



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2023 – 12:26 AM EST

PDB ID : 2HWF  
Title : A COMPARISON OF THE ANTI-RHINOVIRAL DRUG BINDING  
POCKET IN HRV14 AND HRV1A  
Authors : Kim, K.H.; Rossmann, M.G.  
Deposited on : 1994-01-25  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

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

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
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) : 2.32.1

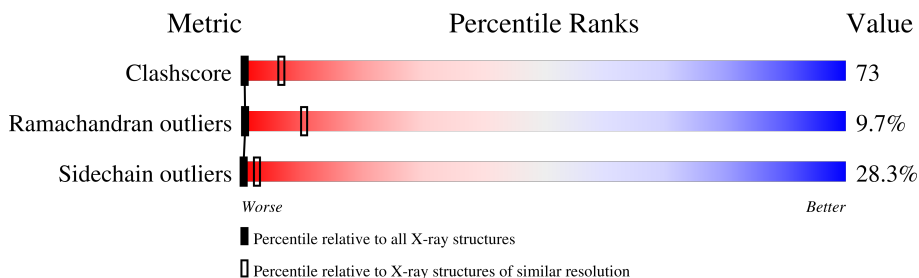
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1	287	15% 43% 27% 14% .
2	2	263	19% 37% 31% 10% .
3	3	238	18% 47% 26% 8%
4	4	44	7% 18% 9% 9% 57%

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
5	JEN	1	700	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6244 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 HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	283	2262	1431	389	430	12	0	0	0

- Molecule 2 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	253	1979	1249	349	371	10	0	0	0

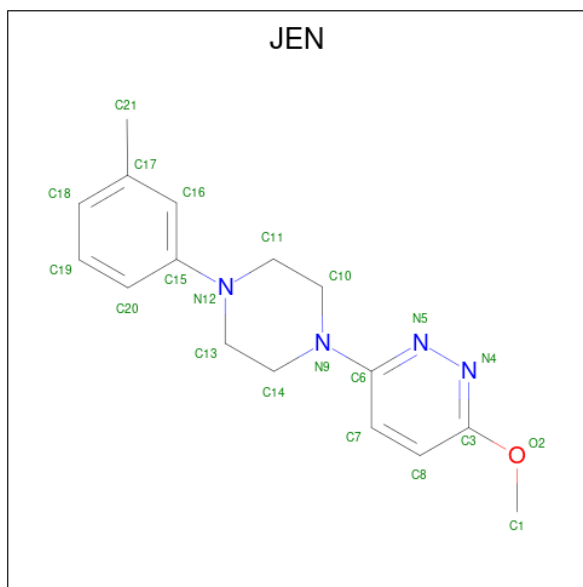
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	238	1831	1169	297	348	17	0	0	0

- Molecule 4 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	4	19	151	96	25	30	0	0	0

- Molecule 5 is 3-METHOXY-6-[4-(3-METHYLPHENYL)-1-PIPERAZINYL]PYRIDAZINE (three-letter code: JEN) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	1	1	21	16	4	1	0	0

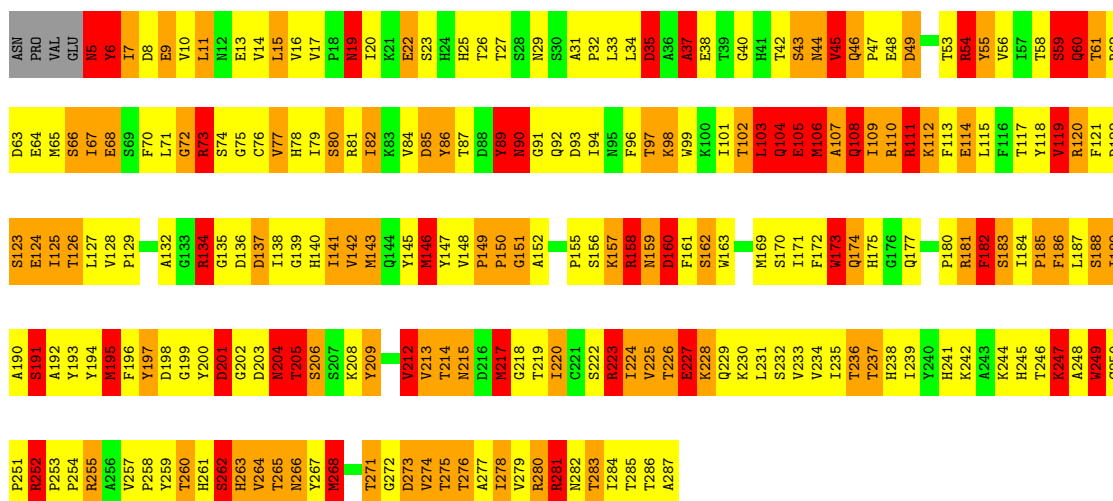
### 3 Residue-property plots

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

Note EDS was not executed.

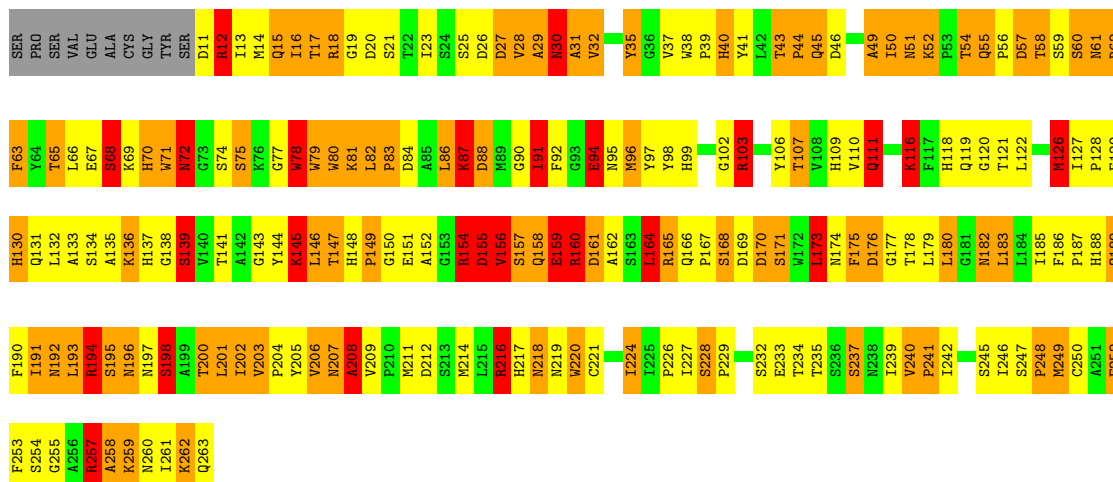
- Molecule 1: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)

Chain 1: 

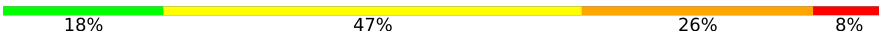


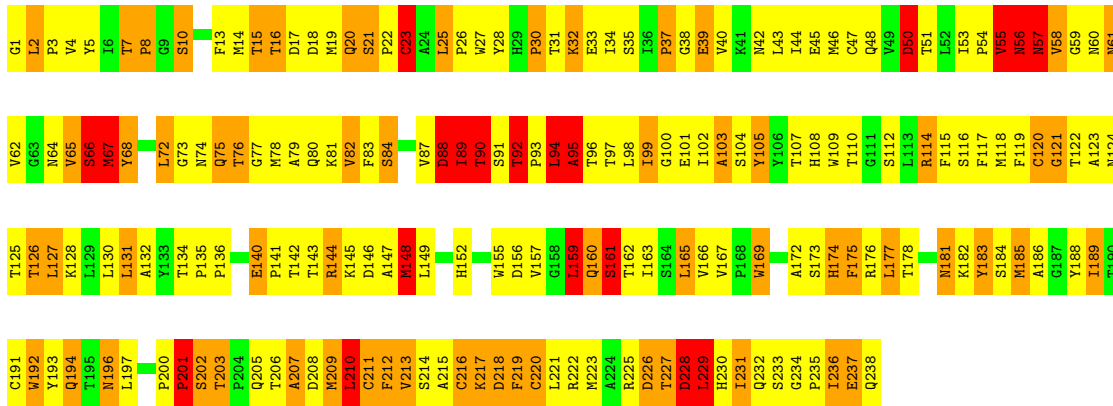
- Molecule 2: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2)

Chain 2: 




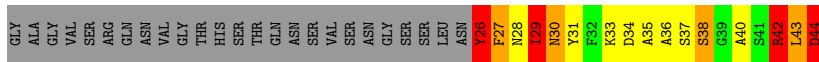
- Molecule 3: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3)

Chain 3: 



- Molecule 4: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4)

Chain 4: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	341.30Å 341.30Å 465.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	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: JEN

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	1	1.08	4/2322 (0.2%)	2.39	97/3162 (3.1%)
2	2	0.95	0/2033	2.60	151/2770 (5.5%)
3	3	0.97	1/1878 (0.1%)	2.43	106/2570 (4.1%)
4	4	1.25	0/154	3.16	21/206 (10.2%)
All	All	1.01	5/6387 (0.1%)	2.49	375/8708 (4.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	185	PRO	CA-C	-7.88	1.37	1.52
1	1	118	TYR	C-N	-7.51	1.16	1.34
1	1	186	PHE	N-CA	-7.10	1.32	1.46
1	1	185	PRO	N-CA	-6.48	1.36	1.47
3	3	20	GLN	C-N	-5.11	1.22	1.34

