	ALA	N-CA-C	-7.68	90.26	111.00
2	B	94	LYS	N-CA-CB	7.68	124.42	110.60
1	A	225	GLU	CB-CG-CD	-7.67	93.48	114.20
1	A	250	HIS	N-CA-CB	-7.67	96.79	110.60
1	A	11	SER	C-N-CA	7.66	140.85	121.70
1	A	16	SER	O-C-N	7.66	134.95	122.70
2	B	5	ASP	CB-CG-OD1	7.65	125.19	118.30
1	A	217	GLU	O-C-N	7.62	134.90	122.70
1	A	207	ILE	N-CA-C	7.62	131.57	111.00
1	A	280	TYR	CB-CG-CD2	7.61	125.57	121.00
2	B	5	ASP	CA-C-O	7.61	136.08	120.10
1	A	145	ILE	CA-CB-CG1	-7.61	96.55	111.00
1	A	219	MET	CA-CB-CG	7.60	126.22	113.30
1	A	221	ARG	CG-CD-NE	7.59	127.75	111.80
2	B	129	ARG	CD-NE-CZ	7.59	134.23	123.60
1	A	238	GLN	N-CA-CB	7.58	124.25	110.60
1	A	242	ARG	CA-C-N	-7.58	100.53	117.20
2	B	129	ARG	NH1-CZ-NH2	-7.58	111.06	119.40
1	A	212	HIS	O-C-N	7.56	134.79	122.70
1	A	45	ALA	CA-C-O	-7.53	104.29	120.10
1	A	290	ALA	N-CA-CB	7.51	120.62	110.10
1	A	273	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	29	LYS	CB-CA-C	-7.51	95.38	110.40
1	A	52	SER	N-CA-CB	-7.50	99.26	110.50
1	A	264	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	A	144	THR	CA-CB-CG2	-7.47	101.94	112.40
1	A	90	ASN	N-CA-C	-7.46	90.84	111.00
1	A	20	LEU	CB-CA-C	-7.46	96.03	110.20
1	A	216	GLU	N-CA-CB	-7.45	97.19	110.60
2	B	146	HIS	CB-CA-C	-7.45	95.50	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	SER	N-CA-CB	-7.45	99.33	110.50
2	B	117	HIS	CB-CA-C	-7.44	95.53	110.40
1	A	153	ASN	N-CA-CB	-7.41	97.27	110.60
2	B	65	PHE	CB-CG-CD1	7.37	125.96	120.80
1	A	188	ALA	N-CA-CB	7.36	120.41	110.10
2	B	94	LYS	CB-CG-CD	7.36	130.74	111.60
2	B	147	ASN	CA-C-N	-7.33	101.06	117.20
1	A	38	LEU	CB-CA-C	-7.33	96.27	110.20
1	A	291	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	67	GLY	O-C-N	-7.32	110.99	122.70
1	A	226	ARG	CD-NE-CZ	-7.31	113.36	123.60
2	B	4	ASN	C-N-CA	7.31	139.97	121.70
2	B	105	ASP	CB-CA-C	7.28	124.96	110.40
1	A	149	GLU	CG-CD-OE2	-7.23	103.84	118.30
1	A	221	ARG	CD-NE-CZ	7.21	133.69	123.60
2	B	65	PHE	CB-CG-CD2	-7.20	115.76	120.80
1	A	81	LEU	CA-CB-CG	7.18	131.82	115.30
2	B	142	LYS	N-CA-CB	7.18	123.53	110.60
2	B	108	VAL	CG1-CB-CG2	7.18	122.39	110.90
2	B	18	ILE	C-N-CA	7.17	139.64	121.70
1	A	270	THR	N-CA-CB	-7.15	96.71	110.30
1	A	104	MET	CA-CB-CG	7.14	125.43	113.30
1	A	109	GLU	CA-CB-CG	7.14	129.10	113.40
2	B	72	ASP	CA-CB-CG	-7.13	97.71	113.40
1	A	106	HIS	CA-CB-CG	7.11	125.68	113.60
2	B	68	GLU	O-C-N	7.10	134.07	122.70
1	A	121	ASN	CA-CB-CG	7.10	129.02	113.40
2	B	78	ALA	CB-CA-C	7.05	120.68	110.10
1	A	155	LEU	CA-C-O	7.05	134.91	120.10
1	A	69	SER	CB-CA-C	7.04	123.47	110.10
2	B	1	MET	CA-C-O	7.03	134.87	120.10
1	A	105	ARG	CD-NE-CZ	7.03	133.44	123.60
1	A	159	MET	CB-CA-C	7.02	124.43	110.40
2	B	46	LEU	O-C-N	-7.01	111.48	122.70
1	A	108	GLN	CA-C-O	-7.01	105.38	120.10
1	A	280	TYR	CB-CA-C	7.00	124.39	110.40
2	B	46	LEU	CB-CA-C	6.99	123.48	110.20
1	A	200	ASP	O-C-N	6.99	133.88	122.70
2	B	62	GLU	O-C-N	6.99	133.88	122.70
2	B	6	LYS	N-CA-CB	6.98	123.17	110.60
1	A	292	GLN	CG-CD-OE1	6.98	135.56	121.60
2	B	127	VAL	CB-CA-C	-6.97	98.16	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	TYR	CB-CG-CD2	-6.96	116.83	121.00
1	A	224	LYS	CB-CA-C	6.95	124.30	110.40
1	A	94	VAL	CA-C-O	6.95	134.69	120.10
2	B	70	GLU	CG-CD-OE2	-6.95	104.41	118.30
1	A	298	VAL	O-C-N	-6.94	111.60	122.70
1	A	152	LEU	CA-CB-CG	6.93	131.24	115.30
2	B	137	CYS	CA-C-O	-6.93	105.55	120.10
2	B	37	GLU	CG-CD-OE1	6.92	132.15	118.30
2	B	84	ASN	CA-CB-CG	6.92	128.63	113.40
1	A	226	ARG	CB-CG-CD	-6.90	93.66	111.60
2	B	35	LEU	CB-CA-C	6.90	123.31	110.20
2	B	126	ALA	N-CA-CB	-6.90	100.44	110.10
1	A	179	PHE	N-CA-CB	6.90	123.01	110.60
2	B	149	VAL	N-CA-C	-6.90	92.38	111.00
2	B	71	VAL	CB-CA-C	-6.89	98.31	111.40
2	B	37	GLU	N-CA-C	-6.88	92.42	111.00
1	A	77	ALA	N-CA-CB	6.88	119.73	110.10
1	A	237	ALA	CB-CA-C	6.88	120.42	110.10
1	A	228	ASP	CB-CG-OD2	6.84	124.46	118.30
1	A	192	LEU	CA-C-O	6.82	134.42	120.10
1	A	257	LYS	CA-CB-CG	6.82	128.40	113.40
2	B	151	ALA	N-CA-C	-6.82	92.60	111.00
2	B	117	HIS	C-N-CA	-6.80	104.69	121.70
1	A	231	GLU	N-CA-CB	-6.79	98.38	110.60
1	A	102	ILE	CA-C-N	6.78	132.12	117.20
1	A	144	THR	CB-CA-C	6.78	129.90	111.60
1	A	169	VAL	C-N-CA	6.77	138.61	121.70
1	A	52	SER	C-N-CA	6.76	138.61	121.70
2	B	111	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	273	ASP	N-CA-CB	6.76	122.77	110.60
1	A	22	LEU	CA-CB-CG	6.75	130.82	115.30
1	A	25	ALA	CA-C-O	-6.74	105.94	120.10
1	A	211	LEU	O-C-N	-6.74	111.92	122.70
2	B	31	SER	CA-C-N	-6.74	102.38	117.20
2	B	129	ARG	N-CA-C	6.74	129.18	111.00
1	A	98	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	A	126	ASN	O-C-N	6.72	133.46	122.70
1	A	258	VAL	CA-C-O	-6.72	105.98	120.10
1	A	5	TYR	CB-CG-CD1	6.72	125.03	121.00
1	A	259	LEU	CB-CA-C	-6.69	97.48	110.20
1	A	206	GLY	C-N-CA	6.67	138.38	121.70
2	B	131	ASP	CB-CG-OD1	6.66	124.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ASP	OD1-CG-OD2	6.65	135.94	123.30
2	B	67	SER	CA-CB-OG	6.65	129.16	111.20
2	B	129	ARG	CB-CA-C	-6.64	97.11	110.40
1	A	72	GLY	O-C-N	6.63	133.31	122.70
1	A	136	THR	N-CA-CB	6.63	122.89	110.30
1	A	217	GLU	CA-C-N	-6.63	102.62	117.20
2	B	34	LYS	CB-CA-C	-6.63	97.14	110.40
1	A	196	GLU	CA-C-O	-6.62	106.20	120.10
1	A	5	TYR	CB-CA-C	-6.62	97.17	110.40
1	A	216	GLU	CB-CA-C	-6.62	97.17	110.40
1	A	33	ASN	CA-CB-CG	-6.61	98.86	113.40
1	A	69	SER	O-C-N	-6.56	112.20	122.70
2	B	103	ASN	CB-CA-C	-6.56	97.28	110.40
1	A	122	VAL	CB-CA-C	6.55	123.85	111.40
2	B	119	GLU	CG-CD-OE1	6.55	131.40	118.30
1	A	209	TRP	CA-C-N	-6.54	102.81	117.20
2	B	146	HIS	N-CA-CB	6.54	122.37	110.60
1	A	183	ARG	CA-C-O	6.52	133.79	120.10
1	A	143	PHE	CA-CB-CG	6.52	129.55	113.90
1	A	23	VAL	CB-CA-C	6.51	123.78	111.40
1	A	172	LEU	CA-CB-CG	-6.51	100.32	115.30
1	A	73	PHE	O-C-N	6.48	133.07	122.70
1	A	251	ASN	CA-C-N	6.45	131.39	117.20
1	A	160	VAL	N-CA-CB	-6.44	97.32	111.50
1	A	17	ARG	NH1-CZ-NH2	6.44	126.49	119.40
1	A	128	GLY	O-C-N	-6.44	112.39	122.70
2	B	127	VAL	CG1-CB-CG2	6.44	121.20	110.90
2	B	68	GLU	CG-CD-OE2	-6.43	105.43	118.30
1	A	273	ASP	O-C-N	6.43	132.98	122.70
2	B	131	ASP	CB-CG-OD2	6.43	124.08	118.30
2	B	106	VAL	CA-CB-CG2	-6.42	101.26	110.90
2	B	121	VAL	O-C-N	6.42	132.98	122.70
1	A	237	ALA	CA-C-N	-6.42	103.08	117.20
1	A	233	ALA	CB-CA-C	-6.42	100.48	110.10
2	B	128	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
2	B	88	ASP	CB-CA-C	6.40	123.21	110.40
1	A	238	GLN	N-CA-C	-6.40	93.72	111.00
1	A	43	VAL	N-CA-CB	-6.40	97.42	111.50
2	B	110	PRO	N-CD-CG	-6.40	93.60	103.20
1	A	49	PHE	CB-CA-C	6.39	123.18	110.40
1	A	148	THR	O-C-N	6.39	132.93	122.70
2	B	16	THR	N-CA-C	-6.39	93.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	A	299	LEU	N-CA-C	6.38	128.22	111.00
1	A	218	VAL	N-CA-C	-6.37	93.79	111.00
2	B	48	LEU	N-CA-C	-6.37	93.81	111.00
1	A	114	LEU	N-CA-CB	6.36	123.12	110.40
1	A	35	GLN	CB-CA-C	-6.35	97.70	110.40
1	A	238	GLN	CB-CA-C	6.35	123.11	110.40
1	A	70	VAL	O-C-N	6.35	132.86	122.70
1	A	159	MET	CG-SD-CE	6.35	110.36	100.20
2	B	15	GLY	O-C-N	6.33	132.83	122.70
1	A	153	ASN	CB-CG-ND2	-6.32	101.53	116.70
1	A	299	LEU	N-CA-CB	-6.30	97.80	110.40
1	A	248	GLY	CA-C-O	-6.29	109.27	120.60
1	A	301	ARG	NH1-CZ-NH2	-6.28	112.49	119.40
1	A	207	ILE	CG1-CB-CG2	6.28	125.22	111.40
1	A	10	ILE	CB-CA-C	-6.27	99.06	111.60
1	A	29	LYS	O-C-N	6.27	132.73	122.70
2	B	27	PHE	N-CA-C	-6.27	94.08	111.00
1	A	9	ILE	N-CA-CB	-6.26	96.39	110.80
1	A	241	VAL	CB-CA-C	6.26	123.29	111.40
1	A	223	GLN	OE1-CD-NE2	6.25	136.28	121.90
1	A	165	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	B	16	THR	CA-C-O	-6.25	106.98	120.10
2	B	151	ALA	CB-CA-C	-6.24	100.73	110.10
2	B	62	GLU	CA-C-N	-6.24	103.47	117.20
1	A	272	VAL	CB-CA-C	-6.22	99.58	111.40
1	A	232	TYR	CB-CA-C	-6.21	97.98	110.40
1	A	299	LEU	O-C-N	-6.21	112.77	122.70
2	B	89	TYR	CB-CA-C	6.21	122.81	110.40
2	B	122	SER	CA-C-N	6.19	130.81	117.20
1	A	84	LYS	C-N-CA	6.18	135.29	122.30
1	A	242	ARG	N-CA-C	-6.18	94.31	111.00
2	B	149	VAL	CA-CB-CG2	6.18	120.16	110.90
1	A	185	TYR	O-C-N	6.17	132.57	122.70
2	B	131	ASP	OD1-CG-OD2	-6.17	111.57	123.30
2	B	105	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	298	VAL	C-N-CA	6.16	137.10	121.70
1	A	67	GLY	CA-C-O	-6.16	109.52	120.60
1	A	203	ASP	C-N-CA	6.15	137.09	121.70
2	B	9	VAL	CA-CB-CG1	6.13	120.09	110.90
2	B	70	GLU	CA-C-O	6.12	132.96	120.10
1	A	71	VAL	N-CA-C	-6.12	94.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	LYS	N-CA-CB	-6.12	99.59	110.60
1	A	200	ASP	CA-CB-CG	-6.11	99.95	113.40
1	A	255	ASN	C-N-CA	6.10	136.95	121.70
1	A	269	ALA	N-CA-C	6.08	127.41	111.00
1	A	98	TYR	N-CA-CB	6.07	121.53	110.60
1	A	223	GLN	CG-CD-OE1	-6.07	109.46	121.60
2	B	125	PHE	CA-C-N	6.07	130.56	117.20
1	A	60	GLN	CA-CB-CG	6.07	126.74	113.40
1	A	179	PHE	CA-C-N	6.07	130.54	117.20
1	A	31	LYS	N-CA-CB	6.06	121.51	110.60
1	A	148	THR	N-CA-CB	6.05	121.79	110.30
2	B	6	LYS	CA-C-O	6.03	132.76	120.10
1	A	290	ALA	CA-C-O	-6.02	107.46	120.10
1	A	45	ALA	N-CA-CB	-6.01	101.68	110.10
2	B	29	LEU	CA-C-N	-6.01	103.97	117.20
1	A	19	ASP	CA-CB-CG	5.99	126.57	113.40
2	B	83	VAL	C-N-CA	5.99	136.67	121.70
1	A	65	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	208	ALA	CB-CA-C	5.98	119.07	110.10
2	B	2	THR	N-CA-CB	-5.97	98.95	110.30
1	A	3	PRO	O-C-N	-5.96	113.16	122.70
2	B	79	PRO	O-C-N	5.96	132.23	122.70
1	A	207	ILE	N-CA-CB	-5.95	97.13	110.80
2	B	148	VAL	N-CA-CB	-5.94	98.43	111.50
2	B	125	PHE	CA-C-O	-5.93	107.64	120.10
1	A	70	VAL	CA-C-N	-5.93	104.15	117.20
1	A	73	PHE	CA-C-O	-5.92	107.67	120.10
2	B	71	VAL	N-CA-CB	-5.92	98.49	111.50
1	A	217	GLU	CG-CD-OE2	-5.91	106.47	118.30
1	A	298	VAL	CA-C-N	5.88	130.14	117.20
1	A	125	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	A	189	PRO	N-CD-CG	-5.87	94.39	103.20
2	B	36	THR	O-C-N	5.87	132.09	122.70
1	A	42	LYS	N-CA-CB	-5.87	100.04	110.60
1	A	173	THR	CA-CB-OG1	-5.87	96.68	109.00
1	A	59	PHE	N-CA-CB	5.85	121.13	110.60
2	B	75	ALA	C-N-CA	5.85	136.32	121.70
1	A	69	SER	CA-C-O	5.84	132.37	120.10
1	A	95	ILE	N-CA-CB	-5.84	97.37	110.80
