



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:53 PM GMT

PDB ID : 1R24  
Title : FAB FROM MURINE IGG3 KAPPA  
Authors : Evans, S.V.  
Deposited on : 1998-11-05  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

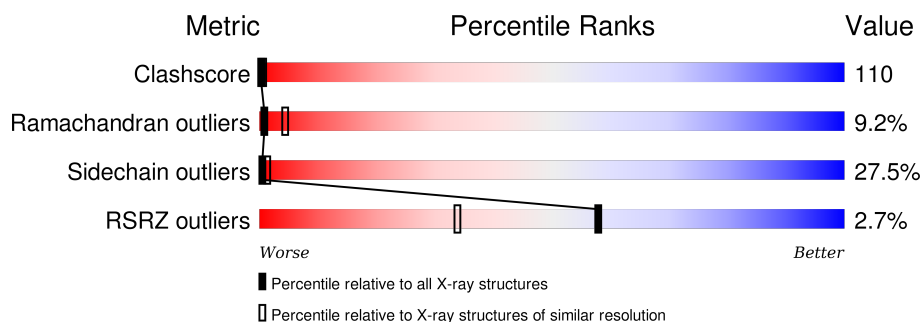
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	
1	C	206	
2	B	217	
2	D	217	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6458 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 PROTEIN (IGG3-KAPPA ANTIBODY (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1605	1004	266	329	6			
1	C	206	Total	C	N	O	S	0	0	0
			1605	1004	266	329	6			

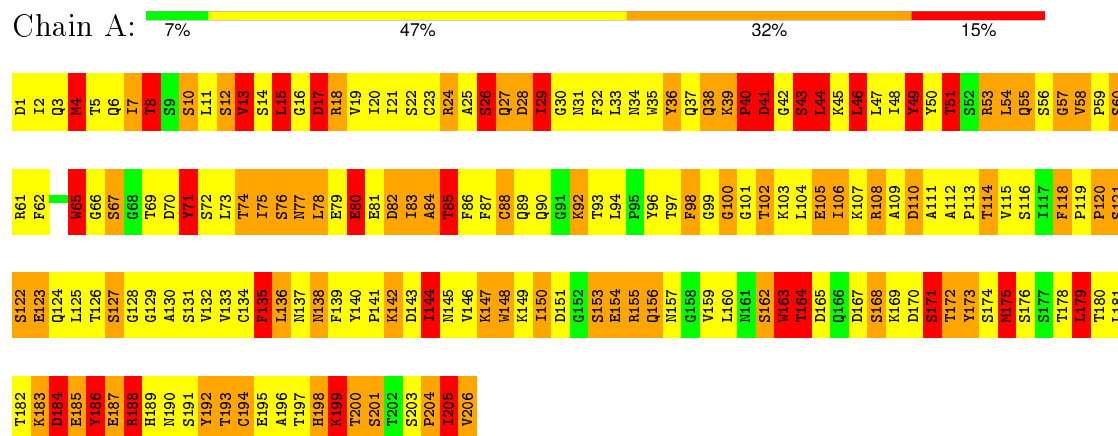
- Molecule 2 is a protein called PROTEIN (IGG3-KAPPA ANTIBODY (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1624	1029	271	317	7			
2	D	217	Total	C	N	O	S	0	0	0
			1624	1029	271	317	7			

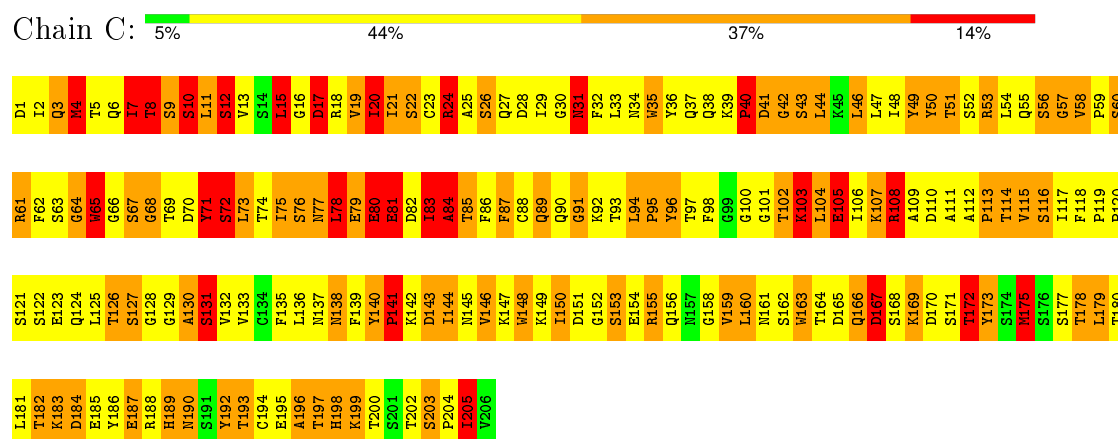
### 3 Residue-property plots

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

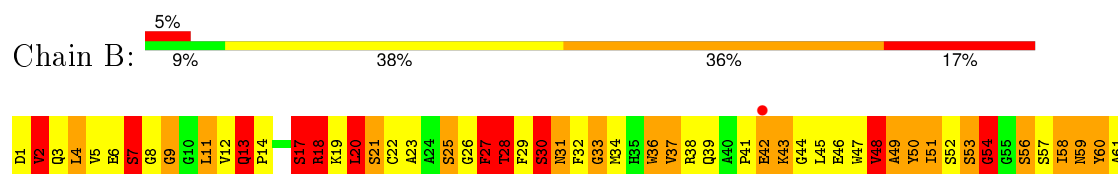
#### • Molecule 1: PROTEIN (IGG3-KAPPA ANTIBODY (LIGHT CHAIN))



#### • Molecule 1: PROTEIN (IGG3-KAPPA ANTIBODY (LIGHT CHAIN))



#### • Molecule 2: PROTEIN (IGG3-KAPPA ANTIBODY (HEAVY CHAIN))





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.24Å 82.07Å 73.58Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	6.00 – 3.10 20.72 – 3.11	Depositor EDS
% Data completeness (in resolution range)	92.0 (6.00-3.10) 88.5 (20.72-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 3.10Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.245 , (Not available) 0.246 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	52.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 127.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 26595 reflections	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	6458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.36	9/1639 (0.5%)	2.74	152/2223 (6.8%)
1	C	1.36	7/1639 (0.4%)	2.81	168/2223 (7.6%)
2	B	1.43	10/1665 (0.6%)	2.69	161/2269 (7.1%)
2	D	1.37	6/1665 (0.4%)	2.89	185/2269 (8.2%)
All	All	1.38	32/6608 (0.5%)	2.78	666/8984 (7.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	4
2	B	0	5
2	D	0	8
All	All	0	19

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	VAL	CA-CB	-7.57	1.38	1.54
1	A	12	SER	CA-CB	7.49	1.64	1.52
1	C	153	SER	CA-CB	-6.70	1.42	1.52
1	C	72	SER	CA-CB	-6.67	1.43	1.52
2	D	140	THR	CA-CB	6.47	1.70	1.53
1	A	206	VAL	CA-CB	-6.43	1.41	1.54
2	B	202	VAL	CA-CB	6.43	1.68	1.54
2	B	54	GLY	CA-C	6.24	1.61	1.51
2	D	114	GLN	CA-CB	-6.19	1.40	1.53
1	A	12	SER	CB-OG	6.13	1.50	1.42
1	C	18	ARG	NE-CZ	6.08	1.41	1.33
2	B	138	SER	CA-CB	5.93	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	SER	CA-CB	-5.80	1.44	1.52
2	B	157	GLY	CA-C	5.61	1.60	1.51
2	B	199	SER	CB-OG	5.54	1.49	1.42
1	C	53	ARG	CZ-NH2	5.50	1.40	1.33
2	D	169	SER	CB-OG	5.45	1.49	1.42
1	A	148	TRP	CG-CD2	-5.42	1.34	1.43
1	A	153	SER	CA-CB	5.38	1.61	1.52
2	B	56	SER	CB-OG	5.38	1.49	1.42
2	B	163	TRP	CD1-NE1	-5.38	1.28	1.38
1	C	35	TRP	CA-CB	5.37	1.65	1.53
2	D	78	THR	CA-CB	-5.32	1.39	1.53
2	B	197	TRP	CD1-NE1	-5.26	1.29	1.38
2	D	137	CYS	CA-CB	5.22	1.65	1.53
1	A	65	TRP	CG-CD2	-5.20	1.34	1.43
1	A	114	THR	CA-CB	-5.15	1.40	1.53
2	B	195	SER	CA-CB	-5.13	1.45	1.52
1	C	163	TRP	CD1-NE1	-5.09	1.29	1.38
1	A	76	SER	CA-CB	5.09	1.60	1.52
1	A	185	GLU	CG-CD	5.05	1.59	1.51
2	D	156	PRO	CA-CB	-5.01	1.43	1.53

All (666) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ARG	NE-CZ-NH2	20.01	130.31	120.30
1	C	53	ARG	NE-CZ-NH1	-18.47	111.07	120.30
1	A	114	THR	N-CA-CB	-17.90	76.30	110.30
1	C	1	ASP	N-CA-C	-16.77	65.71	111.00
1	A	13	VAL	N-CA-C	-16.39	66.74	111.00
2	D	116	ALA	N-CA-C	-16.36	66.84	111.00
2	D	169	SER	CA-C-N	-16.18	81.61	117.20
2	D	98	ARG	NE-CZ-NH1	-14.26	113.17	120.30
1	C	24	ARG	NE-CZ-NH2	13.37	126.98	120.30
2	B	87	ARG	NE-CZ-NH2	13.32	126.96	120.30
2	D	169	SER	N-CA-C	-13.29	75.13	111.00
1	C	53	ARG	NE-CZ-NH2	13.23	126.91	120.30
1	C	192	TYR	CB-CG-CD1	-12.93	113.24	121.00
1	C	65	TRP	N-CA-C	-12.62	76.92	111.00
2	B	54	GLY	O-C-N	-11.73	103.26	123.20
1	A	206	VAL	N-CA-C	-11.39	80.24	111.00
2	D	38	ARG	NE-CZ-NH2	-11.36	114.62	120.30