All (375) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	249	TRP	O-C-N	-45.13	50.49	122.70
2	2	62	ARG	CD-NE-CZ	24.85	158.39	123.60
1	1	134	ARG	NE-CZ-NH1	24.00	132.30	120.30
2	2	216	ARG	NE-CZ-NH2	-22.09	109.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	280	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	1	247	LYS	CA-C-O	-20.00	78.09	120.10
3	3	146	ASP	CB-CG-OD2	-17.26	102.77	118.30
1	1	247	LYS	CA-C-N	17.06	154.72	117.20
2	2	257	ARG	NE-CZ-NH2	-16.52	112.04	120.30
3	3	222	ARG	CD-NE-CZ	15.92	145.89	123.60
4	4	42	ARG	NE-CZ-NH1	15.10	127.85	120.30
1	1	249	TRP	C-N-CA	-14.94	84.35	121.70
2	2	155	ASP	CB-CG-OD2	-14.70	105.07	118.30
1	1	81	ARG	NE-CZ-NH1	14.06	127.33	120.30
1	1	281	ARG	NE-CZ-NH2	-13.91	113.35	120.30
2	2	154	ARG	NE-CZ-NH1	13.89	127.25	120.30
3	3	226	ASP	CB-CG-OD1	13.80	130.72	118.30
2	2	62	ARG	NE-CZ-NH1	13.79	127.19	120.30
1	1	247	LYS	N-CA-C	13.66	147.88	111.00
3	3	228	ASP	CB-CG-OD2	-13.33	106.31	118.30
1	1	247	LYS	CB-CA-C	-13.08	84.24	110.40
3	3	183	TYR	CB-CG-CD1	12.41	128.45	121.00
3	3	144	ARG	CD-NE-CZ	12.32	140.85	123.60
1	1	281	ARG	CA-CB-CG	12.20	140.23	113.40
1	1	6	TYR	CB-CG-CD1	-11.99	113.81	121.00
3	3	114	ARG	NE-CZ-NH1	-11.82	114.39	120.30
3	3	144	ARG	NE-CZ-NH1	11.43	126.02	120.30
3	3	225	ARG	NE-CZ-NH1	-11.26	114.67	120.30
3	3	50	ASP	CB-CG-OD2	-11.21	108.21	118.30
2	2	67	GLU	OE1-CD-OE2	10.99	136.49	123.30
3	3	50	ASP	CB-CG-OD1	10.99	128.19	118.30
1	1	54	ARG	CG-CD-NE	10.81	134.50	111.80
2	2	35	TYR	CB-CG-CD2	10.78	127.47	121.00
4	4	44	ASP	CB-CG-OD2	-10.74	108.63	118.30
2	2	12	ARG	NE-CZ-NH2	-10.30	115.15	120.30
3	3	218	ASP	CB-CG-OD2	-10.29	109.04	118.30
2	2	162	ALA	CB-CA-C	10.23	125.44	110.10
2	2	12	ARG	CD-NE-CZ	10.20	137.88	123.60
2	2	205	TYR	CB-CG-CD2	10.17	127.10	121.00
2	2	62	ARG	NH1-CZ-NH2	-9.96	108.45	119.40
2	2	11	ASP	CB-CG-OD1	9.86	127.18	118.30
2	2	216	ARG	NE-CZ-NH1	9.85	125.23	120.30
2	2	31	ALA	N-CA-CB	9.82	123.85	110.10
1	1	249	TRP	CA-C-N	9.64	138.42	117.20
3	3	67	MET	N-CA-CB	-9.62	93.29	110.60
1	1	8	ASP	CB-CG-OD2	-9.57	109.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	154	ARG	C-N-CA	9.56	145.60	121.70
2	2	29	ALA	N-CA-CB	9.55	123.48	110.10
4	4	42	ARG	CD-NE-CZ	9.44	136.81	123.60
2	2	212	ASP	CB-CG-OD2	9.37	126.73	118.30
2	2	176	ASP	CB-CG-OD2	9.36	126.72	118.30
2	2	165	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	1	182	PHE	O-C-N	-9.29	107.83	122.70
1	1	59	SER	N-CA-CB	-9.20	96.70	110.50
1	1	281	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	1	9	GLU	OE1-CD-OE2	9.12	134.24	123.30
1	1	134	ARG	NH1-CZ-NH2	-9.04	109.46	119.40
1	1	185	PRO	O-C-N	9.04	137.16	122.70
3	3	148	MET	CG-SD-CE	9.04	114.66	100.20
3	3	18	ASP	CB-CG-OD1	-8.95	110.25	118.30
2	2	28	VAL	CA-CB-CG1	8.94	124.31	110.90
2	2	165	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	2	154	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	1	60	GLN	O-C-N	8.73	136.68	122.70
2	2	35	TYR	CB-CG-CD1	-8.70	115.78	121.00
1	1	55	TYR	CB-CG-CD2	-8.69	115.79	121.00
3	3	232	GLN	N-CA-CB	8.68	126.22	110.60
2	2	11	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	1	11	LEU	O-C-N	8.64	136.52	122.70
3	3	222	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	2	233	GLU	CG-CD-OE2	8.45	135.19	118.30
1	1	68	GLU	CB-CG-CD	8.36	136.77	114.20
2	2	12	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	2	57	ASP	N-CA-CB	-8.30	95.66	110.60
3	3	226	ASP	OD1-CG-OD2	-8.24	107.65	123.30
2	2	97	TYR	CB-CG-CD2	8.18	125.91	121.00
2	2	126	MET	CA-CB-CG	-8.11	99.52	113.30
2	2	12	ARG	CG-CD-NE	7.99	128.58	111.80
2	2	241	PRO	C-N-CA	7.95	141.57	121.70
2	2	26	ASP	CB-CG-OD2	7.89	125.40	118.30
2	2	194	ARG	NE-CZ-NH2	-7.88	116.36	120.30
2	2	160	ARG	NE-CZ-NH1	-7.83	116.39	120.30
2	2	189	GLN	CA-CB-CG	7.82	130.60	113.40
1	1	49	ASP	CB-CG-OD1	-7.81	111.28	118.30
2	2	161	ASP	N-CA-CB	7.78	124.61	110.60
2	2	61	ASN	CB-CA-C	7.75	125.89	110.40
3	3	56	ASN	C-N-CA	7.75	141.06	121.70
1	1	55	TYR	CB-CG-CD1	7.74	125.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	235	PRO	C-N-CA	7.72	141.01	121.70
2	2	94	GLU	OE1-CD-OE2	7.70	132.54	123.30
2	2	159	GLU	OE1-CD-OE2	7.68	132.51	123.30
1	1	158	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	1	73	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	1	280	ARG	NH1-CZ-NH2	7.59	127.75	119.40
2	2	71	TRP	CB-CA-C	7.57	125.55	110.40
3	3	68	TYR	CB-CG-CD2	7.56	125.54	121.00
1	1	134	ARG	CD-NE-CZ	7.55	134.17	123.60
1	1	85	ASP	CB-CG-OD1	-7.54	111.51	118.30
1	1	6	TYR	CB-CG-CD2	7.54	125.52	121.00
2	2	161	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	1	252	ARG	NE-CZ-NH2	7.52	124.06	120.30
3	3	207	ALA	O-C-N	7.51	134.71	122.70
1	1	120	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	1	181	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	1	111	ARG	NE-CZ-NH2	7.43	124.02	120.30
2	2	232	SER	N-CA-CB	7.42	121.62	110.50
1	1	61	THR	CA-CB-OG1	-7.41	93.44	109.00
2	2	252	GLU	OE1-CD-OE2	7.39	132.16	123.30
1	1	110	ARG	NE-CZ-NH2	7.36	123.98	120.30
3	3	92	THR	CB-CA-C	7.35	131.44	111.60
1	1	89	TYR	CB-CG-CD1	-7.31	116.61	121.00
3	3	161	SER	CB-CA-C	-7.31	96.21	110.10
4	4	34	ASP	CB-CG-OD1	-7.30	111.73	118.30
4	4	37	SER	O-C-N	7.28	134.35	122.70
2	2	147	THR	N-CA-CB	7.21	124.01	110.30
3	3	88	ASP	CB-CG-OD2	7.19	124.77	118.30
1	1	173	TRP	CA-CB-CG	7.17	127.32	113.70
3	3	95	ALA	CA-C-N	7.16	132.95	117.20
2	2	152	ALA	N-CA-CB	-7.16	100.08	110.10
2	2	233	GLU	CG-CD-OE1	-7.16	103.98	118.30
4	4	40	ALA	O-C-N	7.14	134.13	122.70
2	2	78	TRP	CA-CB-CG	7.12	127.23	113.70
2	2	62	ARG	NE-CZ-NH2	7.12	123.86	120.30
3	3	232	GLN	O-C-N	7.10	134.05	122.70
2	2	237	SER	CB-CA-C	7.08	123.54	110.10
3	3	120	CYS	CA-CB-SG	-7.04	101.32	114.00
2	2	164	LEU	O-C-N	7.03	133.95	122.70
1	1	223	ARG	NE-CZ-NH2	7.01	123.81	120.30
3	3	218	ASP	N-CA-CB	-7.01	97.98	110.60
2	2	80	TRP	N-CA-CB	7.00	123.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	45	VAL	CB-CA-C	6.97	124.65	111.40
2	2	160	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	2	103	ARG	CD-NE-CZ	6.96	133.34	123.60
4	4	42	ARG	NH1-CZ-NH2	-6.96	111.75	119.40
4	4	31	TYR	CB-CG-CD1	6.91	125.15	121.00
3	3	222	ARG	NH1-CZ-NH2	-6.90	111.81	119.40
2	2	81	LYS	O-C-N	6.85	133.66	122.70
2	2	160	ARG	N-CA-CB	-6.84	98.30	110.60
1	1	5	ASN	N-CA-CB	6.80	122.84	110.60
2	2	72	ASN	OD1-CG-ND2	6.80	137.54	121.90
2	2	106	TYR	C-N-CA	6.78	138.65	121.70
1	1	203	ASP	CB-CG-OD1	-6.74	112.24	118.30
2	2	198	SER	CB-CA-C	-6.72	97.33	110.10
3	3	193	TYR	O-C-N	6.68	133.38	122.70
2	2	52	LYS	CA-CB-CG	6.67	128.07	113.40
3	3	90	THR	N-CA-CB	6.65	122.94	110.30
3	3	73	GLY	CA-C-O	6.64	132.56	120.60
3	3	218	ASP	CA-CB-CG	-6.63	98.81	113.40
4	4	40	ALA	N-CA-CB	6.62	119.37	110.10
3	3	57	ASN	CB-CG-ND2	-6.59	100.88	116.70
2	2	135	ALA	N-CA-CB	-6.59	100.88	110.10
1	1	19	ASN	CB-CG-OD1	-6.58	108.45	121.60
1	1	37	ALA	N-CA-CB	-6.56	100.91	110.10
1	1	70	PHE	O-C-N	6.54	133.17	122.70
2	2	196	ASN	N-CA-CB	-6.53	98.86	110.60
3	3	55	VAL	CB-CA-C	6.51	123.78	111.40
1	1	5	ASN	O-C-N	6.51	133.11	122.70
2	2	50	ILE	CA-CB-CG2	6.48	123.86	110.90
2	2	187	PRO	CB-CA-C	6.46	128.14	112.00
3	3	16	THR	CA-CB-CG2	6.45	121.44	112.40
1	1	260	THR	O-C-N	6.44	133.01	122.70
2	2	183	LEU	O-C-N	6.43	132.99	122.70
3	3	222	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	1	64	GLU	CA-CB-CG	6.42	127.52	113.40
2	2	16	ILE	O-C-N	6.39	132.93	122.70
2	2	28	VAL	CG1-CB-CG2	-6.39	100.68	110.90
1	1	13	GLU	O-C-N	6.38	132.91	122.70
3	3	172	ALA	CB-CA-C	6.38	119.67	110.10
2	2	68	SER	N-CA-CB	6.35	120.02	110.50
2	2	26	ASP	OD1-CG-OD2	-6.34	111.26	123.30
3	3	235	PRO	CA-C-N	-6.33	103.26	117.20
3	3	160	GLN	N-CA-CB	6.33	121.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	185	PRO	CA-C-N	-6.32	103.30	117.20
3	3	235	PRO	CA-C-O	6.30	135.32	120.20
2	2	196	ASN	OD1-CG-ND2	6.28	136.34	121.90
3	3	37	PRO	N-CA-CB	6.26	110.81	103.30
1	1	201	ASP	CB-CG-OD2	6.26	123.93	118.30
2	2	248	PRO	N-CA-C	-6.25	95.85	112.10
2	2	161	ASP	O-C-N	6.25	132.69	122.70
4	4	44	ASP	CB-CG-OD1	6.22	123.90	118.30
1	1	77	VAL	O-C-N	6.21	132.64	122.70
2	2	19	GLY	C-N-CA	6.21	137.21	121.70
2	2	94	GLU	CG-CD-OE1	-6.20	105.89	118.30