1	A	178	LYS	CA-C-O	-5.83	107.85	120.10
1	A	41	HIS	N-CA-CB	-5.82	100.12	110.60
1	A	158	ALA	N-CA-CB	-5.82	101.95	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LYS	CA-CB-CG	5.82	126.20	113.40
1	A	88	LEU	CA-C-O	-5.82	107.88	120.10
1	A	175	ALA	N-CA-CB	5.82	118.24	110.10
2	B	103	ASN	N-CA-CB	5.82	121.07	110.60
1	A	281	PHE	N-CA-CB	5.81	121.06	110.60
1	A	192	LEU	CA-C-N	-5.81	104.42	117.20
1	A	115	ALA	CA-C-N	5.80	129.97	117.20
1	A	143	PHE	CB-CG-CD1	5.80	124.86	120.80
1	A	223	GLN	CA-CB-CG	-5.80	100.64	113.40
1	A	278	ALA	CA-C-O	-5.79	107.94	120.10
1	A	65	ARG	N-CA-CB	5.79	121.02	110.60
2	B	29	LEU	CB-CG-CD1	5.79	120.84	111.00
1	A	167	ARG	C-N-CA	5.79	136.17	121.70
1	A	229	PRO	CA-N-CD	-5.79	103.40	111.50
1	A	207	ILE	C-N-CA	-5.78	107.25	121.70
1	A	290	ALA	CA-C-N	5.78	129.91	117.20
2	B	44	ILE	O-C-N	5.77	133.01	123.20
2	B	127	VAL	N-CA-C	5.76	126.55	111.00
1	A	138	THR	CA-CB-OG1	-5.75	96.92	109.00
1	A	89	ALA	CA-C-N	-5.75	104.56	117.20
1	A	209	TRP	CA-C-O	5.75	132.17	120.10
2	B	61	ILE	CA-CB-CG2	5.75	122.39	110.90
1	A	138	THR	OG1-CB-CG2	5.74	123.20	110.00
2	B	142	LYS	CD-CE-NZ	-5.74	98.50	111.70
1	A	165	TYR	CA-C-N	5.74	127.67	116.20
2	B	37	GLU	CA-C-O	-5.73	108.07	120.10
1	A	125	LEU	N-CA-C	-5.72	95.56	111.00
1	A	90	ASN	CB-CA-C	5.72	121.83	110.40
1	A	303	LEU	C-N-CA	5.72	135.99	121.70
1	A	117	GLU	CB-CA-C	-5.71	98.97	110.40
1	A	231	GLU	O-C-N	5.71	131.84	122.70
2	B	69	ASP	CB-CG-OD1	-5.71	113.16	118.30
2	B	70	GLU	CA-C-N	-5.71	104.64	117.20
2	B	144	PHE	CB-CA-C	5.71	121.82	110.40
1	A	17	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	217	GLU	CG-CD-OE1	5.70	129.69	118.30
1	A	56	ARG	NE-CZ-NH1	-5.69	117.45	120.30
2	B	103	ASN	O-C-N	5.69	131.80	122.70
1	A	242	ARG	CG-CD-NE	5.68	123.73	111.80
1	A	138	THR	CA-CB-CG2	-5.68	104.45	112.40
1	A	261	PRO	N-CD-CG	-5.67	94.69	103.20
2	B	104	ILE	CA-CB-CG1	-5.67	100.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	VAL	C-N-CA	5.67	135.88	121.70
1	A	30	LEU	CB-CA-C	5.67	120.97	110.20
2	B	14	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	B	151	ALA	O-C-N	5.66	131.76	122.70
2	B	123	SER	CA-CB-OG	5.66	126.48	111.20
1	A	19	ASP	CB-CA-C	5.66	121.71	110.40
2	B	27	PHE	CA-C-N	-5.65	104.78	117.20
1	A	249	LEU	O-C-N	5.64	131.73	122.70
1	A	13	ASN	CB-CG-ND2	-5.64	103.16	116.70
1	A	82	GLY	N-CA-C	-5.64	99.01	113.10
1	A	117	GLU	CA-CB-CG	5.63	125.78	113.40
2	B	139	TYR	O-C-N	5.63	131.70	122.70
2	B	150	LEU	CA-CB-CG	5.63	128.24	115.30
1	A	25	ALA	CA-C-N	5.61	129.55	117.20
2	B	139	TYR	CA-CB-CG	-5.61	102.73	113.40
2	B	35	LEU	O-C-N	-5.61	113.72	122.70
2	B	108	VAL	CA-CB-CG2	-5.60	102.50	110.90
1	A	288	ILE	CA-C-O	-5.59	108.36	120.10
1	A	291	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	A	168	THR	N-CA-CB	-5.59	99.69	110.30
1	A	288	ILE	CA-CB-CG2	5.59	122.07	110.90
1	A	75	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	122	VAL	N-CA-C	-5.58	95.93	111.00
1	A	175	ALA	N-CA-C	-5.58	95.95	111.00
1	A	303	LEU	CA-C-O	5.58	131.81	120.10
2	B	135	LEU	O-C-N	5.57	131.62	122.70
1	A	36	PRO	N-CA-C	-5.56	97.63	112.10
1	A	266	ASP	CA-CB-CG	-5.56	101.18	113.40
2	B	74	LEU	CB-CA-C	5.56	120.76	110.20
2	B	105	ASP	CA-CB-CG	-5.55	101.19	113.40
1	A	7	SER	CA-CB-OG	-5.54	96.23	111.20
1	A	274	LYS	CB-CA-C	-5.54	99.32	110.40
2	B	123	SER	O-C-N	-5.53	113.86	122.70
2	B	136	LYS	CA-C-N	5.52	129.35	117.20
2	B	97	PRO	N-CA-C	-5.52	97.75	112.10
1	A	215	ILE	CA-C-N	-5.52	105.07	117.20
2	B	94	LYS	O-C-N	5.51	131.53	122.70
1	A	141	ASP	CB-CA-C	-5.51	99.39	110.40
1	A	185	TYR	N-CA-CB	-5.50	100.69	110.60
1	A	135	PRO	N-CD-CG	-5.50	94.95	103.20
2	B	116	SER	CA-C-N	5.50	129.29	117.20
1	A	56	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LYS	CA-C-N	-5.49	105.12	117.20
1	A	221	ARG	N-CA-C	-5.49	96.17	111.00
2	B	29	LEU	N-CA-CB	-5.49	99.41	110.40
2	B	55	ARG	O-C-N	5.48	131.46	122.70
1	A	126	ASN	CA-C-O	-5.47	108.61	120.10
1	A	65	ARG	CD-NE-CZ	-5.46	115.95	123.60
1	A	109	GLU	CG-CD-OE1	5.45	129.20	118.30
1	A	10	ILE	CA-C-O	-5.44	108.67	120.10
1	A	167	ARG	CG-CD-NE	5.44	123.23	111.80
2	B	97	PRO	CA-C-O	-5.44	107.15	120.20
1	A	257	LYS	O-C-N	5.44	131.40	122.70
1	A	174	GLN	CA-C-O	-5.43	108.69	120.10
2	B	103	ASN	CA-C-O	5.42	131.49	120.10
1	A	99	VAL	CA-C-N	-5.42	105.27	117.20
1	A	223	GLN	N-CA-C	5.42	125.63	111.00
1	A	69	SER	N-CA-CB	-5.42	102.38	110.50
1	A	135	PRO	CB-CA-C	-5.42	98.46	112.00
2	B	122	SER	CA-C-O	-5.41	108.74	120.10
1	A	1	ALA	CA-C-O	5.41	131.45	120.10
1	A	72	GLY	CA-C-O	-5.41	110.87	120.60
1	A	271	ASP	CB-CA-C	5.39	121.18	110.40
2	B	2	THR	CA-C-O	-5.38	108.79	120.10
2	B	73	GLU	N-CA-CB	5.38	120.29	110.60
2	B	125	PHE	CB-CA-C	-5.37	99.67	110.40
2	B	55	ARG	N-CA-C	-5.36	96.54	111.00
1	A	172	LEU	O-C-N	5.35	131.26	122.70
1	A	203	ASP	OD1-CG-OD2	-5.35	113.14	123.30
1	A	33	ASN	CB-CG-ND2	-5.34	103.88	116.70
2	B	6	LYS	O-C-N	5.34	131.25	122.70
2	B	73	GLU	OE1-CD-OE2	-5.34	116.90	123.30
1	A	121	ASN	CB-CG-ND2	5.33	129.50	116.70
2	B	18	ILE	N-CA-CB	-5.33	98.53	110.80
1	A	227	LEU	N-CA-CB	-5.31	99.78	110.40
1	A	174	GLN	O-C-N	5.31	131.20	122.70
1	A	145	ILE	CA-CB-CG2	5.30	121.50	110.90
1	A	200	ASP	N-CA-C	-5.30	96.70	111.00
1	A	99	VAL	O-C-N	5.29	131.17	122.70
1	A	208	ALA	CA-C-O	5.29	131.21	120.10
2	B	50	SER	N-CA-C	-5.29	96.72	111.00
2	B	29	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	A	52	SER	O-C-N	-5.28	114.25	122.70
1	A	240	LEU	N-CA-C	-5.28	96.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ALA	N-CA-C	-5.28	96.74	111.00
2	B	108	VAL	N-CA-CB	-5.28	99.88	111.50
1	A	50	GLU	CA-CB-CG	5.28	125.01	113.40
1	A	250	HIS	CG-ND1-CE1	5.28	115.59	108.20
1	A	182	ASN	CB-CA-C	5.27	120.94	110.40
1	A	273	ASP	N-CA-C	-5.27	96.78	111.00
1	A	180	ASP	N-CA-C	5.26	125.20	111.00
2	B	2	THR	CA-CB-OG1	-5.26	97.96	109.00
1	A	80	SER	N-CA-CB	5.25	118.38	110.50
1	A	209	TRP	CA-CB-CG	-5.24	103.74	113.70
1	A	225	GLU	CA-C-O	5.24	131.10	120.10
2	B	95	SER	CA-C-N	-5.23	105.69	117.20
2	B	79	PRO	CA-C-N	-5.23	105.70	117.20
1	A	130	GLY	O-C-N	5.23	131.06	122.70
1	A	136	THR	CA-CB-CG2	-5.23	105.08	112.40
2	B	106	VAL	CG1-CB-CG2	5.23	119.26	110.90
1	A	207	ILE	O-C-N	-5.22	114.34	122.70
1	A	177	ALA	CB-CA-C	5.22	117.94	110.10
1	A	209	TRP	N-CA-CB	-5.22	101.20	110.60
2	B	119	GLU	CB-CG-CD	-5.22	100.11	114.20
1	A	181	GLY	C-N-CA	-5.22	108.66	121.70
1	A	264	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	A	222	VAL	CA-CB-CG1	5.21	118.71	110.90
2	B	49	PRO	CA-C-N	-5.20	105.76	117.20
1	A	295	LEU	C-N-CA	-5.19	108.72	121.70
2	B	148	VAL	CA-C-O	-5.19	109.21	120.10
2	B	61	ILE	CA-C-O	5.18	130.99	120.10
1	A	158	ALA	CA-C-O	-5.18	109.22	120.10
1	A	38	LEU	CA-C-O	-5.18	109.22	120.10
1	A	218	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	117	GLU	OE1-CD-OE2	5.18	129.51	123.30
1	A	249	LEU	CA-C-N	-5.18	105.81	117.20
2	B	41	ARG	N-CA-CB	5.17	119.91	110.60
1	A	41	HIS	CA-C-O	5.16	130.94	120.10
2	B	18	ILE	CA-CB-CG1	-5.16	101.19	111.00
1	A	163	LEU	CB-CA-C	-5.16	100.40	110.20
2	B	26	GLY	N-CA-C	-5.16	100.20	113.10
1	A	228	ASP	CB-CA-C	5.16	120.71	110.40
1	A	128	GLY	CA-C-N	5.15	128.53	117.20
1	A	172	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	A	294	LEU	CB-CG-CD1	5.14	119.74	111.00
1	A	156	HIS	N-CA-CB	-5.14	101.35	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	SER	O-C-N	5.14	130.92	122.70
1	A	6	GLN	CG-CD-OE1	-5.13	111.34	121.60
1	A	154	ASN	CA-C-N	-5.13	105.92	117.20
1	A	235	VAL	CA-CB-CG2	5.13	118.60	110.90
1	A	25	ALA	CB-CA-C	5.12	117.78	110.10
1	A	196	GLU	CG-CD-OE2	-5.10	108.10	118.30
2	B	150	LEU	N-CA-C	-5.10	97.23	111.00
1	A	59	PHE	CB-CG-CD1	5.09	124.36	120.80
1	A	205	LYS	CD-CE-NZ	-5.09	99.99	111.70
2	B	80	GLN	C-N-CA	-5.09	108.97	121.70
1	A	166	GLY	O-C-N	-5.08	114.57	122.70
2	B	103	ASN	OD1-CG-ND2	5.07	133.57	121.90
2	B	24	GLU	CA-C-O	5.07	130.75	120.10
1	A	9	ILE	CG1-CB-CG2	5.07	122.54	111.40
1	A	205	LYS	CB-CG-CD	5.07	124.77	111.60
2	B	98	SER	CA-CB-OG	-5.07	97.52	111.20
2	B	9	VAL	CB-CA-C	5.06	121.02	111.40
1	A	113	ARG	CD-NE-CZ	-5.06	116.52	123.60
1	A	176	LEU	CB-CA-C	5.06	119.81	110.20
2	B	31	SER	N-CA-CB	-5.06	102.91	110.50
2	B	67	SER	O-C-N	5.06	130.79	122.70
1	A	52	SER	CA-C-O	5.06	130.72	120.10
2	B	121	VAL	N-CA-C	5.06	124.65	111.00
1	A	279	TRP	CB-CA-C	5.05	120.51	110.40
2	B	37	GLU	CG-CD-OE2	-5.05	108.19	118.30
2	B	115	ILE	N-CA-CB	5.05	122.41	110.80
1	A	15	LEU	CB-CA-C	5.05	119.79	110.20
1	A	202	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	A	122	VAL	O-C-N	5.04	130.68	121.10
1	A	302	ASP	OD1-CG-OD2	5.03	132.86	123.30
1	A	113	ARG	NH1-CZ-NH2	5.03	124.94	119.40
1	A	214	SER	CB-CA-C	5.03	119.66	110.10
1	A	231	GLU	CA-C-O	-5.03	109.53	120.10
2	B	31	SER	O-C-N	5.03	130.75	122.70
1	A	132	ASN	CB-CG-OD1	-5.02	111.55	121.60
1	A	25	ALA	C-N-CA	-5.02	109.16	121.70
2	B	144	PHE	CA-CB-CG	5.02	125.94	113.90
1	A	26	THR	N-CA-CB	-5.01	100.77	110.30
1	A	225	GLU	C-N-CA	-5.01	109.17	121.70
2	B	142	LYS	CA-CB-CG	5.01	124.43	113.40
1	A	214	SER	N-CA-CB	5.01	118.02	110.50
2	B	61	ILE	O-C-N	-5.01	114.69	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CA-CB-CG	-5.01	102.38	113.40
1	A	8	HIS	CB-CA-C	-5.00	100.39	110.40
1	A	243	ALA	CA-C-N	-5.00	106.19	117.20
1	A	267	GLU	C-N-CA	5.00	134.20	121.70
2	B	85	ARG	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	113	ARG	Sidechain
1	A	151	ARG	Sidechain
1	A	17	ARG	Sidechain
1	A	183	ARG	Sidechain
1	A	221	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	242	ARG	Sidechain
1	A	264	ARG	Sidechain
1	A	291	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	35	GLN	Sidechain
1	A	54	ARG	Sidechain
1	A	56	ARG	Sidechain
1	A	65	ARG	Sidechain
2	B	129	ARG	Sidechain
2	B	14	ARG	Sidechain
2	B	85	ARG	Sidechain
2	B	96	ARG	Sidechain

## 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	2362	0	2360	840	6
2	B	1148	0	1114	518	10
3	B	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3511	0	3474	1348	16

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 194.