2	D	107	TYR	CA-CB-CG	-11.17	92.17	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	18	ARG	N-CA-C	-11.09	81.06	111.00
1	A	13	VAL	O-C-N	11.08	140.42	122.70
1	A	145	ASN	CA-C-N	10.97	141.34	117.20
1	A	88	CYS	N-CA-C	-10.80	81.83	111.00
2	B	199	SER	O-C-N	-10.73	105.53	122.70
1	A	190	ASN	O-C-N	-10.64	105.67	122.70
1	A	12	SER	N-CA-C	-10.64	82.28	111.00
2	D	173	ARG	NE-CZ-NH2	10.35	125.47	120.30
1	C	84	ALA	N-CA-C	-10.34	83.09	111.00
1	C	150	ILE	N-CA-C	-10.28	83.23	111.00
1	C	198	HIS	CA-CB-CG	-10.20	96.27	113.60
1	C	24	ARG	NE-CZ-NH1	-10.02	115.29	120.30
2	D	122	SER	N-CA-CB	-9.99	95.52	110.50
1	C	167	ASP	CA-C-N	-9.96	95.28	117.20
1	A	145	ASN	O-C-N	-9.93	106.82	122.70
1	A	43	SER	CA-C-N	9.84	138.85	117.20
2	D	94	TYR	CB-CG-CD2	-9.75	115.15	121.00
2	D	163	TRP	CD1-CG-CD2	9.74	114.10	106.30
1	A	43	SER	O-C-N	-9.73	107.13	122.70
1	A	100	GLY	CA-C-N	9.68	135.56	116.20
1	A	36	TYR	CB-CG-CD1	-9.62	115.23	121.00
2	D	50	TYR	CB-CG-CD1	-9.51	115.30	121.00
2	D	197	TRP	CD1-CG-CD2	9.50	113.90	106.30
2	D	98	ARG	NE-CZ-NH2	9.49	125.05	120.30
2	B	163	TRP	CD1-CG-CD2	9.47	113.88	106.30
1	C	1	ASP	CA-C-O	-9.38	100.40	120.10
2	B	150	LEU	CA-CB-CG	9.30	136.69	115.30
1	C	61	ARG	CA-C-N	-9.28	96.79	117.20
2	B	195	SER	N-CA-CB	-9.26	96.61	110.50
2	B	197	TRP	CG-CD2-CE3	9.24	142.22	133.90
1	A	144	ILE	N-CA-C	-9.16	86.26	111.00
1	A	65	TRP	CD1-CG-CD2	9.13	113.60	106.30
2	D	33	GLY	O-C-N	-9.08	108.17	122.70
2	D	144	SER	N-CA-C	-9.06	86.52	111.00
2	D	122	SER	C-N-CA	-9.05	99.07	121.70
1	C	163	TRP	CD1-CG-CD2	9.05	113.54	106.30
1	A	74	THR	O-C-N	-9.04	108.23	122.70
2	D	112	TRP	CD1-CG-CD2	8.98	113.49	106.30
1	A	13	VAL	CA-C-O	-8.98	101.24	120.10
2	D	8	GLY	O-C-N	-8.96	107.97	123.20
1	C	148	TRP	CD1-CG-CD2	8.95	113.46	106.30
2	D	122	SER	O-C-N	-8.93	108.42	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	GLY	CA-C-N	8.90	133.99	116.20
1	C	155	ARG	NE-CZ-NH2	8.88	124.74	120.30
2	D	173	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	153	SER	CA-C-N	-8.75	97.94	117.20
2	D	36	TRP	CD1-CG-CD2	8.74	113.30	106.30
1	A	4	MET	CA-CB-CG	8.74	128.16	113.30
1	C	173	TYR	CB-CG-CD1	-8.73	115.76	121.00
2	B	159	VAL	CG1-CB-CG2	-8.67	97.03	110.90
2	D	19	LYS	N-CA-C	-8.60	87.79	111.00
1	A	201	SER	CA-C-N	-8.59	98.31	117.20
2	B	160	THR	O-C-N	-8.57	108.98	122.70
1	A	29	ILE	CA-C-N	8.57	133.34	116.20
1	C	1	ASP	CA-CB-CG	-8.53	94.64	113.40
2	D	72	ARG	O-C-N	-8.53	109.06	122.70
2	B	131	TYR	CB-CG-CD1	-8.51	115.89	121.00
1	C	44	LEU	O-C-N	-8.51	109.09	122.70
2	B	160	THR	CA-C-N	8.50	135.90	117.20
2	D	30	SER	C-N-CA	-8.45	100.57	121.70
2	D	184	TYR	CB-CG-CD1	-8.42	115.95	121.00
2	D	112	TRP	CG-CD2-CE3	8.39	141.45	133.90
2	B	163	TRP	CE2-CD2-CG	-8.39	100.59	107.30
1	C	72	SER	CA-CB-OG	-8.38	88.57	111.20
1	A	38	GLN	O-C-N	-8.38	109.30	122.70
1	A	17	ASP	O-C-N	8.34	136.05	122.70
2	D	137	CYS	CA-CB-SG	8.34	129.01	114.00
2	B	58	ILE	N-CA-C	-8.34	88.48	111.00
1	A	179	LEU	N-CA-C	-8.33	88.50	111.00
1	A	190	ASN	C-N-CA	-8.33	100.88	121.70
2	D	144	SER	CA-C-N	-8.32	98.89	117.20
1	C	192	TYR	CA-CB-CG	-8.31	97.62	113.40
1	C	8	THR	CA-CB-CG2	-8.30	100.77	112.40
1	A	80	GLU	O-C-N	-8.28	109.46	122.70
2	B	168	LEU	N-CA-C	-8.26	88.69	111.00
1	A	29	ILE	O-C-N	-8.24	109.19	123.20
2	B	197	TRP	CE2-CD2-CG	-8.23	100.71	107.30
1	C	163	TRP	CE2-CD2-CG	-8.18	100.76	107.30
2	B	11	LEU	N-CA-C	-8.14	89.01	111.00
2	D	123	ALA	CA-C-N	-8.14	99.28	117.20
1	A	46	LEU	CA-CB-CG	8.13	134.00	115.30
2	B	48	VAL	O-C-N	-8.12	109.71	122.70
1	C	153	SER	C-N-CA	-8.11	101.43	121.70
2	B	197	TRP	CD1-CG-CD2	8.10	112.78	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	173	ARG	CB-CA-C	-8.10	94.20	110.40
1	C	102	THR	CA-CB-CG2	8.08	123.72	112.40
2	D	47	TRP	CD1-CG-CD2	8.05	112.74	106.30
2	B	106	LEU	CA-CB-CG	-8.02	96.85	115.30
2	D	112	TRP	CE2-CD2-CG	-8.02	100.89	107.30
2	B	47	TRP	CD1-CG-CD2	8.00	112.70	106.30
2	D	81	LEU	N-CA-C	-8.00	89.41	111.00
2	D	171	GLY	N-CA-C	-7.99	93.12	113.10
2	B	115	GLY	N-CA-C	-7.97	93.16	113.10
2	D	62	ASP	CB-CG-OD1	7.97	125.47	118.30
1	C	91	GLY	CA-C-N	-7.93	99.74	117.20
2	D	140	THR	N-CA-C	-7.93	89.60	111.00
2	B	165	TYR	CB-CG-CD2	-7.91	116.25	121.00
2	B	199	SER	CA-C-N	7.88	134.53	117.20
1	C	83	ILE	O-C-N	-7.86	110.13	122.70
2	D	163	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	C	161	ASN	O-C-N	-7.83	110.17	122.70