3	3	33	GLU	CG-CD-OE2	-6.20	105.90	118.30
4	4	30	ASN	CB-CA-C	6.19	122.79	110.40
1	1	86	TYR	CB-CA-C	6.17	122.74	110.40
3	3	94	LEU	CA-C-N	6.17	130.77	117.20
3	3	89	ILE	CB-CA-C	-6.16	99.28	111.60
1	1	195	MET	CG-SD-CE	6.16	110.05	100.20
2	2	155	ASP	N-CA-CB	6.14	121.66	110.60
4	4	38	SER	O-C-N	6.14	133.65	123.20
1	1	143	MET	CG-SD-CE	6.14	110.03	100.20
1	1	255	ARG	NE-CZ-NH2	6.14	123.37	120.30
2	2	205	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	1	217	MET	CG-SD-CE	6.13	110.01	100.20
1	1	268	MET	CG-SD-CE	6.13	110.01	100.20
1	1	175	HIS	N-CA-CB	-6.12	99.58	110.60
1	1	16	VAL	CG1-CB-CG2	6.12	120.69	110.90
4	4	35	ALA	CB-CA-C	6.10	119.25	110.10
1	1	106	MET	CG-SD-CE	6.09	109.94	100.20
1	1	206	SER	O-C-N	6.09	132.44	122.70
2	2	154	ARG	CG-CD-NE	6.07	124.56	111.80
2	2	17	THR	CB-CA-C	6.07	127.98	111.60
1	1	146	MET	CG-SD-CE	6.07	109.91	100.20
3	3	185	MET	CA-CB-CG	6.04	123.57	113.30
2	2	155	ASP	CB-CG-OD1	6.04	123.73	118.30
2	2	107	THR	CA-CB-OG1	-6.04	96.32	109.00
2	2	81	LYS	CA-CB-CG	6.03	126.66	113.40
3	3	32	LYS	O-C-N	6.02	132.33	122.70
2	2	57	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	2	194	ARG	NH1-CZ-NH2	6.02	126.02	119.40
2	2	82	LEU	CA-CB-CG	-6.01	101.48	115.30
2	2	57	ASP	CB-CG-OD1	-6.01	112.89	118.30
3	3	183	TYR	CB-CG-CD2	-6.00	117.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	35	ASP	CB-CG-OD2	6.00	123.69	118.30
2	2	262	LYS	CB-CA-C	5.98	122.36	110.40
3	3	15	THR	N-CA-CB	-5.96	98.98	110.30
2	2	160	ARG	CG-CD-NE	5.95	124.29	111.80
4	4	26	TYR	CB-CG-CD1	5.94	124.56	121.00
3	3	30	PRO	O-C-N	5.93	132.19	122.70
1	1	82	ILE	CB-CA-C	-5.92	99.75	111.60
2	2	130	HIS	CA-CB-CG	-5.92	103.53	113.60
3	3	233	SER	CA-C-N	-5.92	104.35	116.20
2	2	130	HIS	O-C-N	5.92	132.17	122.70
1	1	71	LEU	CB-CA-C	5.91	121.43	110.20
2	2	87	LYS	CB-CG-CD	5.90	126.94	111.60
2	2	156	VAL	C-N-CA	5.89	136.43	121.70
2	2	157	SER	N-CA-CB	5.89	119.33	110.50
2	2	208	ALA	N-CA-CB	5.89	118.34	110.10
1	1	68	GLU	OE1-CD-OE2	-5.88	116.25	123.30
2	2	91	ILE	N-CA-CB	5.88	124.31	110.80
2	2	49	ALA	CA-C-O	-5.87	107.77	120.10
1	1	55	TYR	O-C-N	5.87	132.09	122.70
2	2	97	TYR	CB-CG-CD1	-5.86	117.48	121.00
3	3	68	TYR	CB-CG-CD1	-5.86	117.49	121.00
3	3	201	PRO	N-CA-C	5.85	127.31	112.10
2	2	252	GLU	CG-CD-OE1	-5.84	106.61	118.30
3	3	105	TYR	CB-CG-CD2	5.83	124.50	121.00
1	1	85	ASP	CB-CG-OD2	5.83	123.55	118.30
1	1	20	ILE	O-C-N	5.83	132.03	122.70
2	2	234	THR	CA-C-O	5.83	132.33	120.10
1	1	49	ASP	OD1-CG-OD2	5.81	134.33	123.30
1	1	89	TYR	CB-CG-CD2	5.79	124.48	121.00
2	2	147	THR	O-C-N	5.79	131.96	122.70
2	2	257	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	1	54	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	3	185	MET	N-CA-CB	5.79	121.02	110.60
2	2	249	MET	CA-CB-CG	5.78	123.13	113.30
1	1	25	HIS	O-C-N	5.75	131.91	122.70
2	2	57	ASP	OD1-CG-OD2	5.75	134.22	123.30
2	2	218	ASN	CA-CB-CG	5.74	126.03	113.40
1	1	202	GLY	C-N-CA	5.71	135.99	121.70
2	2	134	SER	CA-C-N	-5.71	104.64	117.20
1	1	16	VAL	CB-CA-C	5.68	122.19	111.40
3	3	45	GLU	OE1-CD-OE2	-5.67	116.49	123.30
2	2	249	MET	CG-SD-CE	5.67	109.27	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	81	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
3	3	229	LEU	CA-CB-CG	5.66	128.32	115.30
2	2	83	PRO	C-N-CA	5.66	135.84	121.70
3	3	103	ALA	CB-CA-C	5.65	118.58	110.10
3	3	76	THR	O-C-N	5.65	132.81	123.20
3	3	160	GLN	O-C-N	5.65	131.74	122.70
1	1	90	ASN	CB-CA-C	5.65	121.70	110.40
2	2	139	SER	N-CA-CB	-5.64	102.04	110.50
1	1	204	ASN	CA-C-N	-5.63	104.81	117.20
3	3	77	GLY	CA-C-O	5.63	130.74	120.60
3	3	18	ASP	OD1-CG-OD2	5.62	133.98	123.30
3	3	227	THR	CA-C-O	5.62	131.89	120.10
3	3	212	PHE	CA-CB-CG	5.61	127.35	113.90
2	2	228	SER	N-CA-CB	5.60	118.91	110.50
2	2	26	ASP	CB-CG-OD1	5.59	123.33	118.30
2	2	212	ASP	CB-CG-OD1	-5.59	113.27	118.30
2	2	49	ALA	CA-C-N	5.59	129.50	117.20
3	3	146	ASP	OD1-CG-OD2	5.58	133.91	123.30
2	2	149	PRO	CA-C-N	5.57	127.34	116.20
2	2	134	SER	N-CA-CB	5.57	118.85	110.50
2	2	220	TRP	CA-C-N	-5.57	104.96	117.20
2	2	83	PRO	CB-CA-C	5.56	125.89	112.00
3	3	146	ASP	CB-CG-OD1	5.56	123.30	118.30
2	2	116	LYS	CB-CA-C	-5.55	99.30	110.40
2	2	119	GLN	CB-CA-C	5.53	121.47	110.40
1	1	68	GLU	CA-CB-CG	5.53	125.57	113.40
3	3	79	ALA	O-C-N	5.53	131.54	122.70
3	3	64	ASN	OD1-CG-ND2	5.52	134.60	121.90
1	1	81	ARG	CD-NE-CZ	5.52	131.33	123.60
2	2	194	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	2	54	THR	N-CA-CB	5.49	120.73	110.30
2	2	169	ASP	CA-C-O	5.49	131.62	120.10
2	2	32	VAL	O-C-N	5.47	131.45	122.70
2	2	90	GLY	CA-C-O	5.46	130.43	120.60
2	2	216	ARG	NH1-CZ-NH2	5.45	125.40	119.40
1	1	62	ARG	NE-CZ-NH1	-5.44	117.58	120.30
4	4	40	ALA	N-CA-C	-5.43	96.34	111.00
3	3	169	TRP	CB-CA-C	5.42	121.24	110.40
2	2	70	HIS	CB-CA-C	-5.42	99.57	110.40
3	3	218	ASP	C-N-CA	5.41	135.22	121.70
3	3	228	ASP	CB-CA-C	-5.41	99.58	110.40
2	2	20	ASP	CB-CG-OD2	-5.40	113.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	225	ARG	NE-CZ-NH2	5.40	123.00	120.30
3	3	58	VAL	CA-CB-CG1	-5.40	102.81	110.90
3	3	234	GLY	N-CA-C	-5.39	99.62	113.10
4	4	26	TYR	CB-CG-CD2	-5.39	117.76	121.00
3	3	237	GLU	OE1-CD-OE2	5.38	129.76	123.30
3	3	8	PRO	C-N-CA	5.38	133.60	122.30
3	3	235	PRO	CB-CA-C	-5.38	98.56	112.00
3	3	183	TYR	CG-CD2-CE2	5.37	125.60	121.30
3	3	203	THR	O-C-N	5.35	131.27	121.10
3	3	88	ASP	OD1-CG-OD2	-5.35	113.14	123.30
1	1	172	PHE	CA-C-O	-5.34	108.88	120.10
1	1	283	THR	O-C-N	5.34	131.25	122.70
4	4	44	ASP	CA-C-O	5.33	131.30	120.10
2	2	150	GLY	O-C-N	5.33	131.24	122.70
3	3	175	PHE	CB-CG-CD1	-5.33	117.07	120.80
3	3	95	ALA	CA-C-O	-5.33	108.91	120.10
3	3	233	SER	CA-C-O	5.33	131.29	120.10
2	2	161	ASP	CB-CA-C	-5.33	99.75	110.40
3	3	206	THR	N-CA-C	-5.32	96.64	111.00
2	2	52	LYS	CG-CD-CE	5.31	127.84	111.90
2	2	96	MET	CA-C-N	-5.31	105.51	117.20
2	2	165	ARG	C-N-CA	5.31	134.98	121.70
2	2	111	GLN	CB-CG-CD	5.31	125.40	111.60
2	2	87	LYS	CB-CA-C	5.30	121.00	110.40
3	3	206	THR	OG1-CB-CG2	5.29	122.16	110.00
1	1	201	ASP	CB-CG-OD1	-5.28	113.55	118.30
2	2	150	GLY	CA-C-O	-5.28	111.09	120.60
4	4	29	ILE	O-C-N	5.28	131.15	122.70
3	3	35	SER	N-CA-CB	-5.28	102.58	110.50
2	2	195	SER	CB-CA-C	5.27	120.11	110.10
3	3	108	HIS	CA-CB-CG	5.27	122.56	113.60
3	3	202	SER	CA-C-N	-5.26	105.63	117.20
3	3	10	SER	CB-CA-C	5.25	120.08	110.10
3	3	156	ASP	CB-CG-OD1	-5.25	113.58	118.30
2	2	11	ASP	O-C-N	5.23	131.07	122.70
2	2	182	ASN	O-C-N	5.22	131.06	122.70
2	2	203	VAL	N-CA-CB	-5.22	100.01	111.50
2	2	82	LEU	N-CA-C	5.22	125.09	111.00
2	2	12	ARG	CB-CA-C	-5.21	99.97	110.40
3	3	114	ARG	NE-CZ-NH2	5.21	122.91	120.30
3	3	92	THR	N-CA-C	-5.21	96.94	111.00
3	3	64	ASN	N-CA-CB	-5.20	101.24	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	287	ALA	CA-C-O	-5.20	109.19	120.10
2	2	173	LEU	CB-CA-C	5.19	120.06	110.20
4	4	26	TYR	O-C-N	5.17	130.97	122.70
2	2	30	ASN	N-CA-CB	-5.16	101.31	110.60
3	3	146	ASP	N-CA-CB	5.16	119.89	110.60
3	3	76	THR	CA-C-N	-5.16	105.88	116.20
3	3	165	LEU	O-C-N	5.16	130.96	122.70
2	2	19	GLY	CA-C-N	-5.15	105.86	117.20
1	1	22	GLU	CG-CD-OE2	5.14	128.58	118.30
3	3	181	ASN	O-C-N	5.14	130.92	122.70
2	2	237	SER	CA-C-O	5.13	130.87	120.10
4	4	42	ARG	C-N-CA	-5.13	108.88	121.70
1	1	66	SER	O-C-N	5.11	130.88	122.70
3	3	72	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	1	43	SER	CA-C-N	-5.10	105.98	117.20
4	4	38	SER	CA-C-O	-5.10	109.39	120.10
1	1	46	GLN	O-C-N	5.10	130.78	121.10
2	2	50	ILE	CB-CA-C	5.09	121.77	111.60
1	1	205	THR	OG1-CB-CG2	5.08	121.70	110.00
3	3	78	MET	CB-CA-C	5.08	120.56	110.40
2	2	40	HIS	CA-CB-CG	-5.07	104.98	113.60
3	3	223	MET	CG-SD-CE	5.06	108.30	100.20
2	2	168	SER	C-N-CA	5.06	134.35	121.70
3	3	227	THR	CA-CB-CG2	-5.06	105.32	112.40
1	1	275	THR	O-C-N	5.05	130.79	122.70
2	2	28	VAL	CB-CA-C	-5.05	101.80	111.40
3	3	131	LEU	CA-CB-CG	5.04	126.89	115.30
3	3	64	ASN	CA-CB-CG	-5.03	102.33	113.40
2	2	45	GLN	N-CA-CB	5.03	119.65	110.60
2	2	79	TRP	CA-CB-CG	5.03	123.25	113.70
1	1	204	ASN	N-CA-CB	5.02	119.64	110.60
1	1	80	SER	CA-C-O	5.02	130.64	120.10
2	2	218	ASN	CB-CG-OD1	-5.02	111.57	121.60
3	3	57	ASN	N-CA-CB	-5.02	101.57	110.60
3	3	210	LEU	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	247	LYS	Mainchain
1	1	249	TRP	Mainchain