All (1348) 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)
2:B:66:LEU:H	2:B:66:LEU:CD1	1.34	1.38
2:B:9:VAL:CG1	2:B:14:ARG:HA	1.56	1.32
1:A:282:GLN:HE21	1:A:282:GLN:N	1.23	1.32
2:B:128:ARG:NH1	2:B:143:GLU:OE1	1.60	1.32
1:A:294:LEU:O	1:A:298:VAL:HG23	1.25	1.32
1:A:251:ASN:O	1:A:253:LYS:N	1.60	1.31
1:A:282:GLN:NE2	1:A:282:GLN:H	1.29	1.31
1:A:69:SER:O	1:A:70:VAL:HG13	1.33	1.29
2:B:114:CYS:HB3	2:B:116:SER:OG	1.24	1.26
1:A:231:GLU:HB2	1:A:232:TYR:CE2	1.68	1.26
1:A:157:VAL:O	1:A:185:TYR:HD1	1.14	1.24
2:B:18:ILE:HG23	2:B:62:GLU:OE2	1.37	1.24
1:A:108:GLN:O	1:A:129:ASP:O	1.56	1.24
1:A:140:LEU:HD13	1:A:287:GLY:CA	1.69	1.23
1:A:157:VAL:O	1:A:185:TYR:CD1	1.93	1.22
1:A:20:LEU:O	1:A:24:LEU:HB2	1.40	1.21
1:A:210:SER:C	1:A:211:LEU:HD23	1.60	1.21
2:B:25:ILE:HD12	2:B:25:ILE:O	1.42	1.19
2:B:66:LEU:HD13	2:B:66:LEU:N	1.46	1.19
2:B:4:ASN:OD1	2:B:5:ASP:N	1.75	1.18
1:A:119:SER:O	1:A:120:GLY:O	1.59	1.18
2:B:145:SER:O	2:B:147:ASN:N	1.77	1.18
1:A:145:ILE:O	1:A:145:ILE:HD12	1.40	1.18
2:B:27:PHE:CA	2:B:30:LEU:HD12	1.73	1.17
1:A:294:LEU:C	1:A:298:VAL:HG23	1.62	1.17
1:A:59:PHE:O	1:A:62:SER:HB2	1.44	1.17
2:B:22:PRO:HG2	2:B:25:ILE:HG23	1.22	1.16
1:A:157:VAL:HG11	1:A:184:PHE:CD2	1.80	1.16
1:A:254:MET:O	1:A:255:ASN:OD1	1.63	1.15
1:A:232:TYR:O	1:A:234:ASX:XD1	1.95	1.15
1:A:187:ILE:H	1:A:187:ILE:HD13	1.10	1.14
1:A:201:MET:HA	1:A:204:GLU:HB3	1.20	1.14
2:B:100:PRO:O	2:B:101:GLU:HG2	1.47	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ILE:O	2:B:123:SER:O	1.64	1.14
1:A:264:ARG:NH2	1:A:273:ASP:OD1	1.81	1.14
1:A:303:LEU:HD11	1:A:305:LEU:HA	1.23	1.13
2:B:71:VAL:HA	2:B:74:LEU:HD11	1.26	1.13
2:B:9:VAL:HG13	2:B:14:ARG:CA	1.79	1.13
1:A:197:TYR:CD1	1:A:198:ILE:N	2.15	1.13
1:A:278:ALA:O	1:A:279:TRP:CB	1.95	1.13
2:B:114:CYS:CB	2:B:116:SER:OG	1.96	1.13
2:B:61:ILE:HG23	2:B:62:GLU:HG2	1.29	1.13
2:B:101:GLU:O	2:B:102:ARG:CB	1.97	1.13
1:A:216:GLU:O	1:A:219:MET:HB3	1.47	1.12
1:A:210:SER:O	1:A:211:LEU:HD23	1.46	1.12
1:A:303:LEU:HD21	1:A:305:LEU:HB3	1.31	1.12
1:A:257:LYS:HA	1:A:277:HIS:HA	1.16	1.12
1:A:140:LEU:HD13	1:A:287:GLY:HA2	1.23	1.12
2:B:27:PHE:O	2:B:30:LEU:HB2	1.50	1.11
1:A:56:ARG:CD	1:A:60:GLN:HE22	1.61	1.11
2:B:20:HIS:HD2	2:B:22:PRO:O	1.32	1.11
1:A:274:LYS:HD3	1:A:274:LYS:C	1.69	1.10
1:A:29:LYS:CG	1:A:30:LEU:H	1.57	1.10
1:A:40:LYS:HD3	1:A:41:HIS:NE2	1.65	1.10
1:A:143:PHE:O	1:A:146:GLN:N	1.84	1.10
2:B:128:ARG:O	2:B:134:ALA:HB3	1.49	1.10
1:A:198:ILE:O	1:A:199:LEU:HD12	1.52	1.10
2:B:86:ILE:HG12	2:B:89:TYR:O	1.48	1.10
2:B:61:ILE:HB	2:B:82:THR:O	1.50	1.10
1:A:219:MET:HG3	1:A:219:MET:O	1.51	1.09
2:B:27:PHE:HA	2:B:30:LEU:HD12	1.28	1.09
2:B:32:LEU:HD21	2:B:77:TYR:HE2	1.14	1.09
2:B:70:GLU:N	2:B:71:VAL:HG23	1.66	1.09
2:B:71:VAL:HG12	2:B:72:ASP:H	1.06	1.09
2:B:71:VAL:C	2:B:73:GLU:H	1.50	1.09
1:A:116:THR:HG22	1:A:117:GLU:N	1.58	1.08
1:A:160:VAL:HG12	1:A:187:ILE:HB	1.09	1.08
1:A:87:THR:O	1:A:89:ALA:N	1.87	1.08
1:A:157:VAL:HG11	1:A:184:PHE:HD2	0.92	1.08
2:B:34:LYS:HG2	2:B:35:LEU:H	0.95	1.08
1:A:272:VAL:O	1:A:273:ASP:C	1.89	1.08
2:B:119:GLU:HB3	2:B:120:PRO:HD2	1.32	1.07
2:B:64:THR:O	2:B:64:THR:HG22	1.45	1.07
1:A:162:ASP:N	1:A:228:ASP:OD2	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:THR:O	2:B:17:VAL:HG23	1.55	1.07
2:B:66:LEU:HD22	2:B:67:SER:N	1.69	1.06
1:A:56:ARG:HG2	1:A:60:GLN:NE2	1.70	1.06
2:B:150:LEU:O	2:B:151:ALA:HB2	1.50	1.06
1:A:95:ILE:O	1:A:99:VAL:CG2	2.03	1.06
1:A:70:VAL:O	1:A:71:VAL:HG13	1.54	1.05
2:B:61:ILE:HG22	2:B:62:GLU:N	1.71	1.05
2:B:70:GLU:H	2:B:71:VAL:HG23	1.15	1.05
1:A:231:GLU:CB	1:A:232:TYR:CE2	2.38	1.05
1:A:276:PRO:O	1:A:278:ALA:N	1.90	1.05
2:B:71:VAL:HA	2:B:74:LEU:CD1	1.85	1.05
2:B:74:LEU:N	2:B:74:LEU:HD13	1.71	1.05
1:A:35:GLN:HG3	1:A:38:LEU:HD21	1.38	1.05
1:A:229:PRO:HA	1:A:267:GLU:OE2	1.57	1.05
2:B:67:SER:HB3	2:B:70:GLU:OE2	1.57	1.04
1:A:187:ILE:N	1:A:187:ILE:HD13	1.73	1.04
2:B:71:VAL:O	2:B:73:GLU:N	1.90	1.03
2:B:27:PHE:HA	2:B:30:LEU:CD1	1.87	1.03
1:A:228:ASP:HB2	1:A:229:PRO:HD3	1.07	1.03
1:A:27:ALA:HB2	1:A:293:ALA:HB2	1.37	1.03
2:B:61:ILE:CG1	2:B:82:THR:H	1.72	1.03
1:A:35:GLN:CA	1:A:35:GLN:HE21	1.62	1.03
1:A:249:LEU:O	1:A:250:HIS:ND1	1.92	1.03
1:A:274:LYS:CD	1:A:275:THR:N	2.22	1.03
1:A:187:ILE:N	1:A:187:ILE:CD1	2.21	1.02
2:B:61:ILE:HG13	2:B:82:THR:H	0.90	1.02
1:A:142:LEU:O	1:A:145:ILE:HG23	1.58	1.02
2:B:128:ARG:HH21	2:B:128:ARG:HB3	1.19	1.02
1:A:29:LYS:HG2	1:A:30:LEU:N	1.72	1.01
2:B:131:ASP:O	2:B:132:ASP:OD1	1.76	1.01
1:A:208:ALA:O	1:A:209:TRP:HB3	1.60	1.01
2:B:33:PHE:O	2:B:34:LYS:O	1.78	1.01
1:A:235:VAL:CG2	1:A:238:GLN:HB2	1.89	1.01
1:A:9:ILE:HB	1:A:125:LEU:CD1	1.90	1.01
1:A:260:HIS:H	1:A:283:GLN:HE22	1.05	1.00
2:B:63:ASN:O	2:B:64:THR:OG1	1.77	1.00
1:A:272:VAL:O	1:A:273:ASP:O	1.79	1.00
2:B:119:GLU:CB	2:B:120:PRO:HD2	1.85	1.00
2:B:15:GLY:O	2:B:64:THR:CG2	2.08	1.00
2:B:64:THR:N	2:B:84:ASN:HD22	1.60	1.00
2:B:66:LEU:HD22	2:B:67:SER:H	0.84	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ILE:HG13	2:B:82:THR:N	1.74	0.99
1:A:31:LYS:HE2	1:A:289:PHE:CE2	1.97	0.99
1:A:29:LYS:HG2	1:A:30:LEU:H	0.87	0.99
2:B:34:LYS:CG	2:B:35:LEU:H	1.62	0.99
2:B:86:ILE:HG23	2:B:90:GLU:HB2	1.40	0.99
1:A:138:THR:HG21	1:A:171:SER:CB	1.91	0.99
1:A:67:GLY:O	1:A:68:ALA:HB2	1.57	0.99
1:A:16:SER:O	1:A:17:ARG:O	1.81	0.98
1:A:194:MET:HG2	1:A:199:LEU:HD11	1.44	0.98
1:A:69:SER:O	1:A:70:VAL:CG1	2.11	0.98
1:A:202:LEU:HD12	1:A:207:ILE:HG21	1.44	0.98
2:B:128:ARG:NH1	2:B:143:GLU:CD	2.16	0.98
1:A:228:ASP:HB2	1:A:229:PRO:CD	1.92	0.98
1:A:80:SER:O	1:A:81:LEU:HD12	1.63	0.98
1:A:303:LEU:CD1	1:A:305:LEU:HA	1.94	0.98
1:A:31:LYS:HE2	1:A:289:PHE:CD2	1.98	0.98
1:A:145:ILE:HD12	1:A:145:ILE:C	1.76	0.98
1:A:8:HIS:HB2	1:A:10:ILE:HD11	1.43	0.97
1:A:10:ILE:HG22	1:A:10:ILE:O	1.60	0.97
2:B:28:LYS:O	2:B:32:LEU:N	1.96	0.97
2:B:34:LYS:HG2	2:B:35:LEU:N	1.80	0.97
1:A:191:ALA:O	1:A:192:LEU:HD13	1.63	0.97
2:B:32:LEU:CD2	2:B:77:TYR:HE2	1.77	0.97
1:A:231:GLU:HB2	1:A:232:TYR:CD2	1.99	0.97
1:A:81:LEU:HD22	1:A:82:GLY:N	1.78	0.97
2:B:66:LEU:CD2	2:B:67:SER:H	1.76	0.97
1:A:187:ILE:H	1:A:187:ILE:CD1	1.75	0.96
2:B:8:GLN:O	2:B:9:VAL:HG23	1.64	0.96
1:A:31:LYS:NZ	1:A:147:GLN:OE1	1.96	0.96
1:A:43:VAL:HA	1:A:69:SER:HB2	1.48	0.96
2:B:74:LEU:H	2:B:74:LEU:HD13	1.27	0.96
1:A:164:LYS:HD3	1:A:165:TYR:CE2	1.99	0.96
1:A:5:TYR:HE2	1:A:300:ASN:O	1.49	0.95
2:B:34:LYS:O	2:B:35:LEU:HG	1.67	0.95
1:A:5:TYR:O	1:A:7:SER:N	1.98	0.95
1:A:56:ARG:CG	1:A:60:GLN:NE2	2.30	0.95
2:B:73:GLU:HA	2:B:73:GLU:OE1	1.66	0.95
1:A:14:ASP:OD1	1:A:14:ASP:O	1.85	0.95
1:A:81:LEU:HD22	1:A:82:GLY:H	1.30	0.94
1:A:303:LEU:HD11	1:A:305:LEU:CA	1.96	0.94
2:B:107:LEU:C	2:B:108:VAL:HG22	1.84	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PRO:O	1:A:262:LEU:O	1.85	0.94
1:A:40:LYS:HB3	1:A:41:HIS:CD2	2.03	0.94
1:A:262:LEU:HB3	1:A:263:PRO:HA	1.50	0.94
1:A:88:LEU:HD22	1:A:88:LEU:O	1.68	0.94
1:A:217:GLU:O	1:A:218:VAL:HG23	1.66	0.94
1:A:279:TRP:O	1:A:281:PHE:N	2.01	0.94
1:A:67:GLY:O	1:A:68:ALA:CB	2.14	0.93
2:B:128:ARG:HB3	2:B:128:ARG:NH2	1.83	0.93
2:B:23:ALA:O	2:B:24:GLU:HB2	1.65	0.93
1:A:303:LEU:HD21	1:A:305:LEU:CD2	1.98	0.93
1:A:92:ILE:O	1:A:96:SER:OG	1.85	0.93
2:B:23:ALA:O	2:B:24:GLU:CB	2.17	0.93
1:A:214:SER:HB3	1:A:216:GLU:HG3	1.50	0.93
1:A:202:LEU:CD1	1:A:207:ILE:HG21	1.97	0.93
2:B:114:CYS:HG	3:B:153:ZN:ZN	0.75	0.93
2:B:101:GLU:O	2:B:102:ARG:HB3	1.12	0.93
1:A:44:ILE:O	1:A:71:VAL:CG2	2.17	0.92
1:A:8:HIS:HB2	1:A:10:ILE:CD1	1.97	0.92
1:A:251:ASN:O	1:A:253:LYS:CA	2.17	0.92
1:A:260:HIS:N	1:A:283:GLN:HE22	1.67	0.92
1:A:95:ILE:HG22	1:A:96:SER:N	1.82	0.92
2:B:4:ASN:CG	2:B:5:ASP:H	1.70	0.92
1:A:138:THR:HG21	1:A:171:SER:HB3	1.52	0.92
2:B:20:HIS:CD2	2:B:22:PRO:O	2.21	0.92
1:A:201:MET:HA	1:A:204:GLU:CB	2.00	0.92
1:A:49:PHE:HB2	1:A:105:ARG:O	1.68	0.91
1:A:159:MET:HE1	1:A:172:LEU:HD23	1.49	0.91
1:A:56:ARG:HG2	1:A:60:GLN:HE21	1.24	0.91
1:A:269:ALA:HB3	1:A:272:VAL:HG23	1.53	0.91
1:A:274:LYS:HD3	1:A:275:THR:N	1.82	0.91
1:A:201:MET:CA	1:A:204:GLU:HB3	2.00	0.91
1:A:94:VAL:O	1:A:97:THR:OG1	1.89	0.91
1:A:230:SER:C	1:A:231:GLU:HG2	1.91	0.91
1:A:234:ASX:XD1	1:A:239:PHE:HE1	1.84	0.91
2:B:108:VAL:HG21	2:B:152:ASN:HB3	1.52	0.91
2:B:38:THR:O	2:B:38:THR:HG22	1.71	0.91
2:B:66:LEU:N	2:B:66:LEU:CD1	2.13	0.91
2:B:32:LEU:HD21	2:B:106:VAL:HG21	1.50	0.91
2:B:140:CYS:HG	3:B:153:ZN:ZN	0.77	0.91
2:B:32:LEU:CD2	2:B:106:VAL:HG21	2.00	0.90
1:A:235:VAL:HG23	1:A:238:GLN:HB2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:HG12	2:B:72:ASP:N	1.86	0.90
1:A:24:LEU:HD21	1:A:142:LEU:HD23	1.52	0.90
1:A:110:GLY:HA2	2:B:139:TYR:O	1.70	0.90
2:B:32:LEU:HD21	2:B:77:TYR:CE2	2.06	0.90
2:B:25:ILE:O	2:B:25:ILE:CD1	2.18	0.90
1:A:197:TYR:O	1:A:199:LEU:N	2.04	0.90
2:B:71:VAL:O	2:B:73:GLU:HB2	1.72	0.90
1:A:95:ILE:O	1:A:99:VAL:HG23	1.72	0.89
2:B:18:ILE:CA	2:B:62:GLU:OE1	2.19	0.89
2:B:72:ASP:OD1	2:B:98:SER:N	2.05	0.89
1:A:159:MET:CE	1:A:172:LEU:HD23	2.01	0.89
2:B:22:PRO:HG2	2:B:25:ILE:CG2	2.01	0.89
2:B:86:ILE:HG23	2:B:90:GLU:CB	2.03	0.89
1:A:281:PHE:O	1:A:284:ALA:N	2.04	0.89
2:B:71:VAL:CG1	2:B:72:ASP:H	1.82	0.89
1:A:75:ASP:O	1:A:76:SER:HB2	1.72	0.89
2:B:105:ASP:C	2:B:105:ASP:OD2	2.07	0.89
2:B:64:THR:O	2:B:64:THR:CG2	2.21	0.89
1:A:303:LEU:O	1:A:303:LEU:HD23	1.73	0.89
1:A:70:VAL:C	1:A:71:VAL:HG22	1.87	0.89
2:B:1:MET:CE	2:B:41:ARG:HH22	1.85	0.89
2:B:17:VAL:HG22	2:B:43:THR:CB	2.01	0.89
2:B:15:GLY:O	2:B:64:THR:HG21	1.69	0.88
1:A:303:LEU:HG	1:A:305:LEU:N	1.88	0.88
1:A:250:HIS:O	1:A:251:ASN:C	2.09	0.88
2:B:17:VAL:HG13	2:B:43:THR:HB	1.55	0.88
1:A:216:GLU:O	1:A:219:MET:CB	2.21	0.88
1:A:88:LEU:C	1:A:88:LEU:HD22	1.93	0.88
2:B:61:ILE:CG2	2:B:62:GLU:N	2.30	0.88
1:A:254:MET:C	1:A:255:ASN:OD1	2.10	0.88
2:B:111:ASP:O	2:B:117:HIS:HE1	1.57	0.88
1:A:235:VAL:HG23	1:A:238:GLN:N	1.88	0.88
1:A:293:ALA:O	1:A:297:LEU:HD12	1.74	0.88
1:A:35:GLN:CA	1:A:35:GLN:NE2	2.37	0.88
2:B:18:ILE:HA	2:B:62:GLU:OE1	1.73	0.88
2:B:91:VAL:O	2:B:92:VAL:HG23	1.73	0.88
1:A:29:LYS:HD2	1:A:29:LYS:H	1.37	0.87
1:A:231:GLU:CB	1:A:232:TYR:CD2	2.55	0.87
1:A:294:LEU:C	1:A:298:VAL:CG2	2.43	0.87
2:B:71:VAL:HG13	2:B:74:LEU:HD21	1.57	0.87
1:A:50:GLU:O	1:A:51:ALA:O	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD2	1:A:60:GLN:HE22	1.40	0.87
2:B:9:VAL:CG1	2:B:14:ARG:CA	2.45	0.87
1:A:152:LEU:HD22	1:A:176:LEU:HD21	1.54	0.87
2:B:132:ASP:O	2:B:146:HIS:CE1	2.27	0.87
1:A:68:ALA:O	1:A:69:SER:OG	1.91	0.87
2:B:86:ILE:O	2:B:90:GLU:CG	2.22	0.87
2:B:107:LEU:O	2:B:108:VAL:HG13	1.74	0.87
2:B:9:VAL:HG12	2:B:10:ALA:H	1.40	0.87