1	A	153	SER	N-CA-CB	7.82	122.24	110.50
1	A	8	THR	CA-CB-CG2	-7.81	101.47	112.40
1	C	127	SER	O-C-N	-7.80	109.94	123.20
1	C	18	ARG	NE-CZ-NH1	-7.76	116.42	120.30
2	D	197	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	D	165	TYR	CB-CG-CD1	-7.72	116.36	121.00
2	D	112	TRP	CB-CG-CD1	-7.72	116.97	127.00
1	C	138	ASN	CA-C-N	7.72	134.18	117.20
1	C	91	GLY	O-C-N	7.70	135.01	122.70
2	B	60	TYR	CB-CG-CD1	-7.68	116.39	121.00
2	D	95	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	96	TYR	N-CA-C	-7.66	90.31	111.00
2	B	168	LEU	CA-C-N	-7.66	100.34	117.20
1	C	56	SER	CA-CB-OG	-7.66	90.53	111.20
1	A	201	SER	C-N-CA	-7.63	102.62	121.70
2	B	216	ILE	CA-C-N	-7.62	100.42	117.20
2	B	116	ALA	N-CA-C	-7.61	90.47	111.00
1	A	15	LEU	CA-C-N	7.60	131.40	116.20
1	A	24	ARG	CA-C-N	-7.59	100.50	117.20
1	A	10	SER	N-CA-C	-7.56	90.58	111.00
2	D	116	ALA	CA-C-O	-7.56	104.22	120.10
1	A	44	LEU	CA-CB-CG	-7.54	97.95	115.30
2	B	50	TYR	CA-C-N	7.54	133.80	117.20
1	A	188	ARG	CA-CB-CG	-7.51	96.88	113.40
1	A	87	PHE	O-C-N	-7.50	110.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	CA-CB-CG	-7.48	96.94	113.40
1	C	1	ASP	O-C-N	7.47	134.66	122.70
2	B	95	TYR	CB-CG-CD1	-7.47	116.52	121.00
2	B	70	ILE	CG1-CB-CG2	-7.47	94.96	111.40
2	D	49	ALA	O-C-N	-7.47	110.75	122.70
1	A	186	TYR	N-CA-C	-7.46	90.85	111.00
1	A	184	ASP	O-C-N	-7.46	110.77	122.70
2	B	199	SER	N-CA-CB	-7.45	99.32	110.50
1	A	65	TRP	CE2-CD2-CG	-7.41	101.37	107.30
2	B	17	SER	CA-C-N	-7.40	100.92	117.20
1	C	100	GLY	CA-C-N	7.40	131.00	116.20
1	C	153	SER	CA-C-N	7.40	133.47	117.20
2	D	171	GLY	CA-C-N	7.38	133.44	117.20
1	A	190	ASN	CA-C-N	7.37	133.42	117.20
2	B	153	GLY	O-C-N	-7.37	110.91	122.70
1	A	188	ARG	O-C-N	-7.36	110.92	122.70
2	D	47	TRP	CE2-CD2-CG	-7.36	101.41	107.30
2	B	21	SER	O-C-N	-7.36	110.93	122.70
2	D	22	CYS	CA-C-N	7.35	133.37	117.20
1	C	141	PRO	N-CA-C	7.35	131.21	112.10
1	C	83	ILE	CA-C-N	7.34	133.35	117.20
2	D	165	TYR	N-CA-C	-7.33	91.20	111.00
2	D	171	GLY	O-C-N	-7.32	110.98	122.70
2	B	197	TRP	CB-CG-CD1	-7.31	117.49	127.00
2	D	129	SER	CB-CA-C	-7.31	96.21	110.10
2	D	77	ASN	N-CA-C	7.28	130.66	111.00
2	B	159	VAL	N-CA-C	-7.27	91.36	111.00
1	C	194	CYS	O-C-N	-7.25	111.09	122.70
1	A	148	TRP	CE2-CD2-CG	-7.23	101.51	107.30
2	D	102	GLY	CA-C-N	-7.23	101.28	117.20
2	D	32	PHE	CA-C-N	7.23	130.66	116.20
1	C	15	LEU	N-CA-C	-7.23	91.48	111.00
1	C	11	LEU	N-CA-C	-7.21	91.53	111.00
2	B	112	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	C	115	VAL	O-C-N	-7.21	111.17	122.70
1	A	135	PHE	CB-CG-CD2	7.21	125.84	120.80
2	B	107	TYR	CB-CG-CD1	-7.21	116.68	121.00
2	B	162	LYS	CB-CG-CD	-7.20	92.87	111.60
2	D	173	ARG	N-CA-CB	7.20	123.56	110.60
1	A	105	GLU	CA-C-N	-7.20	101.37	117.20
1	A	179	LEU	CA-CB-CG	7.19	131.83	115.30
2	B	137	CYS	N-CA-C	-7.18	91.60	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	172	VAL	N-CA-C	-7.18	91.61	111.00
2	B	47	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	C	26	SER	O-C-N	-7.15	111.25	122.70
2	D	36	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	C	104	LEU	CA-CB-CG	7.13	131.71	115.30
1	C	172	THR	N-CA-CB	-7.13	96.75	110.30
1	A	10	SER	N-CA-CB	-7.13	99.80	110.50
2	B	72	ARG	N-CA-C	-7.13	91.75	111.00
2	D	197	TRP	CG-CD2-CE3	7.10	140.29	133.90
1	A	14	SER	CA-C-N	7.09	132.80	117.20
2	D	54	GLY	CA-C-N	7.08	130.36	116.20
1	A	148	TRP	CD1-CG-CD2	7.07	111.95	106.30
1	C	4	MET	C-N-CA	-7.07	104.03	121.70
1	C	177	SER	N-CA-C	-7.06	91.93	111.00
2	D	2	VAL	CA-CB-CG1	-7.05	100.33	110.90
1	C	105	GLU	CA-C-N	-7.05	101.70	117.20
1	C	21	ILE	O-C-N	-7.04	111.44	122.70
1	C	94	LEU	CA-CB-CG	-7.04	99.11	115.30
2	D	150	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	152	LYS	CB-CG-CD	-7.03	93.32	111.60
1	A	114	THR	CA-CB-OG1	-7.03	94.25	109.00
2	D	211	SER	CA-C-N	7.02	132.65	117.20
2	D	101	THR	C-N-CA	-7.01	107.57	122.30
1	C	19	VAL	C-N-CA	-7.00	104.19	121.70
1	C	10	SER	N-CA-C	-7.00	92.09	111.00
2	D	8	GLY	C-N-CA	-7.00	107.60	122.30
1	C	188	ARG	O-C-N	-6.99	111.51	122.70
1	A	20	ILE	N-CA-C	-6.97	92.19	111.00
1	A	127	SER	CA-CB-OG	-6.96	92.41	111.20
2	B	216	ILE	O-C-N	6.95	133.81	122.70
2	D	122	SER	CA-CB-OG	-6.93	92.47	111.20
1	A	156	GLN	N-CA-C	-6.91	92.36	111.00
1	C	3	GLN	CA-CB-CG	-6.89	98.24	113.40