## 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	1	2262	0	2191	515	1
2	2	1979	0	1920	243	1
3	3	1831	0	1808	253	0
4	4	151	0	136	19	0
5	1	21	0	20	10	0
All	All	6244	0	6075	894	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 73.

All (894) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:125:ILE:HG21	1:1:182:PHE:CE1	1.52	1.41
1:1:267:TYR:O	1:1:268:MET:CG	1.78	1.29
1:1:183:SER:O	1:1:184:ILE:CG1	1.79	1.29
1:1:261:HIS:CD2	2:2:138:GLY:O	1.85	1.27
1:1:267:TYR:O	1:1:268:MET:HG2	1.11	1.26
1:1:261:HIS:CD2	2:2:138:GLY:C	2.06	1.26
1:1:260:THR:HG22	1:1:261:HIS:N	1.31	1.21
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.54	1.21
1:1:101:ILE:HD11	1:1:217:MET:O	1.36	1.20
1:1:261:HIS:NE2	2:2:138:GLY:C	1.94	1.20
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.19
1:1:255:ARG:HD2	1:1:259:TYR:CE2	1.78	1.17
1:1:125:ILE:CG2	1:1:182:PHE:CE1	2.26	1.17
1:1:163:TRP:CH2	1:1:222:SER:O	1.99	1.14
1:1:98:LYS:O	1:1:98:LYS:HG2	1.43	1.14
1:1:183:SER:O	1:1:184:ILE:HG12	1.44	1.14
1:1:271:THR:O	1:1:273:ASP:N	1.78	1.14
1:1:104:GLN:O	3:3:236:ILE:HD13	1.48	1.13
1:1:125:ILE:CG2	1:1:182:PHE:HE1	1.61	1.13
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.06	1.13
1:1:260:THR:CG2	1:1:261:HIS:H	1.44	1.11
1:1:260:THR:CG2	1:1:261:HIS:N	2.00	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.12	1.09
1:1:215:ASN:HD22	1:1:215:ASN:N	1.47	1.09
1:1:252:ARG:CG	1:1:253:PRO:HD2	1.82	1.09
2:2:18:ARG:HH12	2:2:249:MET:HE2	0.99	1.08
3:3:160:GLN:O	3:3:161:SER:HB3	1.48	1.07
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.31	1.07
1:1:191:SER:OG	2:2:208:ALA:O	1.72	1.07
1:1:125:ILE:O	1:1:181:ARG:HG2	1.55	1.06
1:1:46:GLN:HB3	1:1:47:PRO:CD	1.85	1.06
1:1:103:LEU:HD11	5:1:700:JEN:H8	1.33	1.06
1:1:189:ILE:O	3:3:31:THR:HG21	1.55	1.05
1:1:230:LYS:HG2	1:1:231:LEU:HD22	1.37	1.05
1:1:183:SER:O	1:1:184:ILE:HG13	1.55	1.04
1:1:119:VAL:O	1:1:192:ALA:HB1	1.56	1.04
1:1:189:ILE:O	3:3:31:THR:CG2	2.06	1.04
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.02
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.02
1:1:255:ARG:CD	1:1:259:TYR:CE2	2.42	1.02
2:2:185:ILE:HD13	3:3:98:LEU:HD22	1.41	1.02
1:1:261:HIS:NE2	2:2:138:GLY:CA	2.23	1.01
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.01
1:1:273:ASP:O	1:1:274:VAL:HG12	1.59	1.01
3:3:117:PHE:HD1	3:3:211:CYS:HB3	1.25	1.01
1:1:103:LEU:C	1:1:104:GLN:HG2	1.79	1.01
1:1:129:PRO:HG2	1:1:173:TRP:CE2	1.95	1.00
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.00
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	1.00
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.00
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	1.00
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.99
1:1:124:GLU:HG2	1:1:242:LYS:HB3	1.44	0.99
3:3:75:GLN:HA	3:3:75:GLN:NE2	1.75	0.99
3:3:75:GLN:HA	3:3:75:GLN:HE21	1.26	0.99
1:1:278:ILE:HD12	3:3:67:MET:CE	1.93	0.98
1:1:163:TRP:HH2	1:1:222:SER:O	1.41	0.98
1:1:146:MET:HE2	1:1:162:SER:O	1.64	0.98
1:1:252:ARG:HG3	1:1:253:PRO:HD2	1.46	0.98
1:1:261:HIS:NE2	2:2:138:GLY:HA2	1.79	0.97
3:3:117:PHE:CD1	3:3:211:CYS:HB3	2.00	0.97
1:1:103:LEU:O	1:1:104:GLN:HG2	1.62	0.97
1:1:173:TRP:CD1	1:1:180:PRO:HD3	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:146:MET:CE	1:1:162:SER:O	2.13	0.96
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.96
3:3:28:TYR:O	3:3:30:PRO:HD3	1.64	0.96
1:1:113:PHE:O	1:1:115:LEU:N	1.99	0.95
1:1:103:LEU:O	1:1:104:GLN:CG	2.14	0.95
1:1:249:TRP:HA	3:3:39:GLU:HA	1.44	0.95
1:1:158:ARG:O	1:1:163:TRP:NE1	1.99	0.94
1:1:267:TYR:O	1:1:268:MET:CB	2.13	0.94
1:1:189:ILE:O	3:3:31:THR:CB	2.15	0.94
1:1:108:GLN:CD	3:3:226:ASP:OD2	2.06	0.93
1:1:212:VAL:CG1	1:1:263:HIS:CD2	2.51	0.93
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.93
1:1:142:VAL:HG12	1:1:225:VAL:CB	1.98	0.93
1:1:104:GLN:O	3:3:236:ILE:CD1	2.17	0.93
1:1:248:ALA:O	3:3:40:VAL:N	2.02	0.92
1:1:101:ILE:CD1	1:1:217:MET:HB2	1.98	0.92
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.92
1:1:212:VAL:HG12	1:1:263:HIS:CG	2.04	0.92
1:1:260:THR:HG22	1:1:261:HIS:CA	1.99	0.91
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.50	0.91
1:1:212:VAL:CG1	1:1:263:HIS:CG	2.52	0.91
1:1:117:THR:O	1:1:195:MET:HB2	1.70	0.91
1:1:214:THR:C	1:1:215:ASN:HD22	1.73	0.91
1:1:142:VAL:CG1	1:1:225:VAL:HB	2.01	0.90
1:1:138:ILE:HG13	1:1:139:GLY:N	1.86	0.90
1:1:158:ARG:O	1:1:163:TRP:CD1	2.24	0.90
1:1:173:TRP:HD1	1:1:180:PRO:CD	1.85	0.89
1:1:197:TYR:CD2	1:1:214:THR:HG22	2.07	0.89
1:1:189:ILE:O	3:3:31:THR:HB	1.71	0.89
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.54	0.88
1:1:261:HIS:HD2	2:2:138:GLY:O	1.43	0.88
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.88
1:1:125:ILE:O	1:1:181:ARG:CG	2.22	0.88
1:1:75:GLY:O	1:1:77:VAL:HG13	1.74	0.87
1:1:101:ILE:HD11	1:1:217:MET:HB2	1.56	0.87
1:1:183:SER:C	1:1:184:ILE:HG13	1.94	0.87
1:1:215:ASN:N	1:1:215:ASN:ND2	2.20	0.86
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:96:PHE:CE2	1:1:157:LYS:HA	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.86
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
1:1:248:ALA:O	3:3:39:GLU:CA	2.25	0.85
1:1:125:ILE:HG21	1:1:182:PHE:HE1	0.85	0.85
1:1:122:ASP:OD2	4:4:36:ALA:HA	1.77	0.85
1:1:91:GLY:O	1:1:157:LYS:HB3	1.77	0.84
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.38	0.84
1:1:108:GLN:NE2	3:3:226:ASP:OD2	2.10	0.84
1:1:126:THR:HG23	1:1:181:ARG:HG3	1.57	0.84
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.84
1:1:101:ILE:CD1	1:1:217:MET:O	2.23	0.83
1:1:260:THR:HG22	1:1:261:HIS:H	0.95	0.83
2:2:159:GLU:C	2:2:160:ARG:HG2	1.97	0.83
1:1:183:SER:C	1:1:184:ILE:CG1	2.43	0.83
1:1:260:THR:CG2	1:1:261:HIS:CD2	2.61	0.83
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.14	0.83
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
1:1:112:LYS:O	1:1:115:LEU:HB2	1.79	0.82
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.82
1:1:123:SER:HB3	1:1:241:HIS:NE2	1.95	0.82
1:1:186:PHE:CE1	3:3:31:THR:HG22	2.13	0.82
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.82
1:1:97:THR:HG23	1:1:222:SER:HB3	1.60	0.82
1:1:186:PHE:HE1	3:3:31:THR:HG22	1.42	0.82
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.82
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:158:ARG:NH2	1:1:225:VAL:O	2.13	0.81
1:1:110:ARG:NE	1:1:114:GLU:OE2	2.14	0.80
1:1:108:GLN:OE1	3:3:226:ASP:OD2	1.98	0.80
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.12	0.80
1:1:260:THR:HG22	1:1:261:HIS:CB	2.12	0.80
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:212:VAL:CG1	1:1:263:HIS:HB3	2.12	0.80
1:1:76:CYS:HA	1:1:239:ILE:O	1.81	0.80
1:1:141:ILE:CG2	1:1:141:ILE:O	2.30	0.80
1:1:212:VAL:HB	1:1:263:HIS:CD2	2.17	0.80
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.45	0.79
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.79
1:1:248:ALA:O	3:3:39:GLU:HA	1.82	0.79
1:1:252:ARG:HG2	1:1:253:PRO:HD2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:ARG:HH12	2:2:249:MET:CE	1.90	0.79
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.79
1:1:147:TYR:CD1	5:1:700:JEN:C21	2.66	0.79
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.78
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.78
1:1:142:VAL:CG1	1:1:225:VAL:CG2	2.60	0.78
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.78
1:1:101:ILE:HD11	1:1:217:MET:C	2.04	0.78
1:1:252:ARG:CG	1:1:253:PRO:CD	2.61	0.78
1:1:110:ARG:O	1:1:114:GLU:HG3	1.82	0.78
1:1:126:THR:HG21	3:3:13:PHE:CE1	2.19	0.78
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.78
1:1:89:TYR:HE2	1:1:227:GLU:C	1.87	0.78
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.64	0.77
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.77
2:2:173:LEU:O	2:2:174:ASN:HB2	1.83	0.77
1:1:92:GLN:C	1:1:94:ILE:HD12	2.05	0.77
2:2:146:LEU:HD12	2:2:167:PRO:HD3	1.65	0.77
3:3:231:ILE:H	3:3:231:ILE:CD1	1.97	0.77
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.64	0.77
1:1:197:TYR:H	2:2:131:GLN:HE21	1.31	0.77
1:1:261:HIS:NE2	2:2:139:SER:N	2.33	0.77
1:1:212:VAL:HG11	1:1:263:HIS:CB	2.15	0.77
1:1:252:ARG:HG2	1:1:253:PRO:CD	2.15	0.76
1:1:142:VAL:CG1	1:1:225:VAL:CB	2.62	0.76
1:1:92:GLN:O	1:1:93:ASP:HB2	1.85	0.76
1:1:278:ILE:CD1	3:3:67:MET:CE	2.64	0.76
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.76
1:1:261:HIS:ND1	2:2:139:SER:HB3	2.01	0.76
1:1:101:ILE:HG12	1:1:218:GLY:O	1.86	0.76
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.76
1:1:225:VAL:O	1:1:227:GLU:N	2.15	0.75
1:1:103:LEU:HD21	5:1:700:JEN:H7	1.67	0.75
2:2:68:SER:C	2:2:69:LYS:HG2	2.07	0.75
1:1:184:ILE:HG23	1:1:185:PRO:HD2	1.69	0.75
1:1:149:PRO:HB2	1:1:150:PRO:HD2	1.69	0.75
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.75
4:4:26:TYR:CD1	4:4:29:ILE:HD11	2.22	0.74
2:2:65:THR:OG1	2:2:245:SER:OG	2.05	0.74
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.74
1:1:125:ILE:CG2	1:1:182:PHE:CD1	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:260:THR:HG21	1:1:261:HIS:HD2	1.53	0.74
2:2:257:ARG:HH11	2:2:257:ARG:HG2	1.52	0.74
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.70	0.74
1:1:252:ARG:HG3	2:2:186:PHE:HZ	1.53	0.74
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.74
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.73
1:1:214:THR:C	1:1:215:ASN:ND2	2.41	0.73
1:1:212:VAL:HG11	1:1:263:HIS:CG	2.24	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.73
1:1:99:TRP:NE1	1:1:105:GLU:OE2	2.22	0.73
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.71	0.73
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.73
1:1:138:ILE:CG1	1:1:139:GLY:N	2.51	0.73
1:1:212:VAL:CG1	1:1:263:HIS:CB	2.67	0.73
3:3:53:ILE:O	3:3:55:VAL:HG12	1.89	0.72
3:3:173:SER:O	3:3:175:PHE:N	2.22	0.72
2:2:183:LEU:HD12	2:2:186:PHE:HD2	1.52	0.72
3:3:125:THR:HG22	3:3:126:THR:N	2.03	0.72
2:2:148:HIS:N	2:2:149:PRO:CD	2.52	0.72
1:1:143:MET:HG2	1:1:145:TYR:CE1	2.24	0.72
1:1:117:THR:O	1:1:195:MET:CB	2.38	0.72
1:1:212:VAL:CB	1:1:263:HIS:CD2	2.72	0.72
1:1:242:LYS:NZ	3:3:17:ASP:O	2.22	0.72
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.72
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.71
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.71
2:2:148:HIS:N	2:2:149:PRO:HD3	2.06	0.71
1:1:140:HIS:HE1	1:1:174:GLN:OE1	1.73	0.71
1:1:146:MET:HE1	1:1:162:SER:O	1.90	0.71
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.71
1:1:212:VAL:HG11	1:1:263:HIS:CD2	2.24	0.71
1:1:80:SER:HB3	1:1:237:THR:HG23	1.73	0.71
1:1:278:ILE:HD12	3:3:67:MET:HE3	1.71	0.71
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.71
1:1:91:GLY:C	1:1:94:ILE:HD13	2.12	0.70
1:1:252:ARG:HG2	1:1:253:PRO:N	2.06	0.70
3:3:25:LEU:N	3:3:25:LEU:HD12	2.06	0.70
1:1:124:GLU:OE1	1:1:181:ARG:NH1	2.23	0.70
1:1:138:ILE:HG13	1:1:139:GLY:H	1.57	0.70
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.70
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.70
1:1:252:ARG:HG3	2:2:186:PHE:CZ	2.26	0.70
1:1:101:ILE:HD12	1:1:217:MET:HB2	1.73	0.70
1:1:142:VAL:HG12	1:1:225:VAL:CG2	2.22	0.70
1:1:169:MET:CE	1:1:171:ILE:HB	2.21	0.70
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.70
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.70
1:1:113:PHE:C	1:1:115:LEU:H	1.93	0.70
2:2:78:TRP:N	2:2:78:TRP:CE3	2.60	0.69
1:1:138:ILE:CG1	1:1:139:GLY:H	2.03	0.69
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.69
1:1:249:TRP:CA	3:3:39:GLU:HA	2.22	0.69
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.93	0.69
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.69
2:2:78:TRP:HE3	2:2:78:TRP:H	1.39	0.69
1:1:124:GLU:CG	1:1:242:LYS:HB3	2.22	0.69
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.69
1:1:254:PRO:CG	3:3:101:GLU:HG2	2.23	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
1:1:197:TYR:CD2	1:1:214:THR:CG2	2.76	0.69
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.69
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.68
1:1:44:ASN:C	1:1:44:ASN:HD22	1.96	0.68
1:1:147:TYR:CD1	5:1:700:JEN:H213	2.27	0.68
1:1:124:GLU:CD	1:1:181:ARG:HH11	1.97	0.68
1:1:260:THR:HG21	1:1:261:HIS:CD2	2.28	0.68
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
1:1:197:TYR:HD2	1:1:214:THR:HG22	1.53	0.68
1:1:222:SER:O	1:1:223:ARG:CB	2.42	0.68
1:1:38:GLU:O	2:2:189:GLN:HB2	1.94	0.68
1:1:92:GLN:C	1:1:94:ILE:CD1	2.62	0.68
1:1:271:THR:C	1:1:273:ASP:N	2.47	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
2:2:78:TRP:N	2:2:78:TRP:HE3	1.92	0.68
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.68
1:1:278:ILE:HD12	3:3:67:MET:HE1	1.77	0.67
1:1:200:TYR:CD2	1:1:209:TYR:HB2	2.30	0.67
2:2:171:SER:HA	2:2:175:PHE:CE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:230:LYS:CG	1:1:231:LEU:HD22	2.19	0.67
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.67
1:1:125:ILE:CB	1:1:182:PHE:CE1	2.77	0.67
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	0.67
2:2:51:ASN:HD22	2:2:51:ASN:H	1.41	0.67
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.66
1:1:262:SER:HB2	3:3:238:GLN:HA	1.77	0.66
1:1:197:TYR:HD1	1:1:198:ASP:H	1.43	0.66
1:1:141:ILE:O	1:1:141:ILE:HG22	1.95	0.66
1:1:104:GLN:C	1:1:106:MET:H	1.97	0.66
1:1:268:MET:O	2:2:137:HIS:ND1	2.30	0.65
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
2:2:126:MET:HE3	2:2:126:MET:HA	1.79	0.65
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.31	0.65
1:1:267:TYR:OH	2:2:170:ASP:CB	2.45	0.65
1:1:142:VAL:H	1:1:226:THR:HG23	1.60	0.65
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.65
1:1:145:TYR:HB2	1:1:171:ILE:HG23	1.77	0.65
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.65
1:1:125:ILE:CB	1:1:182:PHE:HE1	2.10	0.65