1:A:116:THR:CG2	1:A:117:GLU:N	2.37	0.86
1:A:115:ALA:O	1:A:116:THR:O	1.92	0.86
1:A:56:ARG:CD	1:A:60:GLN:NE2	2.38	0.86
2:B:21:ILE:HB	2:B:22:PRO:HD3	1.58	0.86
1:A:145:ILE:C	1:A:145:ILE:CD1	2.38	0.86
2:B:72:ASP:OD1	2:B:98:SER:C	2.13	0.86
2:B:63:ASN:HA	2:B:84:ASN:HB2	1.57	0.86
1:A:145:ILE:O	1:A:145:ILE:CD1	2.22	0.86
1:A:235:VAL:HG23	1:A:238:GLN:CA	2.06	0.86
1:A:197:TYR:CD1	1:A:197:TYR:C	2.44	0.86
1:A:35:GLN:HA	1:A:35:GLN:HE21	1.38	0.86
1:A:303:LEU:CD2	1:A:305:LEU:HB3	2.05	0.86
2:B:102:ARG:HD2	2:B:104:ILE:CD1	2.06	0.86
1:A:160:VAL:CG1	1:A:187:ILE:HB	2.03	0.86
1:A:278:ALA:O	1:A:279:TRP:HB2	1.07	0.86
2:B:106:VAL:O	2:B:107:LEU:HG	1.76	0.86
2:B:9:VAL:HG21	2:B:14:ARG:C	1.96	0.86
1:A:2:ASN:OD1	1:A:2:ASN:C	2.12	0.85
1:A:40:LYS:O	1:A:41:HIS:HB2	1.74	0.85
2:B:106:VAL:O	2:B:107:LEU:CB	2.24	0.85
1:A:198:ILE:O	1:A:198:ILE:HD12	1.75	0.85
1:A:136:THR:HB	1:A:291:ARG:HH21	1.41	0.85
1:A:214:SER:HB3	1:A:216:GLU:HB2	1.59	0.85
2:B:38:THR:O	2:B:38:THR:CG2	2.24	0.85
1:A:29:LYS:CG	1:A:30:LEU:N	2.30	0.85
2:B:101:GLU:O	2:B:101:GLU:HG3	1.76	0.85
1:A:9:ILE:C	1:A:10:ILE:HD12	1.97	0.84
1:A:234:ASX:XD2	1:A:234:ASX:H	1.88	0.84
2:B:18:ILE:HD13	2:B:44:ILE:CG1	2.07	0.84
2:B:4:ASN:OD1	2:B:5:ASP:CA	2.26	0.84
1:A:91:THR:HG22	1:A:95:ILE:HD12	1.58	0.84
2:B:67:SER:OG	2:B:68:GLU:N	2.10	0.84
1:A:136:THR:HB	1:A:291:ARG:NH2	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG12	1:A:187:ILE:CB	2.03	0.83
1:A:235:VAL:HG22	1:A:238:GLN:HB2	1.60	0.83
1:A:249:LEU:C	1:A:250:HIS:ND1	2.31	0.83
2:B:128:ARG:HH21	2:B:128:ARG:CB	1.90	0.83
1:A:212:HIS:ND1	1:A:212:HIS:N	2.22	0.83
2:B:114:CYS:SG	2:B:116:SER:OG	2.31	0.83
2:B:106:VAL:O	2:B:107:LEU:CG	2.27	0.83
1:A:92:ILE:O	1:A:95:ILE:HG22	1.77	0.83
1:A:5:TYR:CE2	1:A:300:ASN:O	2.31	0.83
1:A:95:ILE:HG22	1:A:96:SER:H	1.39	0.83
2:B:106:VAL:O	2:B:107:LEU:HB2	1.78	0.83
2:B:119:GLU:CB	2:B:120:PRO:CD	2.55	0.83
1:A:211:LEU:C	1:A:212:HIS:ND1	2.32	0.83
1:A:279:TRP:HA	1:A:282:GLN:NE2	1.94	0.83
2:B:28:LYS:C	2:B:32:LEU:HB2	1.99	0.82
1:A:189:PRO:HG2	1:A:189:PRO:O	1.76	0.82
2:B:66:LEU:H	2:B:66:LEU:HD13	0.66	0.82
1:A:228:ASP:O	1:A:267:GLU:HG2	1.78	0.82
2:B:69:ASP:CG	2:B:69:ASP:O	2.16	0.82
1:A:202:LEU:HD12	1:A:207:ILE:CG2	2.08	0.82
1:A:250:HIS:O	1:A:252:ALA:N	2.12	0.82
1:A:260:HIS:H	1:A:283:GLN:NE2	1.78	0.82
2:B:9:VAL:CG2	2:B:14:ARG:C	2.48	0.82
1:A:22:LEU:O	1:A:26:THR:N	2.13	0.82
2:B:29:LEU:HD23	2:B:33:PHE:HE1	1.45	0.82
1:A:262:LEU:CB	1:A:263:PRO:HA	2.07	0.82
1:A:162:ASP:HA	1:A:192:LEU:HB3	1.61	0.82
1:A:191:ALA:C	1:A:192:LEU:HD13	2.00	0.82
1:A:201:MET:HA	1:A:204:GLU:HG3	1.62	0.82
2:B:145:SER:O	2:B:146:HIS:C	2.18	0.82
2:B:22:PRO:CG	2:B:25:ILE:HG23	2.09	0.81
1:A:228:ASP:CB	1:A:229:PRO:HD3	2.01	0.81
2:B:18:ILE:O	2:B:43:THR:O	1.99	0.81
1:A:208:ALA:O	1:A:209:TRP:CB	2.27	0.81
1:A:95:ILE:CG2	1:A:96:SER:N	2.42	0.81
1:A:187:ILE:HG21	1:A:214:SER:O	1.80	0.81
1:A:235:VAL:HG23	1:A:238:GLN:CB	2.11	0.81
2:B:18:ILE:HD13	2:B:44:ILE:HG12	1.63	0.81
2:B:29:LEU:O	2:B:33:PHE:N	2.13	0.81
1:A:108:GLN:HG3	2:B:113:ASN:ND2	1.95	0.81
2:B:17:VAL:HA	2:B:18:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ILE:O	2:B:90:GLU:OE2	1.97	0.81
1:A:208:ALA:HA	1:A:209:TRP:HD1	1.44	0.80
2:B:69:ASP:HB2	2:B:72:ASP:HB2	1.61	0.80
2:B:74:LEU:N	2:B:74:LEU:CD1	2.43	0.80
1:A:152:LEU:CD2	1:A:176:LEU:HD21	2.11	0.80
1:A:179:PHE:H	1:A:179:PHE:HD2	1.29	0.80
1:A:35:GLN:HE21	1:A:35:GLN:N	1.79	0.80
2:B:4:ASN:CG	2:B:5:ASP:N	2.23	0.80
1:A:211:LEU:C	1:A:212:HIS:CE1	2.55	0.80
1:A:257:LYS:HA	1:A:277:HIS:CA	2.08	0.80
1:A:31:LYS:NZ	1:A:286:ASN:OD1	2.13	0.79
1:A:75:ASP:CG	1:A:79:THR:HB	2.02	0.79
2:B:83:VAL:HG23	2:B:92:VAL:HG11	1.61	0.79
2:B:9:VAL:HG13	2:B:14:ARG:HA	0.82	0.79
1:A:279:TRP:O	1:A:280:TYR:C	2.19	0.79
2:B:129:ARG:O	2:B:130:ALA:C	2.21	0.79
1:A:230:SER:O	1:A:231:GLU:OE1	2.00	0.79
2:B:100:PRO:O	2:B:101:GLU:CG	2.30	0.79
2:B:26:GLY:O	2:B:30:LEU:CD1	2.29	0.79
1:A:197:TYR:HD1	1:A:197:TYR:C	1.84	0.79
1:A:217:GLU:HG3	1:A:221:ARG:HH12	1.47	0.79
1:A:10:ILE:CG2	1:A:10:ILE:O	2.21	0.79
1:A:8:HIS:CB	1:A:10:ILE:HD11	2.12	0.79
1:A:212:HIS:CG	1:A:218:VAL:HG21	2.18	0.79
1:A:29:LYS:O	1:A:33:ASN:N	2.15	0.79
1:A:254:MET:O	1:A:255:ASN:CG	2.21	0.79
2:B:83:VAL:HG23	2:B:92:VAL:CG1	2.12	0.79
1:A:211:LEU:HD23	1:A:211:LEU:N	1.89	0.78
1:A:22:LEU:O	1:A:26:THR:OG1	2.01	0.78
2:B:29:LEU:HA	2:B:32:LEU:HB3	1.65	0.78
2:B:102:ARG:HD2	2:B:104:ILE:HD11	1.63	0.78
2:B:150:LEU:O	2:B:151:ALA:CB	2.26	0.78
1:A:58:SER:O	1:A:59:PHE:O	2.02	0.78
2:B:61:ILE:CG2	2:B:62:GLU:HG2	2.12	0.78
1:A:198:ILE:CG1	1:A:198:ILE:O	2.28	0.78
2:B:128:ARG:O	2:B:134:ALA:CB	2.32	0.78
1:A:66:LEU:CD1	1:A:292:GLN:HG3	2.14	0.78
2:B:16:THR:HG23	2:B:62:GLU:HB3	1.66	0.78
1:A:155:LEU:O	1:A:182:ASN:O	2.02	0.78
2:B:116:SER:O	2:B:117:HIS:CB	2.29	0.78
1:A:132:ASN:HD21	2:B:141:GLU:HB2	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ASN:C	2:B:49:PRO:N	2.30	0.78
1:A:214:SER:HB3	1:A:216:GLU:CG	2.14	0.78
1:A:274:LYS:HD2	1:A:275:THR:CA	2.14	0.78
2:B:115:ILE:CG2	2:B:119:GLU:HG3	2.14	0.78
2:B:147:ASN:O	2:B:148:VAL:C	2.22	0.78
2:B:28:LYS:O	2:B:32:LEU:HB2	1.82	0.78
2:B:61:ILE:HG23	2:B:62:GLU:CG	2.11	0.78
1:A:251:ASN:O	1:A:253:LYS:HG3	1.83	0.78
2:B:18:ILE:CD1	2:B:18:ILE:N	2.45	0.77
1:A:208:ALA:C	1:A:209:TRP:CD1	2.58	0.77
1:A:207:ILE:HG23	1:A:208:ALA:N	1.98	0.77
1:A:303:LEU:HD11	1:A:305:LEU:CB	2.13	0.77
2:B:77:TYR:N	2:B:77:TYR:CD1	2.51	0.77
1:A:81:LEU:CD2	1:A:82:GLY:H	1.96	0.77
1:A:82:GLY:HA3	1:A:86:GLN:HB3	1.66	0.77
2:B:26:GLY:O	2:B:30:LEU:HD12	1.84	0.77
2:B:61:ILE:CB	2:B:82:THR:O	2.30	0.77
1:A:109:GLU:HA	1:A:129:ASP:HB3	1.65	0.77
1:A:119:SER:OG	1:A:119:SER:O	1.94	0.77
1:A:210:SER:O	1:A:211:LEU:CD2	2.29	0.77
2:B:17:VAL:CG1	2:B:43:THR:HB	2.15	0.77
2:B:115:ILE:HG22	2:B:119:GLU:HG3	1.66	0.77
2:B:137:CYS:SG	2:B:139:TYR:HB2	2.24	0.77
1:A:136:THR:CG2	1:A:291:ARG:NH2	2.48	0.77
1:A:141:ASP:O	1:A:145:ILE:HG22	1.85	0.77
2:B:86:ILE:O	2:B:90:GLU:HG3	1.84	0.77
2:B:27:PHE:O	2:B:30:LEU:CB	2.32	0.76
1:A:136:THR:CB	1:A:291:ARG:HH21	1.98	0.76
1:A:39:LEU:O	1:A:42:LYS:HB2	1.84	0.76
2:B:34:LYS:C	2:B:35:LEU:HG	2.03	0.76
1:A:294:LEU:O	1:A:298:VAL:CG2	2.21	0.76
1:A:75:ASP:OD1	1:A:79:THR:HB	1.84	0.76
2:B:30:LEU:O	2:B:33:PHE:O	2.02	0.76
2:B:72:ASP:CG	2:B:98:SER:O	2.24	0.76
2:B:5:ASP:OD1	2:B:6:LYS:N	2.17	0.76
1:A:164:LYS:HD3	1:A:165:TYR:HE2	1.49	0.76
1:A:9:ILE:HD13	1:A:294:LEU:HD22	1.67	0.76
1:A:111:ALA:O	1:A:112:ALA:C	2.22	0.76
1:A:16:SER:HB3	1:A:19:ASP:OD1	1.85	0.76
1:A:87:THR:C	1:A:89:ALA:H	1.90	0.76
2:B:71:VAL:C	2:B:73:GLU:N	2.28	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ILE:HD12	2:B:18:ILE:N	1.99	0.76
1:A:194:MET:HG3	1:A:195:PRO:HD2	1.68	0.75
1:A:194:MET:CE	1:A:198:ILE:HG13	2.16	0.75
1:A:52:SER:OG	1:A:55:THR:HG21	1.85	0.75
2:B:67:SER:CB	2:B:70:GLU:OE2	2.33	0.75
1:A:214:SER:HB3	1:A:216:GLU:CB	2.15	0.75
1:A:234:ASX:XD1	1:A:239:PHE:CE1	2.69	0.75
1:A:152:LEU:HD22	1:A:176:LEU:CD2	2.15	0.75
1:A:177:ALA:O	1:A:178:LYS:C	2.23	0.75
1:A:198:ILE:O	1:A:198:ILE:CD1	2.34	0.75
1:A:110:GLY:O	1:A:113:ARG:N	2.20	0.75
1:A:140:LEU:CD1	1:A:287:GLY:CA	2.59	0.75
1:A:303:LEU:HG	1:A:305:LEU:H	1.51	0.75
2:B:28:LYS:O	2:B:31:SER:OG	2.04	0.75
1:A:93:SER:C	1:A:96:SER:OG	2.25	0.75
2:B:16:THR:O	2:B:17:VAL:CG2	2.33	0.75
2:B:1:MET:HE1	2:B:41:ARG:HH22	1.51	0.75
1:A:179:PHE:HD2	1:A:179:PHE:N	1.85	0.75
1:A:194:MET:HE2	1:A:198:ILE:HG13	1.67	0.75
1:A:159:MET:HE1	1:A:172:LEU:CD2	2.17	0.74
2:B:60:LYS:O	2:B:82:THR:O	2.04	0.74
1:A:116:THR:HG22	1:A:117:GLU:H	1.52	0.74
1:A:266:ASP:O	1:A:267:GLU:C	2.18	0.74
1:A:87:THR:C	1:A:89:ALA:N	2.39	0.74
2:B:146:HIS:O	2:B:150:LEU:HB2	1.87	0.74
2:B:5:ASP:CG	2:B:6:LYS:N	2.40	0.74
1:A:195:PRO:O	1:A:199:LEU:HD13	1.88	0.74
1:A:230:SER:H	1:A:231:GLU:HG2	1.50	0.74
2:B:72:ASP:OD1	2:B:98:SER:O	2.05	0.74
2:B:137:CYS:O	2:B:137:CYS:SG	2.45	0.74
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.68	0.74
1:A:132:ASN:ND2	2:B:141:GLU:HB2	2.02	0.74
1:A:253:LYS:C	1:A:254:MET:HG2	2.08	0.74
2:B:16:THR:CG2	2:B:62:GLU:HB3	2.18	0.74
1:A:232:TYR:O	1:A:234:ASX:CG	2.26	0.73
1:A:246:LEU:O	1:A:268:ILE:HA	1.88	0.73
1:A:29:LYS:N	1:A:29:LYS:HD2	2.02	0.73
2:B:18:ILE:HD12	2:B:43:THR:O	1.87	0.73
1:A:175:ALA:O	1:A:177:ALA:N	2.22	0.73
1:A:80:SER:O	1:A:81:LEU:CD1	2.35	0.73
1:A:294:LEU:O	1:A:298:VAL:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:N	1:A:41:HIS:CD2	2.53	0.73
1:A:115:ALA:O	1:A:116:THR:C	2.19	0.73
2:B:147:ASN:O	2:B:149:VAL:HB	1.89	0.73
2:B:32:LEU:CD2	2:B:77:TYR:CE2	2.65	0.73
1:A:59:PHE:O	1:A:62:SER:CB	2.31	0.73
1:A:199:LEU:C	1:A:201:MET:N	2.36	0.73
1:A:42:LYS:O	1:A:69:SER:OG	2.02	0.73
1:A:81:LEU:HD13	1:A:82:GLY:O	1.89	0.73
1:A:232:TYR:CD2	1:A:232:TYR:N	2.57	0.73
2:B:61:ILE:HG22	2:B:62:GLU:CA	2.19	0.72
1:A:259:LEU:CD1	1:A:259:LEU:N	2.52	0.72
1:A:80:SER:O	1:A:81:LEU:HB3	1.88	0.72
1:A:198:ILE:C	1:A:198:ILE:HD12	2.10	0.72
1:A:257:LYS:CA	1:A:277:HIS:HA	2.10	0.72
1:A:303:LEU:HD21	1:A:305:LEU:HD22	1.71	0.72
1:A:95:ILE:O	1:A:99:VAL:HG22	1.89	0.72
1:A:240:LEU:HD22	1:A:241:VAL:HG22	1.72	0.72
2:B:25:ILE:HD12	2:B:25:ILE:C	2.09	0.72
2:B:74:LEU:O	2:B:76:LEU:N	2.22	0.72
1:A:29:LYS:C	1:A:31:LYS:N	2.40	0.72
1:A:251:ASN:C	1:A:253:LYS:N	2.34	0.72
1:A:17:ARG:O	1:A:19:ASP:N	2.23	0.72
1:A:274:LYS:HD2	1:A:275:THR:HA	1.72	0.72
1:A:56:ARG:NE	1:A:60:GLN:HE22	1.86	0.72
2:B:9:VAL:CG1	2:B:10:ALA:H	2.02	0.72
1:A:148:THR:OG1	1:A:149:GLU:HG2	1.89	0.72
1:A:184:PHE:CE1	1:A:202:LEU:HD11	2.25	0.72
1:A:17:ARG:O	1:A:18:ASP:C	2.27	0.72
2:B:71:VAL:O	2:B:73:GLU:CB	2.38	0.72
2:B:64:THR:N	2:B:84:ASN:ND2	2.38	0.72
2:B:18:ILE:O	2:B:44:ILE:HG12	1.89	0.72
2:B:16:THR:HA	2:B:64:THR:OG1	1.90	0.72
2:B:79:PRO:HG2	2:B:80:GLN:N	2.05	0.72
1:A:303:LEU:HG	1:A:304:VAL:N	2.05	0.71
1:A:274:LYS:HD2	1:A:275:THR:N	2.05	0.71
2:B:145:SER:C	2:B:147:ASN:N	2.44	0.71
2:B:29:LEU:CD2	2:B:33:PHE:HE1	2.03	0.71
2:B:61:ILE:HG22	2:B:62:GLU:O	1.91	0.71
1:A:119:SER:C	1:A:120:GLY:O	2.25	0.71
1:A:18:ASP:O	1:A:19:ASP:C	2.28	0.71
2:B:36:THR:CG2	2:B:36:THR:O	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:O	1:A:176:LEU:C	2.24	0.71
2:B:1:MET:HE3	2:B:41:ARG:HH22	1.56	0.71
2:B:77:TYR:N	2:B:77:TYR:HD1	1.88	0.71
1:A:35:GLN:HA	1:A:35:GLN:NE2	2.02	0.70
1:A:208:ALA:C	1:A:209:TRP:HD1	1.94	0.70
2:B:29:LEU:HD23	2:B:33:PHE:CE1	2.26	0.70
2:B:46:LEU:O	2:B:46:LEU:HD23	1.91	0.70
1:A:273:ASP:HA	1:A:280:TYR:OH	1.92	0.70
1:A:293:ALA:O	1:A:297:LEU:CD1	2.39	0.70
1:A:35:GLN:HB3	1:A:38:LEU:CD2	2.20	0.70