1	C	145	ASN	CA-C-N	6.89	132.36	117.20
1	C	141	PRO	CA-C-N	-6.88	102.05	117.20
1	A	49	TYR	CB-CG-CD1	-6.88	116.87	121.00
1	A	1	ASP	CA-C-N	6.87	132.31	117.20
2	B	65	LYS	C-N-CA	-6.87	107.88	122.30
2	B	204	CYS	O-C-N	-6.87	111.72	122.70
2	D	18	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	C	78	LEU	O-C-N	-6.85	111.74	122.70
1	A	187	GLU	O-C-N	-6.85	111.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	TRP	CE2-CD2-CG	-6.84	101.83	107.30
2	B	83	MET	CA-CB-CG	6.83	124.91	113.30
2	B	36	TRP	CD1-CG-CD2	6.83	111.76	106.30
1	C	163	TRP	CG-CD2-CE3	6.83	140.05	133.90
1	A	200	THR	O-C-N	-6.83	111.78	122.70
2	D	169	SER	O-C-N	6.83	133.62	122.70
2	D	147	LEU	CA-C-N	6.82	129.84	116.20
2	D	53	SER	O-C-N	-6.80	111.65	123.20
1	A	153	SER	O-C-N	6.78	133.55	122.70
1	C	64	GLY	O-C-N	-6.77	111.86	122.70
1	C	148	TRP	CG-CD1-NE1	-6.77	103.33	110.10
2	D	45	LEU	CB-CG-CD2	-6.77	99.49	111.00
1	A	163	TRP	CE2-CD2-CG	-6.77	101.89	107.30
2	B	17	SER	O-C-N	6.75	133.50	122.70
2	D	158	PRO	CA-C-N	-6.75	102.36	117.20
2	B	143	SER	CA-C-N	-6.74	102.37	117.20
1	C	73	LEU	CA-C-N	-6.69	102.48	117.20
1	C	153	SER	O-C-N	-6.69	112.00	122.70
2	B	44	GLY	CA-C-O	6.69	132.63	120.60
1	A	176	SER	CB-CA-C	-6.67	97.42	110.10
1	A	153	SER	CB-CA-C	-6.67	97.44	110.10
1	C	35	TRP	CE2-CD2-CG	-6.67	101.97	107.30
2	D	168	LEU	CA-C-O	6.67	134.10	120.10
2	D	211	SER	N-CA-C	6.66	128.99	111.00
1	C	46	LEU	O-C-N	-6.65	112.06	122.70
2	D	69	THR	O-C-N	-6.65	112.06	122.70
2	B	43	LYS	O-C-N	-6.63	111.92	123.20
2	D	207	ALA	CB-CA-C	-6.61	100.19	110.10
2	B	140	THR	CA-C-N	-6.59	102.70	117.20
1	A	26	SER	O-C-N	-6.58	112.17	122.70
2	D	197	TRP	CG-CD1-NE1	-6.57	103.53	110.10
1	C	85	THR	N-CA-C	-6.57	93.26	111.00
2	B	184	TYR	O-C-N	6.57	133.21	122.70
2	D	204	CYS	CA-C-N	-6.56	102.77	117.20
2	B	48	VAL	N-CA-CB	-6.54	97.11	111.50
2	B	165	TYR	N-CA-C	-6.53	93.36	111.00
2	B	65	LYS	CA-CB-CG	-6.53	99.03	113.40
1	C	161	ASN	CA-C-N	6.52	131.54	117.20
2	B	181	SER	CA-C-N	6.51	129.22	116.20
1	C	75	ILE	N-CA-C	-6.51	93.42	111.00
2	D	117	THR	N-CA-C	-6.51	93.43	111.00
2	B	110	ASP	N-CA-CB	-6.51	98.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	THR	CA-CB-OG1	-6.50	95.36	109.00
2	B	53	SER	CA-C-N	6.48	129.16	116.20
1	C	64	GLY	CA-C-N	6.48	131.45	117.20
2	B	211	SER	N-CA-C	6.47	128.47	111.00
1	C	189	HIS	O-C-N	-6.47	112.35	122.70
1	C	166	GLN	O-C-N	-6.47	112.36	122.70
2	D	113	GLY	CA-C-N	6.45	131.40	117.20
1	A	114	THR	CB-CA-C	6.45	129.00	111.60
2	B	112	TRP	CD1-CG-CD2	6.44	111.45	106.30
1	C	7	ILE	N-CA-C	-6.44	93.62	111.00
1	C	51	THR	O-C-N	-6.43	112.41	122.70
1	A	176	SER	N-CA-CB	6.43	120.14	110.50
1	C	9	SER	CA-CB-OG	-6.42	93.86	111.20
2	B	98	ARG	CB-CG-CD	-6.42	94.91	111.60
1	C	167	ASP	O-C-N	6.42	132.97	122.70
2	B	140	THR	O-C-N	6.41	132.96	122.70
1	C	153	SER	CA-CB-OG	-6.41	93.90	111.20
1	A	84	ALA	N-CA-C	-6.41	93.70	111.00
1	A	45	LYS	O-C-N	-6.38	112.49	122.70
1	A	57	GLY	O-C-N	-6.37	112.50	122.70
2	D	168	LEU	CA-C-N	-6.37	103.18	117.20
1	C	122	SER	CA-C-N	-6.35	103.23	117.20
2	D	139	ASP	N-CA-C	6.35	128.15	111.00
1	C	161	ASN	CB-CA-C	-6.35	97.70	110.40
2	B	181	SER	O-C-N	-6.35	112.41	123.20
1	C	194	CYS	CA-C-N	6.34	131.15	117.20
1	A	35	TRP	CD1-CG-CD2	6.33	111.36	106.30
1	A	8	THR	N-CA-CB	6.32	122.31	110.30
2	B	159	VAL	CB-CA-C	-6.32	99.39	111.40
1	C	146	VAL	O-C-N	-6.32	112.59	122.70
1	C	87	PHE	N-CA-C	-6.31	93.97	111.00
2	B	49	ALA	CA-C-N	6.30	131.06	117.20
2	D	185	SER	O-C-N	6.30	132.78	122.70
2	B	169	SER	CA-C-N	-6.29	103.36	117.20
2	B	130	VAL	CG1-CB-CG2	-6.28	100.84	110.90
2	D	18	ARG	CA-CB-CG	6.28	127.22	113.40
2	D	175	VAL	CA-CB-CG2	-6.27	101.49	110.90
1	A	85	THR	CA-CB-CG2	6.27	121.18	112.40
2	D	11	LEU	N-CA-C	-6.27	94.07	111.00
2	B	126	THR	N-CA-CB	-6.27	98.39	110.30
2	D	178	VAL	CA-CB-CG2	-6.26	101.50	110.90
2	D	138	SER	N-CA-C	6.26	127.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	173	ARG	CA-CB-CG	6.26	127.17	113.40
1	A	163	TRP	CD1-CG-CD2	6.25	111.30	106.30
1	C	1	ASP	CB-CG-OD1	-6.25	112.67	118.30
2	D	107	TYR	CB-CG-CD1	-6.24	117.26	121.00
1	A	76	SER	CA-CB-OG	6.24	128.03	111.20
2	D	4	LEU	O-C-N	-6.23	112.73	122.70
2	D	120	VAL	CA-CB-CG2	-6.23	101.55	110.90
1	A	1	ASP	N-CA-C	-6.22	94.21	111.00
2	B	142	GLY	CA-C-N	-6.22	103.52	117.20
2	D	127	ALA	CA-C-N	6.21	134.50	117.10