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
1:1:149:PRO:CB	1:1:150:PRO:HD2	2.27	0.64
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.77	0.64
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.64
1:1:173:TRP:CD1	1:1:180:PRO:CD	2.70	0.64
1:1:222:SER:O	1:1:223:ARG:HB3	1.96	0.64
2:2:155:ASP:O	2:2:156:VAL:HB	1.98	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
1:1:101:ILE:HB	5:1:700:JEN:H131	1.79	0.64
1:1:156:SER:C	1:1:157:LYS:HG3	2.16	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.64
1:1:201:ASP:OD1	1:1:208:LYS:HB2	1.98	0.64
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.27	0.64
1:1:171:ILE:HD11	1:1:180:PRO:CB	2.27	0.64
1:1:136:ASP:O	1:1:137:ASP:HB2	1.97	0.63
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.63
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.63
1:1:129:PRO:HG2	1:1:173:TRP:CZ2	2.31	0.63
1:1:142:VAL:CG1	1:1:225:VAL:HG21	2.29	0.63
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:199:GLY:HA2	2:2:216:ARG:O	1.99	0.63
2:2:174:ASN:C	2:2:175:PHE:HD1	2.02	0.63
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.63
1:1:212:VAL:HG11	1:1:263:HIS:HB3	1.77	0.63
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.62
1:1:7:ILE:HD13	1:1:7:ILE:N	2.14	0.62
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.62
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.62
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.34	0.62
1:1:281:ARG:NH2	3:3:84:SER:O	2.33	0.62
1:1:283:THR:HG22	1:1:285:THR:N	2.15	0.62
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.62
1:1:147:TYR:CD1	5:1:700:JEN:H212	2.33	0.62
1:1:163:TRP:CZ3	1:1:223:ARG:HB3	2.35	0.62
1:1:255:ARG:HD2	1:1:259:TYR:CD2	2.34	0.62
1:1:255:ARG:HD3	1:1:259:TYR:CZ	2.35	0.62
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.15	0.61
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.61
1:1:124:GLU:O	1:1:124:GLU:HG3	1.98	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	0.61
1:1:146:MET:O	1:1:146:MET:HG3	1.99	0.61
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.16	0.61
1:1:209:TYR:OH	2:2:131:GLN:HA	2.00	0.61
2:2:91:ILE:O	2:2:92:PHE:C	2.38	0.61
2:2:183:LEU:HD12	2:2:186:PHE:CD2	2.34	0.61
1:1:92:GLN:N	1:1:94:ILE:CD1	2.63	0.61
3:3:91:SER:O	3:3:92:THR:C	2.39	0.61
1:1:158:ARG:HG2	1:1:159:ASN:N	2.14	0.61
1:1:261:HIS:CE1	2:2:139:SER:CB	2.84	0.61
1:1:190:ALA:C	3:3:31:THR:HG21	2.21	0.60
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
1:1:78:HIS:O	1:1:239:ILE:HB	2.02	0.60
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.84	0.60
1:1:255:ARG:NE	1:1:257:VAL:O	2.34	0.60
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.60
1:1:91:GLY:O	1:1:157:LYS:CB	2.47	0.60
1:1:101:ILE:HG23	1:1:220:ILE:CG2	2.30	0.60
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.60
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:145:LYS:HA	3:3:148:MET:HE2	1.83	0.60
1:1:113:PHE:HD2	1:1:195:MET:HE2	1.67	0.60
1:1:113:PHE:HB3	1:1:195:MET:CE	2.32	0.60
1:1:255:ARG:CD	1:1:259:TYR:CD2	2.83	0.60
2:2:84:ASP:OD1	2:2:87:LYS:HE2	2.02	0.60
3:3:95:ALA:O	3:3:97:THR:N	2.34	0.60
1:1:113:PHE:HB3	1:1:195:MET:HE2	1.84	0.60
2:2:207:ASN:HD21	2:2:209:VAL:HG22	1.67	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.59
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.59
3:3:44:ILE:O	3:3:47:CYS:HB2	2.02	0.59
1:1:145:TYR:HE2	1:1:237:THR:HG1	1.47	0.59
3:3:25:LEU:HD12	3:3:25:LEU:H	1.68	0.59
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.59
1:1:260:THR:HG22	1:1:261:HIS:CG	2.36	0.59
1:1:67:ILE:HD13	1:1:248:ALA:HB3	1.84	0.59
1:1:226:THR:O	1:1:227:GLU:CB	2.50	0.59
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.59
1:1:103:LEU:CD2	5:1:700:JEN:H7	2.33	0.59
2:2:77:GLY:HA2	2:2:78:TRP:CE3	2.37	0.59
3:3:46:MET:O	3:3:98:LEU:HD23	2.03	0.59
1:1:271:THR:C	1:1:273:ASP:H	2.04	0.58
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.58
1:1:89:TYR:HE2	1:1:228:LYS:N	2.01	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.58
1:1:244:LYS:HE3	4:4:38:SER:O	2.03	0.58
1:1:278:ILE:HA	3:3:92:THR:HG21	1.86	0.58
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.58
1:1:184:ILE:CG2	1:1:187:LEU:HD21	2.33	0.58
1:1:44:ASN:C	1:1:44:ASN:ND2	2.58	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:85:ASP:OD1	1:1:86:TYR:N	2.36	0.58
1:1:149:PRO:CB	1:1:150:PRO:CD	2.81	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.58
2:2:235:THR:C	2:2:237:SER:H	2.06	0.57
3:3:192:TRP:CD1	3:3:192:TRP:N	2.73	0.57
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:261:HIS:CE1	2:2:139:SER:OG	2.58	0.57
2:2:49:ALA:O	2:2:50:ILE:HG13	2.04	0.57
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.57
1:1:125:ILE:HB	1:1:182:PHE:CD1	2.40	0.57
1:1:193:TYR:CE1	1:1:217:MET:CE	2.88	0.57
1:1:224:ILE:O	1:1:224:ILE:HG23	2.05	0.57
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.57
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.57
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.57
1:1:273:ASP:O	1:1:274:VAL:CG1	2.43	0.57
1:1:189:ILE:HG23	1:1:190:ALA:H	1.70	0.56
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.56
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.56
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.56
1:1:103:LEU:CD1	5:1:700:JEN:H8	2.23	0.56
1:1:101:ILE:CG1	1:1:218:GLY:O	2.53	0.56
1:1:113:PHE:CD2	1:1:195:MET:HE2	2.40	0.56
3:3:25:LEU:N	3:3:25:LEU:CD1	2.68	0.56
1:1:113:PHE:CD2	1:1:195:MET:CE	2.88	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.56
1:1:74:SER:HA	1:1:241:HIS:O	2.06	0.56
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
1:1:267:TYR:OH	2:2:168:SER:OG	2.21	0.56
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.87	0.56
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.56
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.56
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.55
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.55
1:1:89:TYR:CE2	1:1:227:GLU:C	2.75	0.55
1:1:225:VAL:C	1:1:227:GLU:H	2.05	0.55
1:1:101:ILE:CG2	1:1:220:ILE:CG2	2.85	0.55
1:1:271:THR:O	1:1:273:ASP:CA	2.52	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
1:1:141:ILE:O	1:1:141:ILE:HG23	2.07	0.55
1:1:248:ALA:O	3:3:39:GLU:C	2.44	0.55
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	0.55
3:3:14:MET:HG2	3:3:16:THR:HG22	1.88	0.55
3:3:83:PHE:CE1	3:3:191:CYS:CB	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:104:SER:O	3:3:227:THR:HA	2.06	0.55
3:3:107:THR:O	3:3:177:LEU:HD23	2.06	0.55
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.55
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	0.55
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.55
1:1:19:ASN:HA	1:1:58:THR:HG23	1.88	0.55
1:1:150:PRO:O	1:1:151:GLY:C	2.45	0.55
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.55
1:1:260:THR:CG2	1:1:261:HIS:HD2	2.08	0.54
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.54
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.54
3:3:80:GLN:HA	3:3:80:GLN:NE2	2.23	0.54
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.54
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.54
1:1:224:ILE:O	1:1:225:VAL:O	2.26	0.54
1:1:250:CYS:HB3	2:2:35:TYR:CZ	2.42	0.54
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.54
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.54
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.54
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
1:1:197:TYR:HE1	2:2:217:HIS:CG	2.26	0.54
1:1:200:TYR:HA	1:1:208:LYS:O	2.07	0.54
3:3:81:LYS:HB2	3:3:192:TRP:CZ3	2.43	0.54
3:3:103:ALA:O	3:3:178:THR:HG21	2.08	0.54
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.54
1:1:257:VAL:HG13	1:1:258:PRO:HD2	1.90	0.54
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
2:2:168:SER:HG	2:2:170:ASP:HB2	1.73	0.54
1:1:104:GLN:C	1:1:106:MET:N	2.61	0.54
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.54
2:2:174:ASN:HB3	2:2:176:ASP:OD2	2.08	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
1:1:107:ALA:O	1:1:109:ILE:N	2.41	0.54
1:1:195:MET:O	1:1:196:PHE:CG	2.61	0.54
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.54
1:1:125:ILE:CG2	1:1:126:THR:N	2.71	0.54
1:1:126:THR:HG23	1:1:181:ARG:CG	2.32	0.54
1:1:171:ILE:HD11	1:1:180:PRO:HB3	1.90	0.54
1:1:193:TYR:CE1	1:1:217:MET:HE2	2.43	0.54
1:1:248:ALA:O	3:3:39:GLU:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:237:GLU:CG	3:3:238:GLN:H	2.20	0.53
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.53
1:1:80:SER:O	1:1:236:THR:HA	2.07	0.53
1:1:261:HIS:C	1:1:262:SER:O	2.45	0.53
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.53
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
1:1:124:GLU:HB3	1:1:244:LYS:HD3	1.89	0.53
1:1:197:TYR:HD1	1:1:198:ASP:N	2.06	0.53
1:1:197:TYR:CD1	1:1:198:ASP:N	2.77	0.53
1:1:209:TYR:CD1	1:1:209:TYR:C	2.80	0.53
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
1:1:94:ILE:HD12	1:1:94:ILE:N	2.23	0.53
2:2:174:ASN:C	2:2:175:PHE:CD1	2.82	0.53
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
1:1:244:LYS:NZ	4:4:38:SER:H	2.07	0.53
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.53
1:1:255:ARG:HD2	1:1:259:TYR:HE2	1.60	0.53
1:1:284:ILE:HG13	1:1:285:THR:N	2.24	0.53
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.53
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.53
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.53
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.52
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.52
1:1:128:VAL:HG12	1:1:128:VAL:O	2.07	0.52
1:1:184:ILE:CG2	1:1:185:PRO:HD2	2.37	0.52
1:1:194:TYR:HB2	1:1:214:THR:OG1	2.08	0.52
4:4:26:TYR:CD1	4:4:29:ILE:CD1	2.91	0.52
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.52
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.91	0.52
1:1:181:ARG:O	3:3:21:SER:HB3	2.09	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
3:3:26:PRO:HB2	3:3:27:TRP:CE3	2.44	0.52
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.44	0.52
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.52
1:1:169:MET:HE2	1:1:171:ILE:HB	1.91	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	0.52
1:1:92:GLN:O	1:1:94:ILE:HD11	2.10	0.52
1:1:93:ASP:N	1:1:94:ILE:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:HG23	1:1:220:ILE:HG22	1.92	0.52
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.52
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.52
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.52
1:1:148:VAL:CG1	1:1:152:ALA:HB3	2.40	0.51
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.51
1:1:103:LEU:O	1:1:104:GLN:CB	2.58	0.51
1:1:200:TYR:CE2	1:1:209:TYR:HB2	2.46	0.51
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.51
1:1:97:THR:HG23	1:1:222:SER:CB	2.38	0.51
2:2:110:VAL:O	2:2:198:SER:HA	2.11	0.51
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
2:2:202:ILE:HD13	2:2:249:MET:HE3	1.93	0.51
1:1:96:PHE:CZ	1:1:155:PRO:O	2.64	0.51
1:1:261:HIS:CE1	2:2:139:SER:N	2.79	0.51
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.51
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.51
2:2:145:LYS:HZ1	2:2:263:GLN:HG2	1.74	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
1:1:86:TYR:OH	1:1:229:GLN:HB2	2.10	0.51
1:1:96:PHE:HE2	1:1:157:LYS:HA	1.72	0.51
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.43	0.51
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.51
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
1:1:185:PRO:HB2	1:1:186:PHE:O	2.11	0.51
4:4:42:ARG:HH12	4:4:44:ASP:HB3	1.76	0.51
1:1:7:ILE:O	1:1:11:LEU:HD23	2.11	0.51
1:1:149:PRO:HB2	1:1:150:PRO:CD	2.38	0.51
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.46	0.51
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.26	0.51
1:1:126:THR:HG21	3:3:13:PHE:CD1	2.46	0.50
1:1:101:ILE:HD11	1:1:217:MET:CB	2.36	0.50
1:1:188:SER:OG	1:1:193:TYR:CD1	2.56	0.50
1:1:255:ARG:NE	1:1:259:TYR:CD2	2.79	0.50
1:1:265:THR:HG1	2:2:133:ALA:HB2	1.75	0.50
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:ASN:ND2	1:1:44:ASN:O	2.34	0.50
2:2:154:ARG:HH11	2:2:154:ARG:CG	2.24	0.50
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.12	0.50
1:1:91:GLY:C	1:1:94:ILE:CD1	2.78	0.50
1:1:261:HIS:CD2	2:2:138:GLY:CA	2.86	0.50
2:2:175:PHE:CD1	2:2:175:PHE:N	2.79	0.50
1:1:111:ARG:HA	1:1:259:TYR:OH	2.11	0.50
3:3:72:LEU:HD12	3:3:72:LEU:N	2.26	0.50
3:3:102:ILE:O	3:3:105:TYR:N	2.44	0.50
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.50
1:1:186:PHE:CZ	1:1:188:SER:HB2	2.47	0.50
1:1:191:SER:HB3	3:3:34:ILE:HG12	1.92	0.50
1:1:254:PRO:O	2:2:178:THR:HG22	2.11	0.50
1:1:145:TYR:N	1:1:145:TYR:CD1	2.80	0.50
1:1:260:THR:CG2	1:1:261:HIS:CG	2.95	0.50
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.50
2:2:159:GLU:OE1	2:2:159:GLU:HA	2.11	0.50
1:1:111:ARG:NH2	3:3:101:GLU:OE2	2.39	0.49
1:1:197:TYR:H	2:2:131:GLN:NE2	2.07	0.49
3:3:62:VAL:HA	3:3:67:MET:HG3	1.94	0.49
3:3:140:GLU:HB3	3:3:188:TYR:CD2	2.48	0.49
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.49
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.49
3:3:200:PRO:O	3:3:203:THR:OG1	2.22	0.49
1:1:99:TRP:CZ3	1:1:101:ILE:HA	2.48	0.49
1:1:191:SER:N	3:3:31:THR:HG21	2.28	0.49
1:1:125:ILE:HG23	1:1:126:THR:N	2.28	0.49
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.49
3:3:25:LEU:O	3:3:25:LEU:HD13	2.12	0.49
3:3:117:PHE:CE2	3:3:131:LEU:HG	2.47	0.49
3:3:14:MET:C	3:3:16:THR:H	2.16	0.49
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.49
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.49
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.49