2:B:62:GLU:C	2:B:63:ASN:OD1	2.29	0.70
2:B:69:ASP:OD1	2:B:69:ASP:O	2.09	0.70
1:A:136:THR:CB	1:A:291:ARG:NH2	2.54	0.70
1:A:138:THR:HG21	1:A:171:SER:HB2	1.72	0.70
1:A:276:PRO:C	1:A:278:ALA:H	1.95	0.70
1:A:137:GLN:O	1:A:140:LEU:HB3	1.92	0.70
1:A:161:GLY:HA3	1:A:228:ASP:CG	2.11	0.70
2:B:18:ILE:CD1	2:B:44:ILE:HG12	2.20	0.70
1:A:214:SER:CB	1:A:216:GLU:HG3	2.20	0.70
1:A:251:ASN:O	1:A:253:LYS:CB	2.40	0.70
1:A:230:SER:O	1:A:231:GLU:CG	2.40	0.70
1:A:249:LEU:O	1:A:250:HIS:CG	2.43	0.70
2:B:114:CYS:HG	2:B:140:CYS:HG	1.38	0.70
1:A:114:LEU:HD23	1:A:114:LEU:C	2.12	0.70
1:A:260:HIS:O	1:A:262:LEU:N	2.23	0.70
1:A:38:LEU:HB3	1:A:39:LEU:HD23	1.74	0.70
1:A:157:VAL:HG12	1:A:183:ARG:O	1.92	0.69
1:A:76:SER:O	1:A:77:ALA:CB	2.38	0.69
2:B:134:ALA:O	2:B:135:LEU:HD12	1.91	0.69
2:B:98:SER:O	2:B:99:LEU:O	2.10	0.69
1:A:272:VAL:C	1:A:273:ASP:O	2.29	0.69
2:B:108:VAL:CG2	2:B:152:ASN:HB3	2.21	0.69
1:A:35:GLN:CG	1:A:38:LEU:HD21	2.19	0.69
1:A:304:VAL:HG23	1:A:304:VAL:O	1.92	0.69
2:B:107:LEU:HB3	2:B:125:PHE:CE1	2.26	0.69
2:B:75:ALA:HB1	2:B:99:LEU:HD22	1.74	0.69
1:A:81:LEU:HD22	1:A:82:GLY:O	1.92	0.69
1:A:88:LEU:CD2	1:A:88:LEU:O	2.41	0.69
1:A:297:LEU:O	1:A:298:VAL:C	2.30	0.69
2:B:17:VAL:HG22	2:B:43:THR:OG1	1.92	0.69
2:B:86:ILE:CG2	2:B:90:GLU:HB2	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:CD1	1:A:287:GLY:HA2	2.13	0.69
1:A:60:GLN:O	1:A:63:MET:N	2.26	0.69
1:A:83:LYS:O	1:A:84:LYS:C	2.31	0.69
1:A:211:LEU:O	1:A:212:HIS:CD2	2.46	0.69
1:A:141:ASP:HA	1:A:144:THR:HG21	1.75	0.69
2:B:111:ASP:HB2	2:B:144:PHE:HZ	1.58	0.69
2:B:68:GLU:O	2:B:70:GLU:N	2.25	0.69
2:B:124:SER:HB3	2:B:138:LYS:HE3	1.73	0.68
2:B:46:LEU:HD21	2:B:48:LEU:HG	1.75	0.68
1:A:158:ALA:HA	1:A:185:TYR:HB2	1.74	0.68
2:B:92:VAL:HG12	2:B:92:VAL:O	1.92	0.68
1:A:219:MET:O	1:A:219:MET:CG	2.24	0.68
2:B:15:GLY:O	2:B:64:THR:CB	2.40	0.68
1:A:163:LEU:HD22	1:A:188:ALA:HB2	1.76	0.68
1:A:88:LEU:C	1:A:88:LEU:CD2	2.62	0.68
1:A:68:ALA:C	1:A:69:SER:OG	2.28	0.68
2:B:11:GLU:O	2:B:12:ILE:C	2.30	0.68
2:B:72:ASP:O	2:B:100:PRO:HG3	1.92	0.68
2:B:76:LEU:HB3	2:B:77:TYR:CD1	2.28	0.68
1:A:184:PHE:CD1	1:A:202:LEU:HD11	2.29	0.68
1:A:77:ALA:C	1:A:79:THR:H	1.97	0.68
2:B:107:LEU:HD21	2:B:150:LEU:HD22	1.75	0.68
1:A:280:TYR:O	1:A:283:GLN:HB3	1.92	0.67
2:B:106:VAL:HG13	2:B:106:VAL:O	1.95	0.67
2:B:39:GLN:NE2	2:B:40:ASP:H	1.92	0.67
1:A:215:ILE:HG21	1:A:246:LEU:HD23	1.76	0.67
1:A:276:PRO:C	1:A:278:ALA:N	2.48	0.67
1:A:71:VAL:HG23	1:A:71:VAL:O	1.93	0.67
2:B:111:ASP:O	2:B:117:HIS:CE1	2.43	0.67
1:A:179:PHE:CD2	1:A:179:PHE:N	2.62	0.67
1:A:274:LYS:CD	1:A:275:THR:CA	2.72	0.67
1:A:272:VAL:O	1:A:275:THR:HG23	1.95	0.67
1:A:44:ILE:HG22	1:A:45:ALA:H	1.59	0.67
1:A:209:TRP:N	1:A:209:TRP:CD1	2.61	0.67
2:B:81:ALA:O	2:B:82:THR:HG23	1.95	0.67
2:B:25:ILE:C	2:B:25:ILE:CD1	2.62	0.67
2:B:20:HIS:CE1	2:B:47:ASN:HB2	2.30	0.67
1:A:113:ARG:O	1:A:116:THR:N	2.28	0.66
1:A:114:LEU:O	1:A:114:LEU:HD23	1.95	0.66
1:A:162:ASP:O	1:A:162:ASP:OD1	2.13	0.66
1:A:231:GLU:O	1:A:232:TYR:O	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:OD1	1:A:4:LEU:N	2.28	0.66
2:B:18:ILE:CG2	2:B:62:GLU:OE2	2.31	0.66
2:B:5:ASP:OD1	2:B:5:ASP:C	2.32	0.66
1:A:10:ILE:O	1:A:11:SER:CB	2.42	0.66
2:B:12:ILE:O	2:B:13:LYS:CG	2.43	0.66
2:B:27:PHE:C	2:B:30:LEU:HD12	2.15	0.66
1:A:303:LEU:HD11	1:A:305:LEU:HB2	1.77	0.66
1:A:35:GLN:HB3	1:A:38:LEU:HD23	1.78	0.66
1:A:49:PHE:CE1	1:A:104:MET:HE2	2.30	0.66
1:A:231:GLU:CB	1:A:232:TYR:HE2	2.03	0.66
1:A:34:PRO:O	1:A:35:GLN:NE2	2.28	0.66
1:A:189:PRO:CG	1:A:189:PRO:O	2.36	0.66
1:A:11:SER:HA	1:A:133:GLN:HG2	1.78	0.66
1:A:303:LEU:C	1:A:303:LEU:HD23	2.16	0.66
1:A:136:THR:HG21	1:A:291:ARG:NE	2.10	0.65
1:A:70:VAL:O	1:A:71:VAL:CG1	2.38	0.65
2:B:4:ASN:OD1	2:B:5:ASP:C	2.34	0.65
1:A:44:ILE:O	1:A:71:VAL:HG21	1.94	0.65
1:A:135:PRO:O	1:A:139:LEU:HG	1.95	0.65
1:A:249:LEU:O	1:A:250:HIS:CE1	2.49	0.65
2:B:39:GLN:CG	2:B:40:ASP:H	2.10	0.65
1:A:80:SER:O	1:A:81:LEU:CB	2.44	0.65
1:A:38:LEU:C	1:A:39:LEU:HD23	2.17	0.65
2:B:10:ALA:O	2:B:11:GLU:CB	2.44	0.65
1:A:279:TRP:C	1:A:281:PHE:N	2.44	0.65
2:B:116:SER:HA	2:B:121:VAL:HG11	1.79	0.65
2:B:60:LYS:O	2:B:61:ILE:CB	2.45	0.65
1:A:201:MET:HA	1:A:204:GLU:CG	2.26	0.65
1:A:230:SER:N	1:A:231:GLU:HG2	2.11	0.65
1:A:231:GLU:HB3	1:A:232:TYR:CD2	2.32	0.65
1:A:40:LYS:CB	1:A:41:HIS:CD2	2.79	0.65
2:B:71:VAL:O	2:B:73:GLU:CA	2.44	0.65
2:B:28:LYS:HB3	2:B:32:LEU:HD12	1.79	0.65
2:B:69:ASP:HA	2:B:71:VAL:HB	1.77	0.65
1:A:49:PHE:CE1	1:A:104:MET:CE	2.79	0.64
1:A:18:ASP:O	1:A:21:ASN:N	2.30	0.64
2:B:148:VAL:HG13	2:B:148:VAL:O	1.96	0.64
2:B:17:VAL:CA	2:B:18:ILE:HD12	2.27	0.64
2:B:18:ILE:HG23	2:B:62:GLU:CD	2.17	0.64
2:B:86:ILE:N	2:B:90:GLU:HB2	2.12	0.64
1:A:274:LYS:O	1:A:274:LYS:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:OD1	1:A:3:PRO:N	2.30	0.64
2:B:102:ARG:O	2:B:104:ILE:HD12	1.96	0.64
2:B:116:SER:O	2:B:117:HIS:CG	2.49	0.64
2:B:17:VAL:HG22	2:B:43:THR:HB	1.79	0.64
2:B:39:GLN:HG2	2:B:40:ASP:N	2.12	0.64
2:B:4:ASN:O	2:B:43:THR:HG21	1.96	0.64
1:A:82:GLY:HA3	1:A:86:GLN:CB	2.27	0.64
1:A:9:ILE:HB	1:A:125:LEU:HD12	1.78	0.64
1:A:49:PHE:CD1	1:A:104:MET:HE2	2.32	0.64
2:B:31:SER:C	2:B:33:PHE:N	2.45	0.64
1:A:230:SER:O	1:A:231:GLU:HG2	1.98	0.64
1:A:77:ALA:O	1:A:79:THR:N	2.30	0.64
2:B:147:ASN:O	2:B:148:VAL:O	2.16	0.64
2:B:17:VAL:HA	2:B:18:ILE:CD1	2.28	0.64
2:B:64:THR:H	2:B:84:ASN:HD22	1.44	0.64
1:A:204:GLU:OE2	1:A:205:LYS:NZ	2.31	0.64
1:A:40:LYS:O	1:A:41:HIS:CB	2.44	0.64
1:A:251:ASN:O	1:A:253:LYS:CG	2.46	0.64
1:A:9:ILE:HD13	1:A:294:LEU:CD2	2.28	0.64
2:B:86:ILE:O	2:B:90:GLU:CD	2.36	0.64
1:A:101:ALA:C	1:A:102:ILE:HG12	2.18	0.64
1:A:275:THR:O	1:A:276:PRO:O	2.15	0.64
1:A:34:PRO:C	1:A:35:GLN:HE21	2.01	0.64
1:A:212:HIS:CG	1:A:218:VAL:CG2	2.82	0.63
1:A:58:SER:O	1:A:59:PHE:C	2.37	0.63
2:B:66:LEU:HB2	2:B:70:GLU:HB2	1.80	0.63
2:B:84:ASN:O	2:B:92:VAL:HB	1.99	0.63
1:A:175:ALA:HA	1:A:178:LYS:HD2	1.80	0.63
2:B:20:HIS:CG	2:B:20:HIS:O	2.51	0.63
1:A:231:GLU:O	1:A:234:ASX:XD2	2.46	0.63
1:A:140:LEU:CD1	1:A:287:GLY:N	2.61	0.63
1:A:196:GLU:O	1:A:200:ASP:OD2	2.16	0.63
1:A:253:LYS:HD3	1:A:277:HIS:NE2	2.14	0.63
2:B:18:ILE:HB	2:B:44:ILE:CD1	2.29	0.63
1:A:140:LEU:HD13	1:A:287:GLY:N	2.11	0.63
1:A:159:MET:CE	1:A:172:LEU:CD2	2.75	0.63
2:B:146:HIS:CD2	2:B:147:ASN:OD1	2.52	0.63
1:A:129:ASP:OD1	1:A:132:ASN:OD1	2.17	0.63
1:A:81:LEU:CD1	1:A:82:GLY:O	2.47	0.63
1:A:81:LEU:CD2	1:A:82:GLY:O	2.47	0.63
1:A:200:ASP:O	1:A:204:GLU:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:O	1:A:40:LYS:C	2.37	0.62
2:B:102:ARG:HD2	2:B:104:ILE:HD12	1.80	0.62
1:A:175:ALA:C	1:A:177:ALA:N	2.48	0.62
1:A:218:VAL:O	1:A:222:VAL:CG2	2.47	0.62
1:A:230:SER:C	1:A:231:GLU:CG	2.63	0.62
1:A:258:VAL:C	1:A:259:LEU:CD1	2.68	0.62
2:B:146:HIS:CD2	2:B:147:ASN:N	2.68	0.62
2:B:18:ILE:N	2:B:62:GLU:OE1	2.32	0.62
1:A:189:PRO:O	1:A:191:ALA:N	2.31	0.62
1:A:274:LYS:CD	1:A:275:THR:HA	2.29	0.62
1:A:136:THR:HG21	1:A:291:ARG:CD	2.28	0.62
1:A:201:MET:CG	1:A:204:GLU:HG3	2.29	0.62
1:A:211:LEU:O	1:A:212:HIS:CE1	2.52	0.62
1:A:264:ARG:HG3	1:A:265:VAL:N	2.13	0.62
1:A:8:HIS:H	1:A:8:HIS:CD2	2.18	0.62
2:B:4:ASN:C	2:B:4:ASN:OD1	2.36	0.62
2:B:72:ASP:O	2:B:75:ALA:CB	2.46	0.62
1:A:149:GLU:OE2	1:A:149:GLU:HA	2.00	0.62
2:B:146:HIS:CD2	2:B:147:ASN:H	2.16	0.62
2:B:3:HIS:O	2:B:4:ASN:HB3	2.00	0.62
1:A:249:LEU:C	1:A:250:HIS:CG	2.69	0.62
1:A:292:GLN:O	1:A:293:ALA:C	2.35	0.62
1:A:303:LEU:O	1:A:303:LEU:CD2	2.46	0.62
1:A:81:LEU:HD22	1:A:82:GLY:CA	2.30	0.62
2:B:39:GLN:CG	2:B:40:ASP:N	2.62	0.62
1:A:197:TYR:CE1	1:A:198:ILE:N	2.67	0.61
1:A:200:ASP:O	1:A:204:GLU:HB3	2.00	0.61
1:A:221:ARG:O	1:A:222:VAL:HG23	2.00	0.61
1:A:114:LEU:HD13	2:B:119:GLU:HG3	1.80	0.61
1:A:258:VAL:N	1:A:277:HIS:O	2.30	0.61
1:A:40:LYS:HD3	1:A:41:HIS:CD2	2.33	0.61
2:B:86:ILE:H	2:B:90:GLU:HG3	1.66	0.61
1:A:162:ASP:OD1	1:A:162:ASP:C	2.37	0.61
2:B:12:ILE:O	2:B:13:LYS:CB	2.48	0.61
2:B:60:LYS:O	2:B:61:ILE:HB	1.99	0.61
2:B:72:ASP:C	2:B:100:PRO:HG3	2.19	0.61
2:B:84:ASN:HB3	2:B:92:VAL:HG21	1.82	0.61
2:B:15:GLY:O	2:B:64:THR:OG1	2.17	0.61
2:B:79:PRO:O	2:B:97:PRO:HG2	2.01	0.61
1:A:259:LEU:N	1:A:259:LEU:HD13	2.15	0.61
1:A:276:PRO:O	1:A:277:HIS:C	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:HG21	1:A:288:ILE:HG21	1.82	0.61
1:A:111:ALA:O	1:A:115:ALA:N	2.33	0.61
1:A:184:PHE:CE1	1:A:202:LEU:CD1	2.82	0.61
1:A:251:ASN:O	1:A:252:ALA:C	2.35	0.61
2:B:133:ILE:HB	2:B:146:HIS:ND1	2.15	0.61
2:B:39:GLN:HG2	2:B:40:ASP:H	1.65	0.61
2:B:1:MET:HE1	2:B:41:ARG:NH2	2.16	0.61
1:A:262:LEU:HB3	1:A:263:PRO:CA	2.26	0.61
1:A:274:LYS:HB3	1:A:275:THR:HG22	1.83	0.61
2:B:20:HIS:HB3	2:B:46:LEU:HA	1.81	0.61
1:A:233:ALA:HB3	1:A:234:ASX:XD2	2.31	0.61
1:A:235:VAL:CG2	1:A:238:GLN:CB	2.72	0.61
1:A:224:LYS:NZ	1:A:259:LEU:HD11	2.15	0.61
1:A:45:ALA:HB2	1:A:99:VAL:CG1	2.30	0.61
2:B:115:ILE:CG2	2:B:119:GLU:CG	2.78	0.61
2:B:105:ASP:O	2:B:105:ASP:OD2	2.19	0.61
1:A:12:ILE:HG22	1:A:13:ASN:N	2.16	0.60
1:A:141:ASP:C	1:A:144:THR:CG2	2.69	0.60
1:A:138:THR:O	1:A:142:LEU:HB2	2.01	0.60
1:A:143:PHE:O	1:A:144:THR:C	2.37	0.60
1:A:161:GLY:HA3	1:A:228:ASP:OD1	2.00	0.60
1:A:50:GLU:O	1:A:51:ALA:C	2.40	0.60
1:A:66:LEU:HD12	1:A:292:GLN:HG3	1.82	0.60
1:A:16:SER:CB	1:A:19:ASP:OD1	2.48	0.60
1:A:16:SER:OG	1:A:18:ASP:HB2	2.00	0.60
1:A:281:PHE:O	1:A:283:GLN:N	2.35	0.60
2:B:23:ALA:O	2:B:24:GLU:HB3	1.99	0.60
1:A:163:LEU:HB2	1:A:192:LEU:O	2.02	0.60
1:A:187:ILE:HA	1:A:212:HIS:O	2.00	0.60
1:A:20:LEU:O	1:A:24:LEU:CD2	2.49	0.60
1:A:266:ASP:O	1:A:268:ILE:N	2.35	0.60
1:A:304:VAL:CG2	1:A:304:VAL:O	2.49	0.60
2:B:100:PRO:C	2:B:101:GLU:HG2	2.21	0.60
2:B:17:VAL:CG2	2:B:43:THR:CB	2.77	0.60
2:B:63:ASN:HB3	2:B:84:ASN:HA	1.83	0.60
1:A:164:LYS:HB2	1:A:192:LEU:HA	1.84	0.60
2:B:17:VAL:CG2	2:B:43:THR:HB	2.31	0.60
1:A:217:GLU:HG3	1:A:221:ARG:NH1	2.15	0.60
1:A:232:TYR:O	1:A:234:ASX:XD2	2.50	0.60
2:B:10:ALA:O	2:B:11:GLU:HB3	2.02	0.60
1:A:272:VAL:O	1:A:274:LYS:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ARG:HG2	2:B:64:THR:CG2	2.31	0.59
2:B:66:LEU:HB2	2:B:70:GLU:CB	2.32	0.59
1:A:198:ILE:HD11	1:A:202:LEU:HD21	1.82	0.59
1:A:5:TYR:C	1:A:7:SER:H	2.05	0.59
2:B:140:CYS:SG	2:B:140:CYS:O	2.60	0.59
2:B:31:SER:O	2:B:32:LEU:C	2.38	0.59
2:B:69:ASP:HB2	2:B:72:ASP:CB	2.32	0.59
1:A:110:GLY:O	1:A:111:ALA:C	2.40	0.59
1:A:194:MET:HG3	1:A:195:PRO:CD	2.31	0.59
1:A:44:ILE:O	1:A:71:VAL:HG23	2.00	0.59
1:A:136:THR:HG21	1:A:291:ARG:CZ	2.32	0.59
1:A:31:LYS:HE3	1:A:143:PHE:HZ	1.66	0.59
1:A:75:ASP:OD2	1:A:79:THR:HB	2.03	0.59
1:A:12:ILE:HD13	1:A:175:ALA:HB2	1.84	0.59