2	B	121	SER	CA-C-N	-6.20	103.56	117.20
1	C	197	THR	N-CA-C	-6.20	94.27	111.00
2	D	31	ASN	O-C-N	-6.19	112.79	122.70
2	B	36	TRP	CE2-CD2-CG	-6.19	102.35	107.30
1	C	61	ARG	O-C-N	6.18	132.59	122.70
1	A	87	PHE	CA-C-N	6.18	130.80	117.20
1	C	192	TYR	CA-C-N	6.18	130.79	117.20
1	A	88	CYS	O-C-N	6.17	132.58	122.70
2	D	102	GLY	N-CA-C	-6.17	97.69	113.10
1	C	189	HIS	CA-C-N	6.16	130.75	117.20
2	D	164	ASN	N-CA-CB	6.16	121.68	110.60
2	B	21	SER	C-N-CA	-6.15	106.32	121.70
1	C	165	ASP	N-CA-C	-6.14	94.42	111.00
1	C	41	ASP	N-CA-C	-6.14	94.43	111.00
1	C	105	GLU	O-C-N	6.13	132.50	122.70
1	C	145	ASN	CB-CG-ND2	6.13	131.41	116.70
1	C	175	MET	CB-CG-SD	-6.12	94.03	112.40
2	D	33	GLY	CA-C-N	6.12	130.66	117.20
2	B	43	LYS	CA-C-N	6.12	128.43	116.20
2	B	30	SER	C-N-CA	-6.11	106.42	121.70
2	B	134	VAL	CA-CB-CG2	-6.11	101.73	110.90
2	B	17	SER	CA-CB-OG	-6.10	94.72	111.20
2	D	197	TRP	CB-CG-CD1	-6.10	119.07	127.00
2	D	167	ALA	O-C-N	-6.10	112.94	122.70
2	B	49	ALA	O-C-N	-6.09	112.95	122.70
2	B	163	TRP	CG-CD1-NE1	-6.08	104.02	110.10
1	C	65	TRP	CE2-CD2-CG	-6.08	102.43	107.30
2	D	58	ILE	O-C-N	-6.08	112.97	122.70
2	D	211	SER	O-C-N	-6.08	112.97	122.70
2	B	126	THR	CA-CB-OG1	-6.08	96.24	109.00
1	A	100	GLY	O-C-N	-6.06	112.90	123.20
2	B	215	LEU	N-CA-C	-6.06	94.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	SER	N-CA-CB	6.06	119.58	110.50
2	B	132	PRO	CA-C-N	6.05	130.52	117.20
1	C	167	ASP	N-CA-CB	6.05	121.48	110.60
2	D	103	THR	N-CA-C	6.04	127.32	111.00
2	D	129	SER	N-CA-CB	6.04	119.56	110.50
2	D	158	PRO	O-C-N	6.03	132.35	122.70
1	C	31	ASN	CA-CB-CG	-6.03	100.14	113.40
1	A	205	ILE	N-CA-C	-6.03	94.73	111.00
2	B	153	GLY	CA-C-N	6.01	130.43	117.20
2	D	30	SER	O-C-N	-6.01	113.08	122.70
1	C	100	GLY	O-C-N	-6.00	112.99	123.20
2	D	124	THR	N-CA-C	-6.00	94.79	111.00
1	C	112	ALA	N-CA-C	-6.00	94.80	111.00
1	C	145	ASN	CB-CG-OD1	-6.00	109.60	121.60
2	B	106	LEU	O-C-N	-6.00	113.10	122.70
2	D	114	GLN	O-C-N	-6.00	113.00	123.20
2	B	47	TRP	CG-CD1-NE1	-6.00	104.10	110.10
2	D	172	VAL	CG1-CB-CG2	-5.99	101.31	110.90
1	A	53	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	D	112	TRP	CG-CD1-NE1	-5.98	104.12	110.10
1	C	116	SER	N-CA-C	-5.97	94.89	111.00
1	C	53	ARG	CA-CB-CG	-5.96	100.29	113.40
2	D	32	PHE	O-C-N	-5.96	113.06	123.20
1	C	76	SER	CA-CB-OG	-5.95	95.14	111.20
2	D	214	ASP	CB-CG-OD2	5.95	123.65	118.30
2	B	131	TYR	CG-CD2-CE2	-5.95	116.54	121.30
1	C	60	SER	O-C-N	-5.95	113.19	122.70
1	A	35	TRP	CE2-CD2-CG	-5.94	102.55	107.30
2	D	78	THR	OG1-CB-CG2	5.93	123.64	110.00
2	B	195	SER	CA-C-N	-5.93	104.16	117.20
1	C	196	ALA	CB-CA-C	-5.93	101.21	110.10
1	A	199	LYS	O-C-N	-5.93	113.22	122.70
1	A	67	SER	N-CA-C	-5.91	95.04	111.00
2	B	28	THR	OG1-CB-CG2	5.90	123.58	110.00
1	A	183	LYS	O-C-N	-5.89	113.27	122.70
2	D	20	LEU	CA-CB-CG	5.89	128.85	115.30
1	C	138	ASN	O-C-N	-5.89	113.28	122.70
1	A	206	VAL	CG1-CB-CG2	5.88	120.31	110.90
2	B	214	ASP	O-C-N	-5.88	113.30	122.70
2	D	63	THR	N-CA-CB	-5.88	99.14	110.30
2	B	138	SER	CA-C-N	-5.87	104.28	117.20
1	C	163	TRP	CB-CG-CD1	-5.87	119.36	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASN	C-N-CA	-5.87	107.02	121.70
1	A	55	GLN	O-C-N	-5.87	113.31	122.70
2	B	103	THR	CA-C-N	-5.86	104.31	117.20
2	D	49	ALA	CA-C-N	5.85	130.07	117.20
2	D	7	SER	CA-C-N	5.85	127.90	116.20
1	A	102	THR	CA-C-N	5.85	130.06	117.20
2	D	20	LEU	N-CA-C	-5.85	95.22	111.00
1	A	114	THR	CA-CB-CG2	5.84	120.58	112.40
2	B	189	LEU	O-C-N	-5.84	113.35	122.70
2	D	182	GLY	CA-C-N	-5.84	104.34	117.20
1	A	71	TYR	CB-CG-CD1	5.83	124.50	121.00
1	A	105	GLU	O-C-N	5.83	132.03	122.70
1	C	112	ALA	N-CA-CB	-5.83	101.94	110.10
1	C	192	TYR	N-CA-CB	-5.83	100.12	110.60
1	A	184	ASP	N-CA-C	5.81	126.68	111.00
2	D	159	VAL	N-CA-C	-5.80	95.33	111.00
1	A	14	SER	O-C-N	-5.80	113.42	122.70
2	B	36	TRP	CG-CD1-NE1	-5.80	104.30	110.10
2	D	103	THR	CA-CB-CG2	-5.79	104.29	112.40
2	B	73	ASP	CA-CB-CG	-5.79	100.66	113.40
2	B	119	ILE	O-C-N	-5.79	113.44	122.70
1	A	75	ILE	O-C-N	-5.79	113.44	122.70
2	D	154	TYR	CB-CG-CD2	-5.78	117.53	121.00
2	D	94	TYR	CA-C-N	5.78	129.92	117.20
1	C	20	ILE	N-CA-C	-5.77	95.42	111.00
1	C	167	ASP	CB-CA-C	-5.77	98.86	110.40
2	D	7	SER	O-C-N	-5.77	113.39	123.20
1	C	138	ASN	C-N-CA	-5.77	107.28	121.70