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.49
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.49
1:1:142:VAL:H	1:1:226:THR:CG2	2.23	0.49
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.49
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.49
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:125:ILE:HG22	1:1:182:PHE:CD1	2.47	0.49
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.49
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.49
1:1:120:ARG:HD2	1:1:191:SER:O	2.13	0.48
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.48
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.48
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.48
1:1:163:TRP:CZ3	1:1:222:SER:O	2.62	0.48
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.78	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.48
1:1:200:TYR:CG	1:1:209:TYR:HB2	2.47	0.48
1:1:253:PRO:HB2	2:2:178:THR:HB	1.96	0.48
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.48
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.48
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.48
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.48
1:1:261:HIS:CE1	2:2:139:SER:HB3	2.48	0.48
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.48
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.48
1:1:132:ALA:HB3	1:1:234:VAL:HG13	1.96	0.48
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.79	0.48
1:1:261:HIS:O	1:1:262:SER:O	2.32	0.48
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.48
1:1:143:MET:HG2	1:1:145:TYR:CZ	2.49	0.48
1:1:120:ARG:O	1:1:121:PHE:HB3	2.13	0.48
3:3:82:VAL:HG12	3:3:83:PHE:H	1.77	0.48
1:1:117:THR:HA	1:1:252:ARG:HH21	1.78	0.47
1:1:125:ILE:CB	1:1:182:PHE:CD1	2.97	0.47
1:1:195:MET:O	1:1:196:PHE:CD2	2.67	0.47
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.47
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.47
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.47
1:1:266:ASN:HA	2:2:133:ALA:HB1	1.95	0.47
2:2:128:PRO:HD2	2:2:186:PHE:CD1	2.49	0.47
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	0.47
1:1:101:ILE:CG2	1:1:220:ILE:HG22	2.43	0.47
1:1:182:PHE:HD1	1:1:182:PHE:H	1.60	0.47
2:2:12:ARG:CG	2:2:13:ILE:H	2.26	0.47
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.47
1:1:169:MET:HE1	1:1:171:ILE:CG2	2.44	0.47
1:1:244:LYS:NZ	4:4:38:SER:O	2.47	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
3:3:55:VAL:C	3:3:57:ASN:N	2.67	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
1:1:141:ILE:HA	1:1:226:THR:HG21	1.96	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.47
1:1:137:ASP:O	1:1:231:LEU:HB2	2.14	0.47
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.47
2:2:136:LYS:HA	2:2:136:LYS:HD3	1.59	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
1:1:248:ALA:O	3:3:39:GLU:HB2	2.15	0.47
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.47
1:1:163:TRP:CH2	1:1:223:ARG:HB3	2.50	0.47
1:1:261:HIS:ND1	2:2:139:SER:CB	2.77	0.47
1:1:267:TYR:OH	2:2:170:ASP:HB2	2.14	0.47
1:1:281:ARG:N	3:3:57:ASN:O	2.45	0.47
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.47
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.46
1:1:89:TYR:HD1	1:1:89:TYR:HA	1.49	0.46
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.46
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.46
3:3:22:PRO:C	3:3:23:CYS:O	2.52	0.46
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.50	0.46
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.46
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.46
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.46
1:1:142:VAL:HB	1:1:226:THR:HG23	1.97	0.46
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.46
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.46
1:1:134:ARG:HD3	1:1:234:VAL:HG12	1.97	0.46
1:1:253:PRO:CD	2:2:185:ILE:HG21	2.41	0.46
2:2:206:VAL:O	2:2:207:ASN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:67:ILE:CD1	1:1:248:ALA:HB3	2.46	0.46
1:1:212:VAL:HG12	1:1:263:HIS:CD2	2.33	0.46
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.46
1:1:197:TYR:CE1	2:2:217:HIS:CE1	3.03	0.46
1:1:244:LYS:CE	4:4:38:SER:O	2.64	0.46
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.46
1:1:261:HIS:HB2	1:1:264:VAL:HG21	1.98	0.46
3:3:46:MET:HE3	3:3:102:ILE:HD11	1.97	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.98	0.46
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.46
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.46
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.97	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.45
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.45
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.45
3:3:237:GLU:HG3	3:3:238:GLN:H	1.81	0.45
1:1:249:TRP:HA	3:3:39:GLU:CA	2.31	0.45
1:1:264:VAL:HG12	2:2:141:THR:HG22	1.98	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.45
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.45
1:1:197:TYR:N	2:2:131:GLN:HE21	2.08	0.45
1:1:89:TYR:CE2	1:1:228:LYS:N	2.83	0.45
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.45
2:2:240:VAL:HA	2:2:241:PRO:HD2	1.88	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45
2:2:228:SER:HA	2:2:229:PRO:HD2	1.69	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
1:1:157:LYS:HE2	1:1:157:LYS:HB2	1.40	0.45
1:1:197:TYR:HE2	1:1:213:VAL:CG1	2.29	0.45
1:1:249:TRP:HA	3:3:38:GLY:O	2.17	0.45
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
1:1:257:VAL:HG11	1:1:267:TYR:HB2	1.98	0.45
1:1:261:HIS:CD2	2:2:139:SER:N	2.74	0.45
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.45
3:3:161:SER:OG	3:3:162:THR:N	2.47	0.45
1:1:104:GLN:O	1:1:106:MET:N	2.50	0.45
1:1:126:THR:HG23	1:1:181:ARG:HB2	1.98	0.45
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.45
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.45
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.45
1:1:197:TYR:CE2	1:1:213:VAL:CG1	2.99	0.44
1:1:214:THR:CA	1:1:215:ASN:HD22	2.30	0.44
1:1:140:HIS:HE1	1:1:174:GLN:CD	2.19	0.44
1:1:245:HIS:CE1	4:4:38:SER:OG	2.70	0.44
2:2:91:ILE:HG22	2:2:92:PHE:N	2.32	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE1	2.17	0.44
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.44
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.44
1:1:230:LYS:HG2	1:1:231:LEU:N	2.32	0.44
2:2:18:ARG:HD3	2:2:18:ARG:HA	1.57	0.44
2:2:61:ASN:N	2:2:61:ASN:OD1	2.49	0.44
3:3:66:SER:C	3:3:68:TYR:N	2.69	0.44
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.46	0.44
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.44
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.44
1:1:90:ASN:N	1:1:90:ASN:HD22	2.16	0.44
1:1:214:THR:OG1	1:1:215:ASN:ND2	2.51	0.44
1:1:244:LYS:HZ1	4:4:38:SER:H	1.66	0.44
2:2:80:TRP:NE1	2:2:151:GLU:O	2.50	0.44
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.53	0.44
2:2:43:THR:HA	2:2:44:PRO:HD2	1.80	0.44
2:2:83:PRO:CG	2:2:218:ASN:HA	2.31	0.44
2:2:126:MET:HE2	2:2:126:MET:HB3	1.80	0.44
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.44
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.44
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.44
3:3:130:LEU:C	3:3:130:LEU:HD23	2.38	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
1:1:147:TYR:HD1	5:1:700:JEN:H213	1.81	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.44
1:1:111:ARG:HH21	3:3:101:GLU:HG3	1.83	0.43
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.43
1:1:92:GLN:O	1:1:94:ILE:CD1	2.66	0.43
3:3:25:LEU:HA	3:3:26:PRO:HD2	1.77	0.43
3:3:88:ASP:OD1	3:3:186:ALA:N	2.39	0.43
3:3:159:LEU:HA	3:3:159:LEU:HD23	1.72	0.43
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.43
1:1:155:PRO:CG	1:1:163:TRP:CZ2	3.01	0.43
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.43
2:2:137:HIS:CD2	2:2:137:HIS:C	2.91	0.43
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.43
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.43
1:1:247:LYS:HB3	1:1:249:TRP:CZ3	2.54	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.43
1:1:188:SER:HB3	1:1:189:ILE:H	1.17	0.43
1:1:267:TYR:OH	2:2:170:ASP:HB3	2.18	0.43
2:2:207:ASN:O	2:2:209:VAL:N	2.51	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.18	0.43
1:1:46:GLN:CB	1:1:47:PRO:CD	2.57	0.43
1:1:148:VAL:HG13	1:1:152:ALA:CB	2.48	0.43
2:2:37:VAL:HG12	2:2:204:PRO:HB3	2.01	0.43
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.43
2:2:94:GLU:C	2:2:96:MET:H	2.22	0.43
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.43
4:4:26:TYR:HD1	4:4:29:ILE:HD11	1.78	0.43
3:3:54:PRO:HA	3:3:68:TYR:CD1	2.54	0.43
1:1:182:PHE:CD1	1:1:182:PHE:N	2.83	0.43
1:1:186:PHE:CD1	1:1:186:PHE:C	2.91	0.43
3:3:22:PRO:O	3:3:23:CYS:O	2.36	0.43
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.43
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.43
1:1:251:PRO:HG3	3:3:40:VAL:CG2	2.49	0.43
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.43
2:2:192:ASN:C	2:2:194:ARG:H	2.21	0.43
1:1:184:ILE:HA	1:1:185:PRO:HD3	1.91	0.42
1:1:249:TRP:CD1	3:3:39:GLU:HB3	2.53	0.42
2:2:154:ARG:HH11	2:2:154:ARG:HG2	1.83	0.42
3:3:50:ASP:CA	3:3:214:SER:HB3	2.49	0.42
1:1:98:LYS:O	1:1:98:LYS:CG	2.33	0.42
1:1:125:ILE:O	1:1:181:ARG:HG3	2.15	0.42
1:1:129:PRO:HA	1:1:237:THR:HA	2.02	0.42
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.42
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.42
1:1:249:TRP:CA	3:3:38:GLY:O	2.68	0.42
1:1:160:ASP:H	1:1:163:TRP:HD1	1.66	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:38:TRP:HA	2:2:39:PRO:HD2	1.70	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
2:2:127:ILE:N	2:2:221:CYS:O	2.53	0.42
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.85	0.42
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.42
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.42
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.42
1:1:197:TYR:CE2	1:1:213:VAL:HG11	2.55	0.42
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
3:3:216:CYS:C	3:3:218:ASP:H	2.23	0.42
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.42
1:1:38:GLU:O	2:2:189:GLN:CB	2.66	0.42
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.42
1:1:103:LEU:HD11	5:1:700:JEN:C8	2.23	0.42
1:1:196:PHE:CD2	1:1:252:ARG:NH2	2.88	0.42
2:2:57:ASP:O	2:2:58:THR:CG2	2.67	0.42
1:1:31:ALA:HA	1:1:32:PRO:HD2	1.81	0.42
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.42
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	0.42
3:3:149:LEU:HD23	3:3:149:LEU:HA	1.73	0.42
3:3:217:LYS:HG3	3:3:217:LYS:H	1.64	0.42
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.42
3:3:94:LEU:HA	3:3:94:LEU:HD23	1.83	0.42
2:2:107:THR:OG1	2:2:249:MET:HE3	2.20	0.42
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.42
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.42
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.42
1:1:77:VAL:HG22	1:1:239:ILE:CG2	2.44	0.41
1:1:119:VAL:HG13	1:1:121:PHE:CE1	2.56	0.41
1:1:212:VAL:HG12	1:1:263:HIS:CB	2.41	0.41
1:1:119:VAL:HG13	1:1:120:ARG:N	2.35	0.41
1:1:145:TYR:O	1:1:171:ILE:HG22	2.20	0.41
2:2:175:PHE:HD1	2:2:175:PHE:N	2.18	0.41
1:1:150:PRO:O	1:1:152:ALA:N	2.52	0.41
1:1:197:TYR:HE2	1:1:213:VAL:HG12	1.86	0.41
1:1:225:VAL:C	1:1:227:GLU:N	2.71	0.41
2:2:21:SER:OG	2:2:63:PHE:HB2	2.20	0.41
2:2:158:GLN:CG	2:2:159:GLU:N	2.83	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:2:LEU:HA	3:3:2:LEU:HD23	1.80	0.41
1:1:149:PRO:O	1:1:150:PRO:O	2.39	0.41
1:1:267:TYR:OH	2:2:170:ASP:OD2	2.38	0.41
2:2:63:PHE:CD1	2:2:247:SER:HB2	2.55	0.41
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	0.41
1:1:82:ILE:HD13	1:1:82:ILE:HG21	1.81	0.41
2:2:86:LEU:C	2:2:88:ASP:N	2.74	0.41
3:3:144:ARG:O	3:3:145:LYS:O	2.39	0.41
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.41
1:1:184:ILE:CG2	1:1:185:PRO:CD	2.99	0.41
1:1:235:ILE:HG22	1:1:236:THR:N	2.34	0.41
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.41
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.41
1:1:146:MET:HA	1:1:169:MET:O	2.20	0.41
1:1:169:MET:HE1	1:1:171:ILE:HB	1.99	0.41
2:2:37:VAL:CG2	3:3:37:PRO:HB3	2.47	0.41
2:2:143:GLY:N	2:2:165:ARG:O	2.48	0.41
3:3:43:LEU:HA	3:3:43:LEU:HD23	1.78	0.41
3:3:83:PHE:CE1	3:3:191:CYS:HB2	2.56	0.41
3:3:91:SER:C	3:3:92:THR:O	2.58	0.41
1:1:282:ASN:HD22	1:1:282:ASN:HA	1.55	0.41
3:3:14:MET:C	3:3:16:THR:N	2.74	0.41
3:3:83:PHE:N	3:3:83:PHE:CD1	2.88	0.41
1:1:11:LEU:HD13	1:1:11:LEU:HA	1.77	0.41
1:1:33:LEU:HB3	3:3:163:ILE:CD1	2.51	0.41
1:1:92:GLN:C	1:1:94:ILE:HD11	2.39	0.41
1:1:92:GLN:N	1:1:94:ILE:HD11	2.36	0.41
1:1:128:VAL:HB	1:1:238:HIS:HB2	2.03	0.41
1:1:163:TRP:HB3	1:1:223:ARG:HH21	1.86	0.41
1:1:220:ILE:O	1:1:220:ILE:HG13	2.11	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.41
1:1:86:TYR:CE2	1:1:229:GLN:HB2	2.54	0.41
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.41
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
2:2:51:ASN:H	2:2:51:ASN:ND2	2.15	0.40
2:2:155:ASP:O	2:2:156:VAL:CB	2.68	0.40
1:1:9:GLU:OE2	4:4:42:ARG:HG3	2.21	0.40
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.40
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.02	0.40
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.40
1:1:119:VAL:CG1	1:1:121:PHE:HE1	2.35	0.40
1:1:123:SER:N	1:1:184:ILE:O	2.49	0.40
3:3:15:THR:H	3:3:15:THR:HG22	1.45	0.40
2:2:147:THR:C	2:2:149:PRO:HD3	2.41	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:114:ARG:NH2	3:3:215:ALA:O	2.55	0.40
3:3:115:PHE:CE1	3:3:167:VAL:HG21	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:27:THR:OG1	2:2:18:ARG:NH2[2_655]	2.09	0.11