1:A:29:LYS:CD	1:A:29:LYS:H	1.95	0.59
1:A:303:LEU:HD21	1:A:305:LEU:HD23	1.82	0.59
1:A:189:PRO:HD3	1:A:244:ASN:ND2	2.17	0.59
1:A:155:LEU:HD23	1:A:223:GLN:OE1	2.02	0.59
1:A:303:LEU:C	1:A:303:LEU:CD2	2.66	0.59
1:A:39:LEU:O	1:A:40:LYS:O	2.21	0.59
2:B:85:ARG:HG2	2:B:90:GLU:HG2	1.84	0.59
1:A:178:LYS:O	1:A:179:PHE:O	2.21	0.59
2:B:128:ARG:NH1	2:B:143:GLU:OE2	2.27	0.59
2:B:18:ILE:HB	2:B:44:ILE:HD13	1.85	0.59
1:A:157:VAL:CG1	1:A:184:PHE:HA	2.33	0.58
1:A:208:ALA:HA	1:A:209:TRP:CD1	2.33	0.58
1:A:303:LEU:CG	1:A:305:LEU:HB3	2.32	0.58
2:B:44:ILE:HG22	2:B:45:GLY:H	1.66	0.58
1:A:145:ILE:HG13	1:A:146:GLN:N	2.18	0.58
1:A:171:SER:O	1:A:172:LEU:C	2.38	0.58
1:A:232:TYR:O	1:A:234:ASX:N	2.35	0.58
1:A:143:PHE:O	1:A:146:GLN:CA	2.50	0.58
2:B:116:SER:O	2:B:117:HIS:HB2	2.00	0.58
2:B:145:SER:O	2:B:147:ASN:CA	2.50	0.58
2:B:66:LEU:C	2:B:70:GLU:HG2	2.24	0.58
1:A:184:PHE:HE1	1:A:202:LEU:CD1	2.17	0.58
1:A:198:ILE:HG13	1:A:198:ILE:O	2.03	0.58
1:A:138:THR:CG2	1:A:171:SER:HB2	2.34	0.58
1:A:281:PHE:O	1:A:282:GLN:C	2.42	0.58
1:A:8:HIS:N	1:A:8:HIS:CD2	2.69	0.58
1:A:91:THR:O	1:A:95:ILE:HB	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HH11	1:A:261:PRO:HD3	1.69	0.58
1:A:26:THR:HG21	1:A:297:LEU:HD11	1.84	0.58
2:B:72:ASP:OD2	2:B:98:SER:O	2.22	0.58
1:A:201:MET:CB	1:A:204:GLU:HG3	2.34	0.58
1:A:187:ILE:HD11	1:A:218:VAL:HG11	1.85	0.58
1:A:180:ASP:OD1	1:A:181:GLY:N	2.37	0.58
2:B:25:ILE:CG1	2:B:25:ILE:O	2.49	0.58
1:A:156:HIS:O	1:A:223:GLN:HB2	2.03	0.58
1:A:226:ARG:NH1	1:A:261:PRO:HD3	2.19	0.58
2:B:47:ASN:O	2:B:48:LEU:C	2.42	0.58
1:A:182:ASN:OD1	1:A:182:ASN:N	2.37	0.57
1:A:251:ASN:C	1:A:253:LYS:H	2.03	0.57
1:A:282:GLN:NE2	1:A:282:GLN:N	2.09	0.57
2:B:12:ILE:O	2:B:13:LYS:HG3	2.04	0.57
2:B:39:GLN:HE21	2:B:40:ASP:H	1.50	0.57
1:A:49:PHE:CB	1:A:105:ARG:O	2.48	0.57
1:A:25:ALA:O	1:A:26:THR:C	2.40	0.57
2:B:102:ARG:O	2:B:103:ASN:C	2.40	0.57
2:B:129:ARG:O	2:B:130:ALA:O	2.22	0.57
2:B:76:LEU:HB3	2:B:77:TYR:CE1	2.38	0.57
1:A:200:ASP:O	1:A:204:GLU:CB	2.53	0.57
1:A:9:ILE:HB	1:A:125:LEU:HD11	1.80	0.57
1:A:230:SER:O	1:A:231:GLU:CD	2.42	0.57
1:A:256:ALA:O	1:A:257:LYS:HD2	2.05	0.57
2:B:31:SER:HG	2:B:32:LEU:N	2.02	0.57
1:A:192:LEU:O	1:A:193:ALA:O	2.22	0.57
1:A:303:LEU:CD2	1:A:305:LEU:HD22	2.35	0.57
1:A:49:PHE:HE1	1:A:104:MET:CE	2.17	0.57
2:B:60:LYS:O	2:B:61:ILE:HG13	2.04	0.57
1:A:81:LEU:HD22	1:A:82:GLY:C	2.25	0.57
1:A:86:GLN:HG2	1:A:87:THR:H	1.69	0.57
2:B:72:ASP:O	2:B:75:ALA:HB3	2.04	0.57
2:B:138:LYS:O	2:B:138:LYS:HG3	2.05	0.57
1:A:217:GLU:OE2	1:A:221:ARG:NH1	2.38	0.57
1:A:269:ALA:O	1:A:270:THR:C	2.43	0.57
1:A:40:LYS:C	1:A:41:HIS:CD2	2.78	0.57
2:B:84:ASN:O	2:B:92:VAL:CB	2.53	0.57
1:A:270:THR:O	1:A:273:ASP:HB2	2.05	0.56
1:A:41:HIS:N	1:A:41:HIS:HD2	2.00	0.56
1:A:258:VAL:C	1:A:259:LEU:HD12	2.26	0.56
1:A:234:ASX:HB1	1:A:238:GLN:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:HIS:O	2:B:20:HIS:CD2	2.58	0.56
2:B:29:LEU:CD2	2:B:33:PHE:CE1	2.86	0.56
1:A:16:SER:O	1:A:17:ARG:C	2.44	0.56
1:A:138:THR:CG2	1:A:171:SER:CB	2.77	0.56
2:B:114:CYS:SG	2:B:137:CYS:SG	3.04	0.56
2:B:146:HIS:HD2	2:B:147:ASN:CG	2.09	0.56
2:B:29:LEU:CA	2:B:32:LEU:HB3	2.35	0.56
2:B:72:ASP:OD1	2:B:98:SER:CA	2.52	0.56
2:B:14:ARG:HG2	2:B:64:THR:HG23	1.88	0.56
1:A:11:SER:OG	1:A:133:GLN:CD	2.43	0.56
1:A:258:VAL:C	1:A:259:LEU:HD13	2.26	0.56
2:B:32:LEU:HD23	2:B:106:VAL:HG21	1.84	0.56
1:A:144:THR:O	1:A:145:ILE:C	2.38	0.56
1:A:31:LYS:HG3	1:A:289:PHE:CZ	2.41	0.56
2:B:108:VAL:O	2:B:109:CYS:C	2.45	0.56
2:B:115:ILE:O	2:B:116:SER:C	2.43	0.56
2:B:96:ARG:HB3	2:B:97:PRO:HD2	1.88	0.55
1:A:148:THR:OG1	1:A:149:GLU:N	2.38	0.55
2:B:31:SER:HG	2:B:32:LEU:H	1.54	0.55
2:B:15:GLY:H	2:B:64:THR:HG23	1.70	0.55
2:B:74:LEU:O	2:B:75:ALA:C	2.45	0.55
1:A:202:LEU:HB3	1:A:207:ILE:HG22	1.88	0.55
2:B:111:ASP:HB2	2:B:144:PHE:CZ	2.40	0.55
2:B:118:ALA:C	2:B:119:GLU:HG2	2.27	0.55
1:A:192:LEU:C	1:A:193:ALA:O	2.44	0.55
1:A:69:SER:C	1:A:70:VAL:HG13	2.24	0.55
2:B:71:VAL:CA	2:B:74:LEU:HD11	2.18	0.55
1:A:136:THR:CG2	1:A:291:ARG:CZ	2.85	0.55
1:A:199:LEU:O	1:A:200:ASP:C	2.44	0.55
2:B:5:ASP:O	2:B:6:LYS:HB2	2.06	0.55
2:B:32:LEU:HD13	2:B:77:TYR:HD2	1.72	0.55
1:A:262:LEU:CB	1:A:263:PRO:CA	2.83	0.55
1:A:29:LYS:HA	1:A:32:ALA:HB3	1.88	0.55
1:A:160:VAL:O	1:A:227:LEU:HA	2.07	0.55
2:B:34:LYS:HB3	2:B:35:LEU:HD23	1.89	0.55
1:A:160:VAL:HG11	1:A:215:ILE:CD1	2.37	0.55
1:A:116:THR:O	1:A:118:PHE:N	2.40	0.54
1:A:165:TYR:CD2	1:A:165:TYR:N	2.75	0.54
1:A:148:THR:OG1	1:A:224:LYS:HE3	2.07	0.54
1:A:294:LEU:O	1:A:297:LEU:N	2.40	0.54
1:A:10:ILE:O	1:A:11:SER:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HD12	1:A:125:LEU:HD11	1.89	0.54
1:A:14:ASP:OD2	1:A:113:ARG:NH2	2.40	0.54
1:A:141:ASP:OD1	1:A:226:ARG:NH1	2.38	0.54
1:A:303:LEU:CD1	1:A:305:LEU:CA	2.68	0.54
2:B:71:VAL:HG12	2:B:97:PRO:HA	1.89	0.54
1:A:157:VAL:HG21	1:A:159:MET:HE3	1.89	0.54
1:A:70:VAL:CA	1:A:71:VAL:HG22	2.38	0.54
1:A:198:ILE:CD1	1:A:202:LEU:CD2	2.85	0.54
1:A:231:GLU:HB3	1:A:232:TYR:CE2	2.34	0.54
1:A:77:ALA:C	1:A:79:THR:N	2.61	0.54
2:B:114:CYS:SG	2:B:140:CYS:SG	3.05	0.54
1:A:11:SER:OG	1:A:133:GLN:NE2	2.41	0.54
1:A:92:ILE:HA	1:A:95:ILE:HG21	1.88	0.54
1:A:136:THR:HG21	1:A:291:ARG:NH2	2.22	0.54
2:B:9:VAL:CG2	2:B:14:ARG:O	2.56	0.54
1:A:180:ASP:CG	1:A:181:GLY:N	2.62	0.54
2:B:28:LYS:O	2:B:31:SER:N	2.38	0.54
2:B:21:ILE:HG22	2:B:78:ALA:HB1	1.90	0.54
1:A:204:GLU:CD	1:A:205:LYS:NZ	2.61	0.54
1:A:211:LEU:O	1:A:212:HIS:CG	2.60	0.54
1:A:66:LEU:HG	1:A:292:GLN:HG3	1.91	0.54
2:B:71:VAL:HA	2:B:74:LEU:HD13	1.84	0.54
1:A:138:THR:HA	1:A:141:ASP:HB2	1.90	0.53
2:B:74:LEU:CD2	2:B:97:PRO:HB3	2.37	0.53
2:B:81:ALA:C	2:B:82:THR:OG1	2.46	0.53
1:A:68:ALA:O	1:A:69:SER:CB	2.54	0.53
1:A:190:ASP:OD1	1:A:190:ASP:N	2.42	0.53
1:A:44:ILE:HG23	1:A:101:ALA:HB3	1.89	0.53
2:B:22:PRO:O	2:B:22:PRO:CD	2.51	0.53
2:B:47:ASN:O	2:B:49:PRO:N	2.41	0.53
1:A:11:SER:OG	1:A:133:GLN:OE1	2.27	0.53
2:B:61:ILE:HG22	2:B:62:GLU:C	2.29	0.53
1:A:146:GLN:O	1:A:147:GLN:C	2.47	0.53
1:A:187:ILE:CG2	1:A:214:SER:O	2.55	0.53
1:A:88:LEU:O	1:A:88:LEU:CG	2.56	0.53
2:B:33:PHE:O	2:B:34:LYS:C	2.42	0.53
2:B:63:ASN:C	2:B:64:THR:OG1	2.47	0.53
1:A:136:THR:CG2	1:A:291:ARG:HH21	2.17	0.53
1:A:160:VAL:HG11	1:A:215:ILE:HD13	1.91	0.53
1:A:142:LEU:O	1:A:145:ILE:CG2	2.45	0.53
2:B:107:LEU:O	2:B:108:VAL:CG1	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASN:C	2:B:92:VAL:HG21	2.28	0.53
1:A:142:LEU:HD12	1:A:176:LEU:HD23	1.91	0.53
2:B:69:ASP:C	2:B:71:VAL:N	2.56	0.53
2:B:137:CYS:O	2:B:138:LYS:C	2.47	0.52
2:B:17:VAL:HG22	2:B:43:THR:N	2.23	0.52
2:B:18:ILE:HD11	2:B:42:ILE:HG23	1.91	0.52
2:B:79:PRO:CG	2:B:80:GLN:N	2.70	0.52
2:B:36:THR:HG22	2:B:36:THR:O	2.09	0.52
1:A:109:GLU:CA	1:A:129:ASP:HB3	2.37	0.52
1:A:186:PHE:O	1:A:188:ALA:N	2.43	0.52
2:B:34:LYS:CG	2:B:35:LEU:N	2.38	0.52
2:B:119:GLU:HB2	2:B:120:PRO:CD	2.38	0.52
1:A:132:ASN:HD21	2:B:141:GLU:CB	2.18	0.52
1:A:5:TYR:CE2	1:A:301:ARG:HA	2.45	0.52
2:B:131:ASP:O	2:B:132:ASP:CG	2.47	0.52
2:B:9:VAL:HG21	2:B:15:GLY:N	2.24	0.52
2:B:86:ILE:H	2:B:90:GLU:HB2	1.74	0.52
1:A:20:LEU:HD23	1:A:179:PHE:CE2	2.44	0.52
1:A:201:MET:CA	1:A:204:GLU:HG3	2.35	0.52
1:A:140:LEU:CD1	1:A:286:ASN:C	2.78	0.52
2:B:76:LEU:HB3	2:B:77:TYR:HD1	1.72	0.52
2:B:86:ILE:HG12	2:B:90:GLU:HB3	1.92	0.52
1:A:119:SER:O	1:A:120:GLY:C	2.43	0.52
2:B:39:GLN:H	2:B:39:GLN:CD	2.13	0.52
1:A:84:LYS:N	1:A:84:LYS:HD2	2.25	0.52
2:B:39:GLN:CD	2:B:39:GLN:N	2.62	0.52
1:A:141:ASP:C	1:A:144:THR:HG22	2.30	0.52
1:A:11:SER:OG	2:B:141:GLU:OE1	2.28	0.52
1:A:56:ARG:HG2	1:A:56:ARG:O	2.10	0.52
2:B:16:THR:HG22	2:B:17:VAL:H	1.73	0.52
2:B:18:ILE:O	2:B:44:ILE:HA	2.10	0.52
1:A:60:GLN:C	1:A:62:SER:N	2.63	0.51
1:A:92:ILE:HA	1:A:95:ILE:CG2	2.40	0.51
1:A:197:TYR:HA	1:A:200:ASP:OD2	2.11	0.51
1:A:199:LEU:HA	1:A:202:LEU:HD23	1.91	0.51
1:A:231:GLU:HA	1:A:239:PHE:HZ	1.74	0.51
2:B:17:VAL:CG2	2:B:43:THR:OG1	2.58	0.51
1:A:141:ASP:O	1:A:144:THR:CG2	2.58	0.51
1:A:143:PHE:O	1:A:145:ILE:N	2.43	0.51
1:A:227:LEU:HD21	1:A:246:LEU:HB2	1.92	0.51
2:B:44:ILE:HG22	2:B:45:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:HE3	1:A:198:ILE:HG13	1.91	0.51
1:A:94:VAL:O	1:A:95:ILE:C	2.45	0.51
2:B:109:CYS:N	2:B:125:PHE:HZ	2.09	0.51
2:B:17:VAL:C	2:B:18:ILE:HD12	2.30	0.51
1:A:251:ASN:CA	1:A:253:LYS:HG3	2.41	0.51
1:A:281:PHE:C	1:A:283:GLN:N	2.56	0.51
2:B:14:ARG:HB2	2:B:40:ASP:CG	2.31	0.51
2:B:15:GLY:C	2:B:64:THR:OG1	2.49	0.51
1:A:148:THR:OG1	1:A:224:LYS:CE	2.59	0.51
1:A:198:ILE:HD12	1:A:202:LEU:CD2	2.41	0.51
1:A:208:ALA:CA	1:A:209:TRP:HD1	2.20	0.51
1:A:35:GLN:HG3	1:A:38:LEU:CD2	2.25	0.51
1:A:34:PRO:C	1:A:35:GLN:NE2	2.64	0.51
2:B:128:ARG:CZ	2:B:143:GLU:OE1	2.52	0.51
1:A:214:SER:CB	1:A:216:GLU:HB2	2.37	0.51
1:A:124:VAL:HG23	1:A:125:LEU:O	2.12	0.51
1:A:198:ILE:O	1:A:199:LEU:CD1	2.42	0.51
1:A:258:VAL:HB	1:A:277:HIS:O	2.11	0.51
1:A:95:ILE:O	1:A:96:SER:C	2.49	0.51
2:B:99:LEU:CD1	2:B:127:VAL:HG11	2.40	0.51
1:A:13:ASN:O	1:A:15:LEU:N	2.38	0.50
1:A:224:LYS:HZ2	1:A:259:LEU:HD11	1.75	0.50
1:A:215:ILE:O	1:A:219:MET:HB3	2.12	0.50
1:A:157:VAL:O	1:A:185:TYR:CE1	2.58	0.50
1:A:211:LEU:O	1:A:212:HIS:NE2	2.44	0.50
1:A:23:VAL:O	1:A:24:LEU:C	2.48	0.50
1:A:242:ARG:O	1:A:242:ARG:HG3	2.12	0.50
1:A:93:SER:CA	1:A:96:SER:OG	2.58	0.50
2:B:29:LEU:O	2:B:33:PHE:HD1	1.95	0.50
1:A:187:ILE:N	1:A:187:ILE:HD12	2.22	0.50
2:B:146:HIS:CD2	2:B:147:ASN:CG	2.84	0.50
2:B:148:VAL:O	2:B:149:VAL:HG23	2.11	0.50
2:B:16:THR:HG22	2:B:17:VAL:N	2.27	0.50
2:B:67:SER:HB3	2:B:70:GLU:HG2	1.94	0.50
2:B:9:VAL:HG22	2:B:14:ARG:C	2.29	0.50
1:A:125:LEU:HD21	1:A:298:VAL:HG11	1.93	0.50
1:A:211:LEU:C	1:A:212:HIS:CG	2.84	0.50
1:A:291:ARG:O	1:A:292:GLN:C	2.49	0.50
1:A:80:SER:OG	1:A:81:LEU:N	2.33	0.50
2:B:71:VAL:HG13	2:B:74:LEU:CD2	2.36	0.50
1:A:136:THR:HG21	1:A:291:ARG:CG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:OG1	1:A:139:LEU:N	2.45	0.50
1:A:194:MET:CG	1:A:195:PRO:HD2	2.39	0.50
1:A:267:GLU:OE1	1:A:267:GLU:N	2.43	0.50
1:A:86:GLN:HG2	1:A:87:THR:N	2.26	0.50
1:A:11:SER:HA	1:A:133:GLN:OE1	2.11	0.50
1:A:141:ASP:CA	1:A:144:THR:HG21	2.41	0.50
1:A:279:TRP:C	1:A:281:PHE:H	2.15	0.50
1:A:303:LEU:CD2	1:A:305:LEU:CD2	2.83	0.50
1:A:70:VAL:C	1:A:71:VAL:CG2	2.58	0.50
1:A:199:LEU:H	1:A:201:MET:H	1.60	0.50
1:A:232:TYR:HD2	1:A:232:TYR:N	2.08	0.50
1:A:227:LEU:HD13	1:A:268:ILE:CD1	2.41	0.50
1:A:289:PHE:O	1:A:290:ALA:C	2.50	0.50
1:A:136:THR:HG21	1:A:291:ARG:HG3	1.94	0.50
1:A:56:ARG:HD2	1:A:60:GLN:NE2	2.15	0.50
1:A:56:ARG:NE	1:A:60:GLN:NE2	2.56	0.50