2	D	62	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	162	SER	CA-C-N	-5.76	104.52	117.20
2	D	74	ASN	N-CA-C	5.76	126.57	111.00
1	C	73	LEU	O-C-N	5.76	131.92	122.70
2	D	133	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	206	VAL	CA-C-O	-5.75	108.02	120.10
1	C	163	TRP	CG-CD1-NE1	-5.75	104.35	110.10
2	D	78	THR	N-CA-C	5.75	126.53	111.00
2	D	138	SER	N-CA-CB	-5.75	101.88	110.50
1	A	108	ARG	N-CA-CB	-5.74	100.26	110.60
2	D	5	VAL	CA-CB-CG1	-5.73	102.30	110.90
1	A	175	MET	CG-SD-CE	-5.73	91.03	100.20
1	C	63	SER	CA-C-N	5.72	127.65	116.20
2	D	128	PRO	CA-N-CD	-5.72	103.49	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	THR	N-CA-CB	-5.72	99.44	110.30
1	C	20	ILE	CB-CG1-CD1	5.71	129.90	113.90
2	D	94	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	128	GLY	C-N-CA	-5.70	110.34	122.30
2	D	104	ARG	CG-CD-NE	5.69	123.74	111.80
2	D	196	THR	CA-C-N	-5.69	104.69	117.20
2	D	207	ALA	N-CA-CB	5.69	118.06	110.10
1	A	201	SER	CB-CA-C	-5.67	99.32	110.10
2	B	165	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	172	THR	O-C-N	-5.67	113.63	122.70
1	C	183	LYS	CA-CB-CG	-5.65	100.97	113.40
2	B	7	SER	CA-C-N	5.65	127.50	116.20
2	D	217	LYS	N-CA-C	-5.65	95.75	111.00
2	B	13	GLN	CA-CB-CG	5.64	125.82	113.40
2	B	196	THR	N-CA-C	-5.64	95.78	111.00
1	C	19	VAL	O-C-N	-5.64	113.68	122.70
1	C	88	CYS	CA-CB-SG	-5.63	103.87	114.00
2	D	101	THR	CA-CB-OG1	-5.63	97.18	109.00
2	B	110	ASP	O-C-N	-5.63	113.70	122.70
1	C	44	LEU	N-CA-C	5.62	126.19	111.00
2	B	18	ARG	CA-C-N	-5.62	104.83	117.20
2	D	144	SER	N-CA-CB	5.62	118.93	110.50
1	A	150	ILE	CA-C-N	-5.62	104.84	117.20
1	A	71	TYR	CA-C-N	-5.62	104.85	117.20
1	A	193	THR	N-CA-C	-5.61	95.84	111.00
2	B	202	VAL	N-CA-CB	5.60	123.82	111.50
2	D	31	ASN	CA-C-N	5.59	129.50	117.20
2	B	60	TYR	N-CA-C	5.59	126.09	111.00
2	D	8	GLY	CA-C-N	5.59	127.38	116.20
2	D	178	VAL	CA-CB-CG1	5.59	119.28	110.90
1	A	204	PRO	N-CA-C	-5.58	97.58	112.10
1	A	201	SER	O-C-N	5.58	131.62	122.70
1	C	18	ARG	NH1-CZ-NH2	-5.58	113.27	119.40
2	B	9	GLY	C-N-CA	-5.57	110.61	122.30
2	B	201	THR	CA-C-O	-5.57	108.41	120.10
1	A	76	SER	CB-CA-C	-5.56	99.53	110.10
1	C	131	SER	N-CA-CB	-5.56	102.16	110.50
2	D	54	GLY	O-C-N	-5.56	113.75	123.20
1	A	18	ARG	CA-CB-CG	5.55	125.62	113.40
1	A	51	THR	C-N-CA	-5.55	107.81	121.70
2	B	48	VAL	CA-C-N	5.55	129.42	117.20
1	A	12	SER	C-N-CA	-5.54	107.84	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	THR	O-C-N	-5.54	113.83	122.70
2	D	183	PHE	N-CA-CB	-5.54	100.62	110.60
2	B	164	ASN	CB-CA-C	-5.54	99.33	110.40
1	C	12	SER	O-C-N	5.53	131.54	122.70
1	A	41	ASP	N-CA-C	-5.53	96.08	111.00
2	B	168	LEU	CA-C-O	5.53	131.71	120.10
2	B	54	GLY	N-CA-C	5.52	126.91	113.10
2	D	204	CYS	N-CA-C	-5.52	96.10	111.00
1	A	98	PHE	N-CA-C	5.51	125.88	111.00
2	B	25	SER	O-C-N	-5.51	113.83	123.20
2	B	66	GLY	CA-C-N	5.50	129.30	117.20
2	B	204	CYS	CA-C-N	5.50	129.30	117.20
2	D	206	VAL	CA-C-N	5.50	129.30	117.20
2	D	99	GLY	O-C-N	-5.50	113.86	123.20
2	B	189	LEU	CA-CB-CG	5.47	127.89	115.30
2	B	122	SER	CA-C-N	-5.47	105.17	117.20
1	A	24	ARG	O-C-N	5.47	131.45	122.70
1	C	192	TYR	O-C-N	-5.47	113.95	122.70
1	C	111	ALA	CA-C-N	-5.46	105.18	117.20
1	C	102	THR	CA-CB-OG1	-5.46	97.53	109.00
2	B	27	PHE	O-C-N	-5.45	113.97	122.70
1	A	29	ILE	CA-CB-CG1	-5.45	100.65	111.00
1	A	88	CYS	CA-C-O	-5.45	108.66	120.10
1	A	121	SER	CA-C-N	-5.45	105.21	117.20
1	C	73	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	A	58	VAL	N-CA-C	-5.45	96.29	111.00
1	A	60	SER	N-CA-C	5.44	125.70	111.00
1	A	71	TYR	CB-CG-CD2	-5.44	117.73	121.00
2	D	111	TYR	CB-CG-CD1	-5.44	117.73	121.00
2	B	2	VAL	O-C-N	-5.44	114.00	122.70
2	D	18	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	B	181	SER	C-N-CA	-5.44	110.89	122.30
2	D	16	GLY	O-C-N	-5.43	114.01	122.70
2	D	213	THR	CA-C-N	5.43	129.14	117.20
1	C	65	TRP	CD1-CG-CD2	5.42	110.64	106.30
1	C	205	ILE	O-C-N	-5.42	114.03	122.70
2	B	169	SER	N-CA-C	-5.42	96.38	111.00
1	C	50	TYR	CG-CD1-CE1	5.42	125.63	121.30
2	B	7	SER	O-C-N	-5.41	114.00	123.20
2	B	104	ARG	CB-CG-CD	-5.41	97.53	111.60
1	C	3	GLN	CA-C-N	-5.41	105.29	117.20
1	A	82	ASP	CB-CG-OD2	-5.41	113.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	SER	N-CA-CB	5.41	118.61	110.50
1	C	187	GLU	N-CA-CB	-5.41	100.86	110.60
2	D	98	ARG	CB-CG-CD	-5.41	97.53	111.60
2	D	50	TYR	CB-CG-CD2	5.41	124.25	121.00