## 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	1	281/287 (98%)	196 (70%)	46 (16%)	39 (14%)	<b>0</b> <b>4</b>
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	<b>1</b> <b>20</b>
3	3	236/238 (99%)	176 (75%)	39 (16%)	21 (9%)	<b>1</b> <b>12</b>
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	<b>1</b> <b>21</b>
All	All	785/832 (94%)	582 (74%)	127 (16%)	76 (10%)	<b>0</b> <b>10</b>

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	102	THR
1	1	114	GLU
1	1	151	GLY
1	1	158	ARG
1	1	189	ILE
1	1	191	SER
1	1	223	ARG
1	1	225	VAL
1	1	226	THR
1	1	262	SER
1	1	263	HIS
1	1	264	VAL
1	1	271	THR
1	1	272	GLY
1	1	273	ASP
1	1	274	VAL
2	2	145	LYS
2	2	157	SER
2	2	258	ALA
3	3	23	CYS
3	3	57	ASN
3	3	88	ASP
3	3	89	ILE
3	3	94	LEU
3	3	96	THR
1	1	29	ASN
1	1	37	ALA
1	1	67	ILE
1	1	90	ASN
1	1	104	GLN
1	1	108	GLN
1	1	119	VAL
1	1	137	ASP
1	1	150	PRO
1	1	266	ASN
2	2	91	ILE
2	2	129	GLU
2	2	155	ASP
2	2	193	LEU
2	2	208	ALA
2	2	257	ARG