1:A:12:ILE:O	1:A:13:ASN:C	2.47	0.50
1:A:159:MET:HA	1:A:226:ARG:O	2.12	0.50
1:A:231:GLU:C	1:A:232:TYR:CD2	2.86	0.50
2:B:20:HIS:CD2	2:B:20:HIS:C	2.83	0.50
2:B:84:ASN:O	2:B:92:VAL:CG1	2.60	0.50
1:A:43:VAL:HG13	1:A:43:VAL:O	2.13	0.49
1:A:76:SER:O	1:A:77:ALA:HB2	2.12	0.49
2:B:22:PRO:HD2	2:B:22:PRO:O	2.11	0.49
1:A:11:SER:CB	1:A:133:GLN:CD	2.80	0.49
1:A:159:MET:HE2	1:A:172:LEU:HD23	1.93	0.49
2:B:72:ASP:O	2:B:75:ALA:HB2	2.11	0.49
2:B:86:ILE:O	2:B:90:GLU:CB	2.59	0.49
2:B:91:VAL:O	2:B:92:VAL:CG2	2.54	0.49
1:A:70:VAL:C	1:A:71:VAL:HG13	2.29	0.49
2:B:36:THR:O	2:B:36:THR:HG23	2.12	0.49
1:A:163:LEU:HD21	1:A:186:PHE:HB3	1.94	0.49
1:A:199:LEU:O	1:A:203:ASP:N	2.40	0.49
1:A:222:VAL:O	1:A:254:MET:SD	2.71	0.49
1:A:279:TRP:O	1:A:281:PHE:C	2.50	0.49
2:B:99:LEU:HD12	2:B:127:VAL:HG11	1.94	0.49
2:B:145:SER:O	2:B:147:ASN:C	2.50	0.49
2:B:63:ASN:HB3	2:B:84:ASN:CB	2.43	0.49
2:B:9:VAL:HG11	2:B:15:GLY:N	2.27	0.49
1:A:216:GLU:O	1:A:219:MET:N	2.46	0.49
2:B:33:PHE:CD1	2:B:33:PHE:N	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HG22	1:A:45:ALA:N	2.26	0.49
2:B:145:SER:O	2:B:147:ASN:O	2.30	0.49
1:A:199:LEU:O	1:A:202:LEU:N	2.45	0.49
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.64	0.49
1:A:17:ARG:O	1:A:20:LEU:N	2.46	0.49
1:A:81:LEU:CD2	1:A:82:GLY:N	2.60	0.49
1:A:9:ILE:O	1:A:10:ILE:HD12	2.12	0.49
2:B:86:ILE:CG1	2:B:89:TYR:O	2.41	0.49
1:A:111:ALA:O	1:A:114:LEU:N	2.46	0.49
1:A:185:TYR:C	1:A:186:PHE:CD1	2.86	0.49
2:B:128:ARG:HG3	2:B:129:ARG:N	2.27	0.49
2:B:86:ILE:H	2:B:90:GLU:CG	2.25	0.49
1:A:142:LEU:CD1	1:A:176:LEU:HD23	2.43	0.48
1:A:260:HIS:CD2	1:A:260:HIS:C	2.84	0.48
1:A:60:GLN:O	1:A:62:SER:N	2.45	0.48
2:B:148:VAL:CG1	2:B:148:VAL:O	2.56	0.48
1:A:120:GLY:O	1:A:122:VAL:N	2.45	0.48
1:A:4:LEU:O	1:A:5:TYR:O	2.32	0.48
2:B:32:LEU:HD13	2:B:77:TYR:CD2	2.48	0.48
2:B:60:LYS:O	2:B:61:ILE:CG1	2.61	0.48
1:A:12:ILE:CG2	1:A:13:ASN:N	2.76	0.48
1:A:201:MET:HG2	1:A:201:MET:O	2.13	0.48
1:A:198:ILE:C	1:A:199:LEU:HD12	2.31	0.48
2:B:138:LYS:O	2:B:139:TYR:CG	2.66	0.48
2:B:71:VAL:CG1	2:B:72:ASP:N	2.53	0.48
2:B:75:ALA:CB	2:B:99:LEU:N	2.77	0.48
1:A:194:MET:HE3	1:A:198:ILE:CG1	2.43	0.48
1:A:264:ARG:HD3	1:A:268:ILE:HB	1.95	0.48
2:B:134:ALA:C	2:B:135:LEU:HD12	2.34	0.48
2:B:16:THR:C	2:B:17:VAL:HG23	2.32	0.48
2:B:33:PHE:HB3	2:B:35:LEU:HD21	1.96	0.48
2:B:85:ARG:HG2	2:B:90:GLU:CG	2.42	0.48
1:A:124:VAL:O	1:A:125:LEU:HD13	2.13	0.48
1:A:17:ARG:HG3	1:A:18:ASP:N	2.28	0.48
1:A:143:PHE:C	1:A:145:ILE:N	2.61	0.48
1:A:212:HIS:CD2	1:A:218:VAL:CG2	2.96	0.48
2:B:27:PHE:O	2:B:30:LEU:N	2.47	0.48
1:A:107:PRO:C	1:A:108:GLN:O	2.50	0.48
1:A:149:GLU:HG3	1:A:224:LYS:HG3	1.95	0.48
2:B:14:ARG:HB3	2:B:64:THR:HG23	1.95	0.48
2:B:86:ILE:H	2:B:90:GLU:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:VAL:CG2	2:B:14:ARG:CA	2.92	0.48
1:A:20:LEU:O	1:A:24:LEU:CB	2.35	0.48
1:A:63:MET:HG3	1:A:295:LEU:HD21	1.95	0.48
1:A:295:LEU:N	1:A:298:VAL:HG23	2.26	0.48
2:B:146:HIS:HD2	2:B:147:ASN:N	2.12	0.48
2:B:28:LYS:O	2:B:32:LEU:CB	2.59	0.48
2:B:113:ASN:O	2:B:114:CYS:C	2.53	0.47
2:B:84:ASN:O	2:B:92:VAL:HG11	2.13	0.47
1:A:11:SER:HA	1:A:133:GLN:CG	2.44	0.47
1:A:201:MET:O	1:A:202:LEU:C	2.53	0.47
1:A:20:LEU:O	1:A:24:LEU:HD22	2.13	0.47
1:A:198:ILE:CD1	1:A:202:LEU:HD21	2.44	0.47
1:A:231:GLU:HA	1:A:239:PHE:CZ	2.49	0.47
1:A:26:THR:HB	1:A:297:LEU:HD11	1.96	0.47
1:A:29:LYS:O	1:A:30:LEU:C	2.52	0.47
1:A:227:LEU:HD11	1:A:246:LEU:HG	1.97	0.47
1:A:192:LEU:HD13	1:A:192:LEU:N	2.26	0.47
1:A:259:LEU:N	1:A:259:LEU:HD12	2.28	0.47
1:A:48:PHE:CE2	1:A:56:ARG:HB2	2.49	0.47
1:A:260:HIS:CD2	1:A:262:LEU:HA	2.49	0.47
1:A:31:LYS:HG2	1:A:31:LYS:O	2.14	0.47
1:A:60:GLN:O	1:A:63:MET:HB2	2.15	0.47
1:A:132:ASN:ND2	2:B:141:GLU:CB	2.74	0.47
1:A:185:TYR:O	1:A:186:PHE:HD1	1.98	0.47
2:B:27:PHE:O	2:B:28:LYS:C	2.52	0.47
1:A:137:GLN:HG2	1:A:168:THR:CG2	2.44	0.47
1:A:194:MET:CE	1:A:198:ILE:CG1	2.91	0.47
1:A:83:LYS:O	1:A:83:LYS:HG2	2.14	0.47
1:A:135:PRO:O	1:A:139:LEU:CG	2.61	0.47
1:A:281:PHE:O	1:A:284:ALA:HB3	2.15	0.47
2:B:26:GLY:C	2:B:30:LEU:HD12	2.35	0.47
2:B:86:ILE:CG1	2:B:90:GLU:HB3	2.45	0.47
1:A:157:VAL:HG13	1:A:184:PHE:HA	1.97	0.46
1:A:20:LEU:HD23	1:A:179:PHE:HE2	1.79	0.46
1:A:251:ASN:HA	1:A:253:LYS:HE3	1.97	0.46
1:A:264:ARG:HD2	1:A:268:ILE:O	2.14	0.46
1:A:43:VAL:O	1:A:43:VAL:CG1	2.63	0.46
2:B:76:LEU:C	2:B:77:TYR:HD1	2.19	0.46
2:B:86:ILE:N	2:B:90:GLU:CB	2.78	0.46
2:B:8:GLN:O	2:B:9:VAL:CG2	2.50	0.46
1:A:121:ASN:O	1:A:122:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:SER:H	1:A:231:GLU:CG	2.24	0.46
1:A:51:ALA:HA	1:A:74:SER:OG	2.16	0.46
2:B:9:VAL:HG22	2:B:14:ARG:O	2.14	0.46
1:A:112:ALA:O	1:A:113:ARG:C	2.52	0.46
1:A:163:LEU:HD22	1:A:188:ALA:CB	2.46	0.46
2:B:84:ASN:CB	2:B:92:VAL:HG21	2.44	0.46
1:A:200:ASP:O	1:A:204:GLU:CA	2.64	0.46
1:A:48:PHE:O	1:A:49:PHE:C	2.53	0.46
2:B:100:PRO:O	2:B:101:GLU:CB	2.63	0.46
2:B:102:ARG:CG	2:B:102:ARG:O	2.64	0.46
2:B:5:ASP:OD1	2:B:6:LYS:CA	2.63	0.46
2:B:66:LEU:HD23	2:B:70:GLU:HB2	1.98	0.46
1:A:106:HIS:CD2	1:A:111:ALA:HB2	2.50	0.46
1:A:10:ILE:O	1:A:11:SER:HB3	2.15	0.46
1:A:142:LEU:HA	1:A:145:ILE:CG2	2.45	0.46
1:A:199:LEU:C	1:A:201:MET:H	2.16	0.46
1:A:204:GLU:CD	1:A:205:LYS:HZ1	2.19	0.46
1:A:143:PHE:CE2	1:A:286:ASN:HB3	2.51	0.46
1:A:303:LEU:HD21	1:A:305:LEU:CB	2.23	0.46
2:B:140:CYS:O	2:B:142:LYS:N	2.48	0.46
2:B:32:LEU:CD1	2:B:77:TYR:CD2	2.99	0.46
2:B:75:ALA:HB1	2:B:99:LEU:H	1.81	0.46
1:A:185:TYR:O	1:A:186:PHE:CD1	2.69	0.46
1:A:88:LEU:CD2	1:A:92:ILE:HG12	2.45	0.46
2:B:39:GLN:NE2	2:B:40:ASP:OD2	2.49	0.46
1:A:165:TYR:HD2	1:A:165:TYR:N	2.13	0.46
1:A:261:PRO:C	1:A:262:LEU:O	2.54	0.46
2:B:99:LEU:HA	2:B:100:PRO:HD3	1.65	0.46
2:B:14:ARG:HG2	2:B:64:THR:HG22	1.98	0.46
2:B:18:ILE:HG13	2:B:18:ILE:H	1.00	0.46
2:B:1:MET:CG	2:B:4:ASN:ND2	2.79	0.46
2:B:63:ASN:HB3	2:B:84:ASN:CA	2.47	0.46
1:A:17:ARG:CG	1:A:18:ASP:N	2.79	0.45
2:B:44:ILE:CG2	2:B:45:GLY:H	2.29	0.45
2:B:16:THR:HG22	2:B:18:ILE:HG13	1.98	0.45
2:B:23:ALA:O	2:B:25:ILE:HG22	2.16	0.45
1:A:111:ALA:O	1:A:112:ALA:O	2.34	0.45
1:A:196:GLU:O	1:A:200:ASP:CG	2.55	0.45
1:A:218:VAL:O	1:A:222:VAL:HG23	2.14	0.45
1:A:231:GLU:O	1:A:234:ASX:XD1	2.64	0.45
1:A:284:ALA:C	1:A:286:ASN:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HB	1:A:125:LEU:HD13	1.89	0.45
2:B:61:ILE:CD1	2:B:82:THR:H	2.26	0.45
2:B:86:ILE:CG2	2:B:90:GLU:CB	2.84	0.45
1:A:152:LEU:HD13	1:A:179:PHE:CZ	2.51	0.45
1:A:232:TYR:HB2	1:A:233:ALA:H	1.38	0.45
1:A:279:TRP:HA	1:A:282:GLN:HE22	1.77	0.45
1:A:288:ILE:C	1:A:288:ILE:HD12	2.36	0.45
2:B:140:CYS:O	2:B:142:LYS:HG2	2.16	0.45
1:A:227:LEU:O	1:A:228:ASP:O	2.33	0.45
2:B:83:VAL:HG23	2:B:92:VAL:HG13	1.97	0.45
1:A:172:LEU:O	1:A:176:LEU:N	2.40	0.45
1:A:202:LEU:HB3	1:A:207:ILE:CG2	2.46	0.45
1:A:199:LEU:O	1:A:201:MET:N	2.50	0.45
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.75	0.45
1:A:29:LYS:HB3	1:A:29:LYS:HE2	1.63	0.45
1:A:51:ALA:O	1:A:52:SER:HB2	2.15	0.45
1:A:121:ASN:H	1:A:121:ASN:ND2	2.15	0.45
1:A:11:SER:HA	1:A:133:GLN:CD	2.37	0.45
1:A:16:SER:O	1:A:16:SER:OG	2.35	0.45
2:B:62:GLU:CA	2:B:62:GLU:OE1	2.65	0.45
1:A:156:HIS:CB	1:A:223:GLN:HG3	2.47	0.45
2:B:113:ASN:HA	2:B:113:ASN:HD22	1.68	0.45
2:B:140:CYS:O	2:B:141:GLU:C	2.55	0.45
1:A:187:ILE:HG23	1:A:213:SER:HA	1.97	0.45
1:A:251:ASN:N	1:A:253:LYS:HG3	2.32	0.45
1:A:260:HIS:HD2	1:A:262:LEU:N	2.14	0.45
2:B:21:ILE:CG2	2:B:78:ALA:HB1	2.47	0.45
2:B:107:LEU:HD21	2:B:150:LEU:CD2	2.47	0.44
1:A:109:GLU:O	2:B:139:TYR:O	2.35	0.44
2:B:31:SER:O	2:B:33:PHE:N	2.50	0.44
2:B:14:ARG:CG	2:B:64:THR:HG23	2.47	0.44
2:B:32:LEU:HD22	2:B:77:TYR:CE2	2.52	0.44
1:A:116:THR:O	1:A:117:GLU:C	2.55	0.44
1:A:217:GLU:HA	1:A:217:GLU:OE1	2.11	0.44
1:A:218:VAL:O	1:A:222:VAL:HG21	2.17	0.44
1:A:95:ILE:C	1:A:99:VAL:CG2	2.82	0.44
2:B:9:VAL:CB	2:B:14:ARG:HA	2.40	0.44
1:A:294:LEU:O	1:A:295:LEU:C	2.56	0.44
1:A:44:ILE:CG2	1:A:45:ALA:H	2.27	0.44
2:B:104:ILE:HD11	2:B:124:SER:OG	2.17	0.44
2:B:21:ILE:HB	2:B:22:PRO:CD	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:O	1:A:177:ALA:N	2.51	0.44
1:A:205:LYS:HZ3	1:A:205:LYS:HG2	1.34	0.44
1:A:225:GLU:O	1:A:259:LEU:HB2	2.17	0.44
1:A:240:LEU:O	1:A:242:ARG:N	2.51	0.44
1:A:66:LEU:CG	1:A:292:GLN:HG3	2.46	0.44
1:A:35:GLN:HB3	1:A:38:LEU:HD21	1.99	0.44
2:B:107:LEU:HD23	2:B:107:LEU:HA	1.53	0.44
2:B:15:GLY:O	2:B:64:THR:HG23	2.11	0.44
2:B:86:ILE:O	2:B:90:GLU:HB3	2.18	0.44
1:A:109:GLU:HG2	1:A:132:ASN:HB3	2.00	0.44
1:A:46:SER:O	1:A:72:GLY:HA3	2.17	0.44
2:B:128:ARG:HH11	2:B:143:GLU:CD	1.90	0.44
1:A:192:LEU:N	1:A:192:LEU:HD22	2.33	0.44
1:A:280:TYR:HA	1:A:283:GLN:HE21	1.82	0.44
1:A:295:LEU:O	1:A:299:LEU:HD12	2.18	0.44
2:B:19:ASN:O	2:B:20:HIS:C	2.56	0.44
1:A:135:PRO:O	1:A:139:LEU:CD1	2.65	0.44
1:A:211:LEU:CA	1:A:212:HIS:CE1	3.01	0.44
1:A:141:ASP:CG	1:A:226:ARG:HH12	2.19	0.44
1:A:29:LYS:O	1:A:31:LYS:N	2.49	0.44
2:B:27:PHE:O	2:B:30:LEU:HD12	2.18	0.44
2:B:7:LEU:HD13	2:B:63:ASN:HD22	1.83	0.44
1:A:11:SER:CA	1:A:133:GLN:OE1	2.66	0.43
1:A:235:VAL:N	1:A:238:GLN:HB3	2.32	0.43
1:A:24:LEU:HD11	1:A:143:PHE:HA	2.01	0.43
1:A:71:VAL:CG2	1:A:71:VAL:O	2.64	0.43
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.73	0.43
1:A:52:SER:HB2	1:A:105:ARG:HD3	2.01	0.43
1:A:143:PHE:O	1:A:146:GLN:HB3	2.18	0.43
1:A:235:VAL:HB	1:A:236:LYS:H	1.37	0.43
1:A:166:GLY:O	1:A:170:HIS:ND1	2.51	0.43
1:A:231:GLU:CA	1:A:239:PHE:HZ	2.32	0.43
1:A:76:SER:O	1:A:77:ALA:HB3	2.15	0.43
2:B:71:VAL:CA	2:B:74:LEU:CD1	2.77	0.43
1:A:202:LEU:HD13	1:A:207:ILE:HG21	1.96	0.43
1:A:219:MET:HE2	1:A:219:MET:O	2.18	0.43
1:A:143:PHE:HE2	1:A:286:ASN:HB3	1.82	0.43
1:A:158:ALA:C	1:A:159:MET:HG2	2.38	0.43
1:A:39:LEU:O	1:A:42:LYS:HD2	2.18	0.43
2:B:106:VAL:CG1	2:B:106:VAL:O	2.66	0.43
2:B:61:ILE:HG22	2:B:62:GLU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG22	1:A:158:ALA:N	2.33	0.43
1:A:279:TRP:O	1:A:282:GLN:N	2.52	0.43
1:A:31:LYS:HG3	1:A:289:PHE:CE2	2.54	0.43
2:B:17:VAL:CA	2:B:18:ILE:CD1	2.92	0.43
2:B:17:VAL:HG22	2:B:43:THR:CA	2.48	0.43
1:A:175:ALA:C	1:A:177:ALA:H	2.20	0.43
1:A:303:LEU:CG	1:A:305:LEU:N	2.73	0.43
2:B:12:ILE:O	2:B:13:LYS:HB2	2.17	0.43
2:B:138:LYS:O	2:B:139:TYR:CD2	2.72	0.43
2:B:145:SER:C	2:B:147:ASN:H	2.21	0.43
2:B:4:ASN:ND2	2:B:5:ASP:O	2.52	0.43
2:B:74:LEU:O	2:B:77:TYR:N	2.51	0.43
1:A:15:LEU:HA	1:A:15:LEU:HD12	1.88	0.43
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.58	0.43
1:A:201:MET:HG3	1:A:204:GLU:OE1	2.18	0.43
1:A:216:GLU:HB3	1:A:217:GLU:H	1.10	0.43
2:B:113:ASN:C	2:B:114:CYS:O	2.54	0.43
1:A:114:LEU:CD1	2:B:119:GLU:HG3	2.48	0.43