1	C	17	ASP	N-CA-C	5.41	125.60	111.00
2	D	101	THR	CA-C-N	-5.40	105.40	116.20
1	C	95	PRO	CA-C-N	5.40	129.08	117.20
2	D	215	LEU	CA-C-N	5.40	129.07	117.20
2	B	165	TYR	N-CA-CB	5.39	120.30	110.60
2	B	184	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	74	THR	CA-C-N	5.39	129.05	117.20
1	A	168	SER	N-CA-CB	-5.38	102.42	110.50
2	D	90	ASP	CB-CG-OD2	5.38	123.15	118.30
2	D	198	PRO	N-CA-CB	5.38	109.76	103.30
1	A	172	THR	CA-C-N	5.38	129.04	117.20
2	B	4	LEU	CA-CB-CG	-5.38	102.93	115.30
1	C	56	SER	C-N-CA	-5.38	111.01	122.30
1	A	43	SER	N-CA-CB	-5.37	102.44	110.50
2	B	159	VAL	CA-C-O	-5.37	108.82	120.10
2	B	138	SER	N-CA-C	5.37	125.49	111.00
1	C	71	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	B	111	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	C	84	ALA	O-C-N	5.37	131.29	122.70
2	B	28	THR	N-CA-CB	-5.36	100.11	110.30
1	A	165	ASP	N-CA-C	-5.36	96.53	111.00
1	C	28	ASP	N-CA-C	-5.35	96.54	111.00
1	C	58	VAL	CG1-CB-CG2	-5.35	102.34	110.90
2	D	123	ALA	CA-C-O	5.35	131.33	120.10
2	D	186	LEU	O-C-N	-5.35	114.14	122.70
1	A	43	SER	N-CA-C	5.35	125.44	111.00
1	C	165	ASP	CB-CG-OD1	5.34	123.11	118.30
2	B	204	CYS	C-N-CA	-5.34	108.36	121.70
2	D	164	ASN	CB-CA-C	-5.34	99.73	110.40
1	A	184	ASP	CA-CB-CG	-5.33	101.66	113.40
1	A	104	LEU	CB-CA-C	5.33	120.33	110.20
1	C	182	THR	OG1-CB-CG2	5.33	122.27	110.00
1	C	77	ASN	N-CA-C	-5.33	96.60	111.00
1	A	15	LEU	CB-CG-CD2	5.33	120.05	111.00
2	D	36	TRP	CD2-CE2-CZ2	-5.32	115.92	122.30
1	C	155	ARG	O-C-N	-5.32	114.19	122.70
1	A	45	LYS	CA-C-N	5.31	128.88	117.20
2	B	107	TYR	CA-CB-CG	-5.31	103.32	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	TRP	CD1-CG-CD2	5.30	110.54	106.30
2	D	113	GLY	O-C-N	-5.30	114.22	122.70
2	B	51	ILE	CB-CA-C	-5.30	101.01	111.60
1	C	91	GLY	C-N-CA	5.30	134.94	121.70
1	A	118	PHE	CA-C-N	5.29	131.93	117.10
1	C	40	PRO	CA-CB-CG	-5.29	93.94	104.00
2	D	21	SER	N-CA-C	-5.29	96.71	111.00
1	A	110	ASP	CA-C-N	-5.29	105.56	117.20
1	C	25	ALA	CB-CA-C	-5.29	102.17	110.10
1	C	105	GLU	CB-CA-C	-5.29	99.83	110.40
2	D	192	VAL	CA-CB-CG2	-5.29	102.97	110.90
2	B	197	TRP	NE1-CE2-CZ2	-5.28	124.59	130.40
2	D	72	ARG	CG-CD-NE	-5.27	100.72	111.80
2	D	156	PRO	CA-CB-CG	-5.27	93.98	104.00
2	B	163	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	C	192	TYR	CB-CG-CD2	5.26	124.15	121.00
1	C	121	SER	CA-C-N	-5.25	105.64	117.20
2	D	23	ALA	CB-CA-C	-5.25	102.22	110.10
2	D	120	VAL	N-CA-CB	-5.25	99.95	111.50
2	B	197	TRP	CB-CA-C	-5.25	99.91	110.40
1	C	49	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	206	VAL	CA-CB-CG1	-5.24	103.03	110.90
2	B	208	HIS	CA-CB-CG	5.24	122.51	113.60
1	A	109	ALA	O-C-N	5.24	131.08	122.70
2	B	202	VAL	CB-CA-C	-5.24	101.45	111.40
2	B	148	GLY	CA-C-N	-5.24	105.68	117.20
2	D	97	THR	CA-CB-CG2	-5.23	105.08	112.40
1	C	127	SER	CA-C-N	5.23	126.66	116.20
2	B	194	SER	N-CA-C	5.22	125.11	111.00
2	B	194	SER	O-C-N	-5.22	114.34	122.70
2	D	167	ALA	C-N-CA	-5.22	108.65	121.70
2	B	23	ALA	N-CA-C	5.21	125.07	111.00
2	D	201	THR	CA-CB-CG2	-5.21	105.10	112.40
2	B	196	THR	O-C-N	5.21	131.03	122.70
1	C	184	ASP	O-C-N	-5.21	114.37	122.70
2	D	189	LEU	CA-CB-CG	5.20	127.27	115.30
2	B	4	LEU	O-C-N	-5.20	114.38	122.70
1	A	175	MET	CB-CG-SD	-5.20	96.81	112.40
2	B	152	LYS	N-CA-CB	-5.19	101.25	110.60
1	C	160	LEU	CA-C-N	5.19	128.62	117.20
1	A	44	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	B	20	LEU	CA-CB-CG	5.18	127.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	THR	O-C-N	5.18	130.99	122.70
2	B	147	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	135	PHE	CA-CB-CG	5.16	126.29	113.90
2	D	144	SER	O-C-N	5.16	130.96	122.70
1	C	12	SER	CA-C-N	-5.15	105.86	117.20
2	D	151	VAL	O-C-N	-5.15	114.45	122.70
2	D	77	ASN	N-CA-CB	-5.15	101.33	110.60
2	D	87	ARG	O-C-N	-5.14	114.47	122.70
2	B	120	VAL	N-CA-C	-5.14	97.12	111.00
2	B	173	ARG	CB-CA-C	-5.13	100.13	110.40
2	B	173	ARG	N-CA-CB	5.13	119.84	110.60
2	D	36	TRP	CG-CD1-NE1	-5.13	104.97	110.10
2	D	91	THR	CA-C-N	5.13	128.49	117.20
2	D	135	PRO	CA-N-CD	-5.13	104.32	111.50
2	B	53	SER	O-C-N	-5.13	114.48	123.20
1	C	192	TYR	CG-CD2-CE2	-5.13	117.20	121.30
2	B	33	GLY	N-CA-C	-5.12	100.29	113.10
1	A	28	ASP	CB-CG-OD2	5.12	122.91	118.30
2	D	120	VAL	CA-C-N	5.12	128.46	117.20