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Mol	Chain	Res	Type
3	3	59	GLY
3	3	66	SER
3	3	67	MET
3	3	95	ALA
3	3	159	LEU
3	3	161	SER
3	3	174	HIS
3	3	184	SER
1	1	6	TYR
1	1	103	LEU
1	1	105	GLU
1	1	227	GLU
2	2	30	ASN
2	2	156	VAL
3	3	74	ASN
3	3	201	PRO
3	3	219	PHE
3	3	229	LEU
4	4	27	PHE
1	1	160	ASP
1	1	268	MET
2	2	260	ASN
1	1	107	ALA
1	1	161	PHE
1	1	205	THR
1	1	212	VAL
2	2	87	LYS
2	2	259	LYS
1	1	149	PRO
3	3	220	CYS
3	3	121	GLY
2	2	44	PRO
3	3	82	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	1	254/258 (98%)	177 (70%)	77 (30%)	0	2
2	2	219/227 (96%)	158 (72%)	61 (28%)	0	3
3	3	209/209 (100%)	156 (75%)	53 (25%)	0	4
4	4	15/35 (43%)	9 (60%)	6 (40%)	0	0
All	All	697/729 (96%)	500 (72%)	197 (28%)	0	2

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	ASN
1	1	6	TYR
1	1	7	ILE
1	1	15	LEU
1	1	19	ASN
1	1	26	THR
1	1	35	ASP
1	1	44	ASN
1	1	45	VAL
1	1	54	ARG
1	1	60	GLN
1	1	73	ARG
1	1	87	THR
1	1	89	TYR
1	1	90	ASN
1	1	97	THR
1	1	98	LYS
1	1	102	THR
1	1	103	LEU
1	1	104	GLN
1	1	105	GLU
1	1	106	MET
1	1	108	GLN
1	1	109	ILE
1	1	111	ARG
1	1	112	LYS
1	1	119	VAL
1	1	123	SER
1	1	124	GLU
1	1	125	ILE
1	1	126	THR
1	1	127	LEU
1	1	134	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	141	ILE
1	1	142	VAL
1	1	146	MET
1	1	157	LYS
1	1	159	ASN
1	1	160	ASP
1	1	162	SER
1	1	173	TRP
1	1	174	GLN
1	1	177	GLN
1	1	182	PHE
1	1	183	SER
1	1	188	SER
1	1	191	SER
1	1	195	MET
1	1	197	TYR
1	1	201	ASP
1	1	204	ASN
1	1	209	TYR
1	1	212	VAL
1	1	213	VAL
1	1	214	THR
1	1	215	ASN
1	1	217	MET
1	1	219	THR
1	1	220	ILE
1	1	223	ARG
1	1	224	ILE
1	1	227	GLU
1	1	228	LYS
1	1	232	SER
1	1	236	THR
1	1	237	THR
1	1	246	THR
1	1	247	LYS
1	1	252	ARG
1	1	262	SER
1	1	265	THR
1	1	275	THR
1	1	276	THR
1	1	278	ILE
1	1	279	VAL

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Mol	Chain	Res	Type
1	1	281	ARG
1	1	286	THR
2	2	12	ARG
2	2	15	GLN
2	2	17	THR
2	2	18	ARG
2	2	25	SER
2	2	27	ASP
2	2	30	ASN
2	2	43	THR
2	2	51	ASN
2	2	52	LYS
2	2	55	GLN
2	2	58	THR
2	2	60	SER
2	2	62	ARG
2	2	63	PHE
2	2	65	THR
2	2	68	SER
2	2	72	ASN
2	2	75	SER
2	2	78	TRP
2	2	86	LEU
2	2	87	LYS
2	2	88	ASP
2	2	94	GLU
2	2	103	ARG
2	2	111	GLN
2	2	116	LYS
2	2	126	MET
2	2	136	LYS
2	2	139	SER
2	2	145	LYS
2	2	146	LEU
2	2	154	ARG
2	2	158	GLN
2	2	159	GLU
2	2	160	ARG
2	2	164	LEU
2	2	170	ASP
2	2	171	SER
2	2	173	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	175	PHE
2	2	180	LEU
2	2	191	ILE
2	2	192	ASN
2	2	194	ARG
2	2	195	SER
2	2	197	ASN
2	2	198	SER
2	2	200	THR
2	2	201	LEU
2	2	202	ILE
2	2	206	VAL
2	2	207	ASN
2	2	216	ARG
2	2	219	ASN
2	2	224	ILE
2	2	239	ILE
2	2	240	VAL
2	2	257	ARG
2	2	261	ILE
2	2	262	LYS
3	3	2	LEU
3	3	4	VAL
3	3	5	TYR
3	3	7	THR
3	3	19	MET
3	3	21	SER
3	3	23	CYS
3	3	25	LEU
3	3	32	LYS
3	3	39	GLU
3	3	50	ASP
3	3	55	VAL
3	3	56	ASN
3	3	60	ASN
3	3	61	ASN
3	3	65	VAL
3	3	66	SER
3	3	75	GLN
3	3	84	SER
3	3	90	THR
3	3	92	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	3	99	ILE
3	3	116	SER
3	3	119	PHE
3	3	126	THR
3	3	127	LEU
3	3	134	THR
3	3	140	GLU
3	3	142	THR
3	3	143	THR
3	3	148	MET
3	3	157	VAL
3	3	159	LEU
3	3	161	SER
3	3	177	LEU
3	3	182	LYS
3	3	189	ILE
3	3	192	TRP
3	3	194	GLN
3	3	196	ASN
3	3	201	PRO
3	3	205	GLN
3	3	208	ASP
3	3	209	MET
3	3	210	LEU
3	3	211	CYS
3	3	212	PHE
3	3	213	VAL
3	3	216	CYS
3	3	217	LYS
3	3	228	ASP
3	3	231	ILE
3	3	236	ILE
4	4	26	TYR
4	4	29	ILE
4	4	33	LYS
4	4	42	ARG
4	4	43	LEU
4	4	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:



Mol	Chain	Res	Type
1	1	44	ASN
1	1	90	ASN
1	1	95	ASN
1	1	140	HIS
1	1	159	ASN
1	1	204	ASN
1	1	215	ASN
1	1	261	HIS
1	1	263	HIS
1	1	282	ASN
2	2	15	GLN
2	2	30	ASN
2	2	51	ASN
2	2	72	ASN
2	2	109	HIS
2	2	111	GLN
2	2	131	GLN
2	2	192	ASN
2	2	197	ASN
2	2	207	ASN
2	2	218	ASN
2	2	219	ASN
3	3	20	GLN
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	61	ASN
3	3	75	GLN
3	3	80	GLN
3	3	124	ASN
3	3	194	GLN
3	3	196	ASN
4	4	30	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	JEN	1	700	-	23,23,23	0.78	1 (4%)	30,31,31	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JEN	1	700	-	-	4/10/20/20	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	700	JEN	C8-C7	-2.35	1.34	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

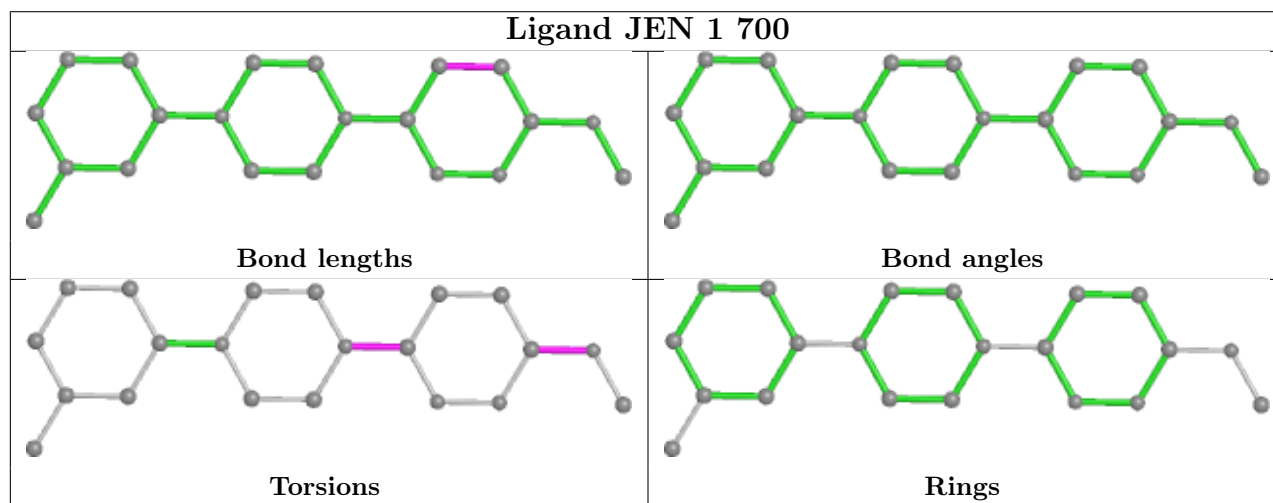
Mol	Chain	Res	Type	Atoms
5	1	700	JEN	N4-C3-O2-C1
5	1	700	JEN	C8-C3-O2-C1
5	1	700	JEN	N5-C6-N9-C10
5	1	700	JEN	C7-C6-N9-C10

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	700	JEN	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	118:TYR	C	119:VAL	N	1.16

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.