2:B:23:ALA:C	2:B:25:ILE:HG22	2.39	0.43
1:A:59:PHE:CD1	1:A:103:VAL:HG21	2.53	0.43
1:A:121:ASN:HD22	1:A:121:ASN:H	1.66	0.43
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.84	0.43
1:A:197:TYR:CE1	1:A:198:ILE:HG22	2.54	0.43
1:A:215:ILE:HG21	1:A:246:LEU:CD2	2.47	0.43
1:A:2:ASN:O	1:A:3:PRO:C	2.57	0.43
1:A:55:THR:HG22	1:A:55:THR:H	1.55	0.43
1:A:92:ILE:O	1:A:95:ILE:CG2	2.60	0.43
2:B:75:ALA:O	2:B:79:PRO:HB3	2.18	0.43
2:B:107:LEU:HB3	2:B:125:PHE:HE1	1.82	0.42
1:A:106:HIS:HA	1:A:107:PRO:HD3	1.64	0.42
2:B:73:GLU:OE1	2:B:100:PRO:HG2	2.18	0.42
1:A:112:ALA:O	1:A:116:THR:N	2.51	0.42
1:A:141:ASP:O	1:A:144:THR:HG23	2.18	0.42
1:A:14:ASP:OD1	1:A:14:ASP:C	2.55	0.42
1:A:80:SER:O	1:A:81:LEU:CG	2.67	0.42
2:B:102:ARG:O	2:B:102:ARG:HG3	2.18	0.42
2:B:70:GLU:OE1	2:B:70:GLU:HA	2.16	0.42
2:B:9:VAL:CG1	2:B:10:ALA:N	2.78	0.42
1:A:240:LEU:HD22	1:A:241:VAL:H	1.84	0.42
1:A:279:TRP:CD1	1:A:282:GLN:HB2	2.53	0.42
2:B:61:ILE:HD11	2:B:81:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ARG:CB	2:B:64:THR:HG23	2.49	0.42
1:A:189:PRO:O	1:A:190:ASP:C	2.57	0.42
1:A:260:HIS:C	1:A:262:LEU:N	2.71	0.42
2:B:104:ILE:CG2	2:B:105:ASP:N	2.83	0.42
2:B:146:HIS:NE2	2:B:147:ASN:OD1	2.53	0.42
2:B:30:LEU:HD21	2:B:44:ILE:CD1	2.49	0.42
2:B:64:THR:O	2:B:65:PHE:HB3	2.20	0.42
1:A:151:ARG:CG	1:A:151:ARG:HH11	2.33	0.42
1:A:253:LYS:O	1:A:254:MET:HG2	2.20	0.42
1:A:274:LYS:HD3	1:A:275:THR:CA	2.43	0.42
2:B:147:ASN:O	2:B:149:VAL:CB	2.66	0.42
1:A:189:PRO:HD3	1:A:244:ASN:HD21	1.85	0.42
1:A:49:PHE:HE1	1:A:104:MET:HE1	1.83	0.42
1:A:50:GLU:HG2	1:A:50:GLU:O	2.18	0.42
1:A:52:SER:OG	1:A:55:THR:CG2	2.64	0.42
1:A:184:PHE:HB3	1:A:186:PHE:CE1	2.55	0.42
1:A:227:LEU:HD13	1:A:268:ILE:HD11	2.02	0.42
2:B:61:ILE:CG1	2:B:82:THR:N	2.57	0.42
2:B:72:ASP:O	2:B:100:PRO:CG	2.65	0.42
1:A:159:MET:HE2	1:A:172:LEU:CD2	2.50	0.41
1:A:149:GLU:CG	1:A:224:LYS:HG3	2.50	0.41
1:A:279:TRP:HA	1:A:282:GLN:CD	2.39	0.41
1:A:303:LEU:CD1	1:A:305:LEU:CB	2.94	0.41
2:B:61:ILE:CG2	2:B:62:GLU:CG	2.86	0.41
2:B:85:ARG:HB3	2:B:90:GLU:HG3	2.02	0.41
1:A:227:LEU:HD11	1:A:246:LEU:CG	2.50	0.41
1:A:284:ALA:O	1:A:285:GLY:C	2.57	0.41
2:B:15:GLY:N	2:B:64:THR:HG23	2.35	0.41
2:B:67:SER:HB3	2:B:70:GLU:CG	2.51	0.41
2:B:68:GLU:HB3	2:B:69:ASP:H	1.44	0.41
1:A:8:HIS:CB	1:A:10:ILE:CD1	2.80	0.41
2:B:75:ALA:CB	2:B:99:LEU:H	2.33	0.41
1:A:258:VAL:O	1:A:259:LEU:HD12	2.19	0.41
1:A:75:ASP:OD1	1:A:79:THR:CB	2.62	0.41
2:B:107:LEU:HA	2:B:108:VAL:HG22	2.01	0.41
1:A:260:HIS:HA	1:A:261:PRO:HD2	1.67	0.41
1:A:140:LEU:HD11	1:A:287:GLY:N	2.36	0.41
1:A:291:ARG:O	1:A:294:LEU:HB2	2.21	0.41
1:A:38:LEU:O	1:A:39:LEU:HD23	2.20	0.41
1:A:60:GLN:C	1:A:62:SER:H	2.22	0.41
2:B:115:ILE:HG22	2:B:119:GLU:CG	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ILE:HD13	2:B:44:ILE:HG13	1.98	0.41
1:A:160:VAL:CG1	1:A:187:ILE:HG12	2.50	0.41
1:A:184:PHE:CD1	1:A:202:LEU:CD1	3.02	0.41
2:B:107:LEU:CB	2:B:125:PHE:CE1	3.01	0.41
2:B:6:LYS:C	2:B:8:GLN:H	2.22	0.41
1:A:176:LEU:HA	1:A:176:LEU:HD22	1.48	0.41
1:A:156:HIS:CE1	1:A:185:TYR:OH	2.74	0.41
1:A:35:GLN:CB	1:A:38:LEU:CD2	2.96	0.41
2:B:79:PRO:HG2	2:B:80:GLN:H	1.84	0.41
2:B:11:GLU:O	2:B:12:ILE:O	2.38	0.41
2:B:14:ARG:HG2	2:B:64:THR:O	2.20	0.41
2:B:69:ASP:CB	2:B:72:ASP:HB2	2.41	0.41
2:B:63:ASN:CA	2:B:84:ASN:HB2	2.41	0.41
1:A:20:LEU:HA	1:A:20:LEU:HD12	1.85	0.41
1:A:282:GLN:O	1:A:283:GLN:C	2.58	0.41
1:A:38:LEU:N	1:A:38:LEU:HD23	2.35	0.41
1:A:88:LEU:HD22	1:A:92:ILE:HG12	2.02	0.41
2:B:115:ILE:O	2:B:118:ALA:N	2.54	0.41
2:B:75:ALA:CB	2:B:99:LEU:HA	2.50	0.41
2:B:92:VAL:CG1	2:B:92:VAL:O	2.62	0.40
1:A:12:ILE:HD11	1:A:138:THR:OG1	2.21	0.40
1:A:212:HIS:CD2	1:A:218:VAL:HG22	2.56	0.40
1:A:38:LEU:CB	1:A:39:LEU:HD23	2.45	0.40
1:A:47:CYS:O	1:A:104:MET:HA	2.21	0.40
2:B:102:ARG:HH11	2:B:104:ILE:HD13	1.86	0.40
2:B:115:ILE:HG21	2:B:115:ILE:HD13	1.62	0.40
2:B:26:GLY:O	2:B:30:LEU:HG	2.21	0.40
1:A:141:ASP:CA	1:A:144:THR:CG2	2.99	0.40
1:A:143:PHE:CG	1:A:144:THR:N	2.86	0.40
1:A:146:GLN:C	1:A:148:THR:N	2.74	0.40
1:A:215:ILE:HA	1:A:215:ILE:HD13	1.79	0.40
1:A:228:ASP:N	1:A:228:ASP:OD1	2.42	0.40
1:A:231:GLU:C	1:A:232:TYR:O	2.58	0.40
2:B:20:HIS:ND1	2:B:47:ASN:HB2	2.36	0.40
2:B:76:LEU:HD13	2:B:150:LEU:HD21	2.03	0.40
2:B:9:VAL:HG22	2:B:14:ARG:CA	2.51	0.40
1:A:137:GLN:HG3	1:A:141:ASP:OD2	2.22	0.40
1:A:267:GLU:HB3	1:A:268:ILE:HG13	2.02	0.40
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.70	0.40
1:A:56:ARG:HD3	1:A:56:ARG:HH11	1.51	0.40
1:A:87:THR:O	1:A:90:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:MET:O	1:A:255:ASN:CB	2.70	0.40
2:B:17:VAL:HA	2:B:43:THR:O	2.20	0.40
2:B:86:ILE:CA	2:B:90:GLU:CB	3.00	0.40

All (16) 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)
2:B:3:HIS:CB	2:B:4:ASN:O[6_555]	0.69	1.51
2:B:3:HIS:O	2:B:4:ASN:CB[6_555]	0.71	1.49
2:B:3:HIS:C	2:B:4:ASN:CA[6_555]	0.72	1.48
2:B:3:HIS:O	2:B:4:ASN:CA[6_555]	1.03	1.17
2:B:4:ASN:N	2:B:4:ASN:N[6_555]	1.46	0.74
1:A:75:ASP:O	1:A:78:ASN:OD1[3_555]	1.46	0.74
2:B:3:HIS:CB	2:B:4:ASN:C[6_555]	1.50	0.70
1:A:54:ARG:NH2	1:A:86:GLN:NE2[3_555]	1.67	0.53
2:B:3:HIS:CG	2:B:4:ASN:O[6_555]	1.76	0.44
2:B:3:HIS:C	2:B:4:ASN:N[6_555]	1.77	0.43
2:B:4:ASN:N	2:B:4:ASN:CA[6_555]	1.77	0.43
1:A:76:SER:C	1:A:78:ASN:ND2[3_555]	2.00	0.20
1:A:75:ASP:C	1:A:78:ASN:OD1[3_555]	2.06	0.14
1:A:76:SER:O	1:A:78:ASN:ND2[3_555]	2.11	0.09
1:A:76:SER:O	1:A:78:ASN:CG[3_555]	2.13	0.07
2:B:3:HIS:NE2	2:B:17:VAL:CG1[6_555]	2.18	0.02

## 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	302/305 (99%)	159 (53%)	71 (24%)	72 (24%)	<b>0</b> <b>0</b>
2	B	150/152 (99%)	66 (44%)	33 (22%)	51 (34%)	<b>0</b> <b>0</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	452/457 (99%)	225 (50%)	104 (23%)	123 (27%)	<b>0</b> <b>0</b>

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	6	GLN
1	A	10	ILE
1	A	11	SER
1	A	17	ARG
1	A	18	ASP
1	A	40	LYS
1	A	51	ALA
1	A	59	PHE
1	A	68	ALA
1	A	76	SER
1	A	77	ALA
1	A	78	ASN
1	A	81	LEU
1	A	88	LEU
1	A	111	ALA
1	A	116	THR
1	A	117	GLU
1	A	120	GLY
1	A	121	ASN
1	A	179	PHE
1	A	183	ARG
1	A	190	ASP
1	A	191	ALA
1	A	193	ALA
1	A	198	ILE
1	A	216	GLU
1	A	218	VAL
1	A	220	THR
1	A	228	ASP
1	A	232	TYR
1	A	237	ALA
1	A	241	VAL
1	A	252	ALA
1	A	254	MET
1	A	255	ASN
1	A	262	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	265	VAL
1	A	273	ASP
1	A	274	LYS
1	A	276	PRO
1	A	277	HIS
1	A	298	VAL
2	B	3	HIS
2	B	4	ASN
2	B	6	LYS
2	B	9	VAL
2	B	13	LYS
2	B	20	HIS
2	B	34	LYS
2	B	36	THR
2	B	58	LEU
2	B	61	ILE
2	B	64	THR
2	B	69	ASP
2	B	72	ASP
2	B	75	ALA
2	B	84	ASN
2	B	85	ARG
2	B	92	VAL
2	B	99	LEU
2	B	101	GLU
2	B	102	ARG
2	B	107	LEU
2	B	108	VAL
2	B	117	HIS
2	B	121	VAL
2	B	130	ALA
2	B	131	ASP
2	B	132	ASP
2	B	139	TYR
2	B	141	GLU
2	B	146	HIS
2	B	147	ASN
2	B	148	VAL
2	B	149	VAL
2	B	151	ALA
1	A	14	ASP
1	A	60	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	61	THR
1	A	181	GLY
1	A	187	ILE
1	A	209	TRP
1	A	229	PRO
1	A	264	ARG
1	A	279	TRP
1	A	280	TYR
1	A	292	GLN
1	A	294	LEU
2	B	11	GLU
2	B	12	ILE
2	B	17	VAL
2	B	22	PRO
2	B	67	SER
2	B	100	PRO
2	B	103	ASN
2	B	122	SER
1	A	37	GLU
1	A	233	ALA
1	A	235	VAL
1	A	267	GLU
1	A	291	ARG
1	A	293	ALA
2	B	26	GLY
2	B	28	LYS
2	B	38	THR
2	B	114	CYS
2	B	133	ILE
1	A	137	GLN
1	A	282	GLN
2	B	94	LYS
1	A	30	LEU
1	A	53	THR
1	A	71	VAL
1	A	143	PHE
1	A	148	THR
1	A	199	LEU
1	A	251	ASN
2	B	25	ILE
1	A	110	GLY
1	A	206	GLY

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Mol	Chain	Res	Type
2	B	71	VAL
2	B	83	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/254 (100%)	136 (54%)	118 (46%)	0	0
2	B	126/136 (93%)	70 (56%)	56 (44%)	0	0
All	All	380/390 (97%)	206 (54%)	174 (46%)	0	0

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	TYR
1	A	12	ILE
1	A	13	ASN
1	A	14	ASP
1	A	15	LEU
1	A	16	SER
1	A	17	ARG
1	A	22	LEU
1	A	23	VAL
1	A	24	LEU
1	A	26	THR
1	A	29	LYS
1	A	35	GLN
1	A	36	PRO
1	A	38	LEU
1	A	39	LEU
1	A	42	LYS
1	A	46	SER
1	A	54	ARG
1	A	55	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	57	LEU
1	A	58	SER
1	A	59	PHE
1	A	60	GLN
1	A	62	SER
1	A	69	SER
1	A	70	VAL
1	A	71	VAL
1	A	74	SER
1	A	75	ASP
1	A	76	SER
1	A	81	LEU
1	A	83	LYS
1	A	84	LYS
1	A	88	LEU
1	A	95	ILE
1	A	96	SER
1	A	98	TYR
1	A	99	VAL
1	A	102	ILE
1	A	104	MET
1	A	116	THR
1	A	117	GLU
1	A	119	SER
1	A	121	ASN
1	A	122	VAL
1	A	125	LEU
1	A	133	GLN
1	A	145	ILE
1	A	147	GLN
1	A	151	ARG
1	A	153	ASN
1	A	156	HIS
1	A	159	MET
1	A	160	VAL
1	A	163	LEU
1	A	165	TYR
1	A	167	ARG
1	A	168	THR
1	A	176	LEU
1	A	178	LYS
1	A	179	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	182	ASN
1	A	187	ILE
1	A	190	ASP
1	A	192	LEU
1	A	194	MET
1	A	196	GLU
1	A	197	TYR
1	A	198	ILE
1	A	199	LEU
1	A	200	ASP
1	A	201	MET
1	A	204	GLU
1	A	205	LYS
1	A	207	ILE
1	A	211	LEU
1	A	217	GLU
1	A	219	MET
1	A	220	THR
1	A	221	ARG
1	A	222	VAL
1	A	225	GLU
1	A	226	ARG
1	A	227	LEU
1	A	228	ASP
1	A	232	TYR
1	A	235	VAL
1	A	236	LYS
1	A	238	GLN
1	A	240	LEU
1	A	241	VAL
1	A	245	SER
1	A	246	LEU
1	A	249	LEU
1	A	254	MET
1	A	255	ASN
1	A	257	LYS
1	A	259	LEU
1	A	264	ARG
1	A	270	THR
1	A	271	ASP
1	A	273	ASP
1	A	274	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	275	THR
1	A	276	PRO
1	A	279	TRP
1	A	280	TYR
1	A	282	GLN
1	A	286	ASN
1	A	297	LEU
1	A	298	VAL
1	A	300	ASN
1	A	301	ARG
1	A	303	LEU
1	A	304	VAL
1	A	305	LEU
2	B	5	ASP
2	B	6	LYS
2	B	8	GLN
2	B	14	ARG
2	B	18	ILE
2	B	20	HIS
2	B	22	PRO
2	B	24	GLU
2	B	25	ILE
2	B	31	SER
2	B	35	LEU
2	B	38	THR
2	B	46	LEU
2	B	61	ILE
2	B	62	GLU
2	B	63	ASN
2	B	66	LEU
2	B	67	SER
2	B	68	GLU
2	B	69	ASP
2	B	70	GLU
2	B	72	ASP
2	B	73	GLU
2	B	74	LEU
2	B	77	TYR
2	B	80	GLN
2	B	82	THR
2	B	85	ARG
2	B	86	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	87	ASN
2	B	88	ASP
2	B	89	TYR
2	B	90	GLU
2	B	102	ARG
2	B	104	ILE
2	B	105	ASP
2	B	108	VAL
2	B	109	CYS
2	B	113	ASN
2	B	114	CYS
2	B	116	SER
2	B	119	GLU
2	B	122	SER
2	B	123	SER
2	B	128	ARG
2	B	129	ARG
2	B	132	ASP
2	B	137	CYS
2	B	138	LYS
2	B	141	GLU
2	B	142	LYS
2	B	143	GLU
2	B	146	HIS
2	B	149	VAL
2	B	150	LEU
2	B	152	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	6	GLN
1	A	8	HIS
1	A	13	ASN
1	A	33	ASN
1	A	35	GLN
1	A	41	HIS
1	A	60	GLN
1	A	121	ASN
1	A	137	GLN
1	A	174	GLN
1	A	260	HIS

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Mol	Chain	Res	Type
1	A	282	GLN
1	A	283	GLN
1	A	292	GLN
2	B	20	HIS
2	B	39	GLN
2	B	84	ASN
2	B	113	ASN
2	B	117	HIS
2	B	146	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

There are no chain breaks in this entry.

## 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.