2	B	163	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	C	103	LYS	N-CA-C	-5.11	97.19	111.00
1	C	51	THR	C-N-CA	-5.11	108.92	121.70
1	C	131	SER	N-CA-C	-5.11	97.22	111.00
2	D	114	GLN	CA-C-N	5.10	126.40	116.20
1	A	155	ARG	CB-CG-CD	-5.09	98.36	111.60
2	D	16	GLY	N-CA-C	5.09	125.83	113.10
1	A	65	TRP	CG-CD1-NE1	-5.09	105.01	110.10
2	D	18	ARG	N-CA-CB	5.08	119.75	110.60
2	D	195	SER	N-CA-CB	-5.08	102.88	110.50
1	C	198	HIS	CB-CG-ND1	5.08	135.89	123.20
2	D	4	LEU	CA-C-N	5.07	128.36	117.20
1	C	65	TRP	NE1-CE2-CD2	5.07	112.37	107.30
1	A	205	ILE	CB-CG1-CD1	-5.07	99.71	113.90
2	D	87	ARG	CA-C-N	5.07	128.35	117.20
1	A	98	PHE	O-C-N	-5.07	114.59	123.20
1	A	164	THR	C-N-CA	-5.07	109.04	121.70
2	B	106	LEU	CA-C-N	5.06	128.33	117.20
2	B	143	SER	N-CA-CB	-5.06	102.91	110.50
1	C	146	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	C	108	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	100	GLY	CA-C-O	-5.04	111.52	120.60
2	D	65	LYS	CA-CB-CG	5.04	124.50	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	TYR	O-C-N	-5.04	114.63	122.70
2	B	137	CYS	CA-CB-SG	5.04	123.07	114.00
1	C	148	TRP	N-CA-C	-5.04	97.39	111.00
2	B	136	GLY	O-C-N	-5.03	114.65	122.70
1	A	150	ILE	CB-CA-C	-5.03	101.54	111.60
2	B	121	SER	O-C-N	5.03	130.75	122.70
1	C	159	VAL	CA-C-N	5.03	128.26	117.20
2	B	72	ARG	O-C-N	5.03	130.75	122.70
2	B	98	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	56	SER	N-CA-CB	-5.02	102.96	110.50
2	D	114	GLN	CA-CB-CG	-5.02	102.35	113.40
1	C	85	THR	OG1-CB-CG2	-5.02	98.45	110.00
1	A	38	GLN	CA-C-N	5.01	128.23	117.20
2	B	196	THR	CA-C-N	-5.01	106.17	117.20
1	C	130	ALA	O-C-N	-5.01	114.69	122.70
1	A	159	VAL	N-CA-CB	-5.00	100.49	111.50
1	A	44	LEU	O-C-N	-5.00	114.70	122.70
2	D	127	ALA	CA-C-O	-5.00	109.60	120.10

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	TYR	Sidechain
1	A	94	LEU	Peptide
2	B	107	TYR	Sidechain
2	B	154	TYR	Sidechain
2	B	157	GLY	Peptide
2	B	195	SER	Mainchain
2	B	208	HIS	Peptide
1	C	140	TYR	Peptide
1	C	167	ASP	Mainchain
1	C	203	SER	Peptide
1	C	96	TYR	Sidechain
2	D	102	GLY	Mainchain
2	D	107	TYR	Sidechain
2	D	123	ALA	Mainchain
2	D	169	SER	Mainchain
2	D	184	TYR	Sidechain
2	D	208	HIS	Peptide
2	D	40	ALA	Peptide
2	D	94	TYR	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	1605	0	1540	373	0
1	C	1605	0	1538	372	2
2	B	1624	0	1583	364	2
2	D	1624	0	1586	353	0
All	All	6458	0	6247	1397	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 110.

All (1397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PRO:CB	1:A:125:LEU:HD21	1.39	1.51
2:B:133:LEU:CD1	2:B:189:LEU:HD11	1.48	1.41
1:C:78:LEU:HD12	1:C:78:LEU:C	1.30	1.38
2:D:163:TRP:CD1	2:D:172:VAL:HG21	1.63	1.34
2:D:11:LEU:CD2	2:D:119:ILE:CG2	2.09	1.31
1:C:78:LEU:CD1	1:C:78:LEU:C	1.99	1.30
2:B:158:PRO:O	2:B:209:PRO:HG2	1.22	1.29
2:D:38:ARG:NE	2:D:46:GLU:OE2	1.65	1.29
2:D:11:LEU:HD23	2:D:119:ILE:CG2	1.63	1.27
2:D:75:PRO:HG2	2:D:77:ASN:OD1	1.09	1.26
1:A:79:GLU:HB3	1:A:81:GLU:OE2	1.31	1.25
2:B:133:LEU:HB2	2:B:148:GLY:CA	1.66	1.24
2:B:204:CYS:N	2:B:216:ILE:O	1.67	1.24
1:A:205:ILE:HD13	1:A:206:VAL:N	1.51	1.24
2:B:106:LEU:HD23	2:B:108:TYR:CD1	1.72	1.23
2:D:147:LEU:HD12	2:D:217:LYS:NZ	1.51	1.22
2:B:133:LEU:HD12	2:B:189:LEU:CD1	1.69	1.21
2:B:166:GLY:O	2:B:168:LEU:CD1	1.88	1.21
1:A:12:SER:OG	1:A:107:LYS:HG3	1.33	1.20
1:A:205:ILE:HD13	1:A:205:ILE:C	1.44	1.20
2:D:163:TRP:CD1	2:D:172:VAL:CG2	2.23	1.20
2:B:13:GLN:HA	2:B:121:SER:O	1.39	1.19
2:B:195:SER:O	2:B:199:SER:OG	1.58	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLN:HG2	1:C:129:GLY:O	1.39	1.18
1:C:15:LEU:HD21	1:C:80:GLU:OE1	1.44	1.18
1:C:92:LYS:HG3	1:C:93:THR:OG1	1.42	1.18
1:C:78:LEU:O	1:C:78:LEU:HD12	1.40	1.17
1:A:18:ARG:HA	1:A:75:ILE:O	1.43	1.17
2:B:152:LYS:HG2	2:B:185:SER:OG	1.43	1.17
2:B:167:ALA:HA	2:B:170:SER:OG	1.40	1.16
1:A:56:SER:HB2	2:D:212:LYS:HD2	1.18	1.16
1:A:150:ILE:HG21	1:A:189:HIS:CD2	1.79	1.16
2:B:133:LEU:CD1	2:B:189:LEU:CD1	2.23	1.16
1:A:147:LYS:NZ	1:A:154:GLU:OE2	1.78	1.16
1:A:120:PRO:HB3	1:A:125:LEU:CD2	1.77	1.15
2:D:60:TYR:OH	2:D:69:THR:HA	1.47	1.14
2:D:34:MET:CE	2:D:34:MET:HA	1.77	1.14
2:B:41:PRO:O	2:B:43:LYS:N	1.79	1.13
1:C:108:ARG:HH21	1:C:108:ARG:HG3	1.06	1.13
1:A:17:ASP:O	1:A:78:LEU:N	1.81	1.12
2:B:88:SER:O	2:B:91:THR:HG22	1.45	1.12
1:C:7:ILE:O	1:C:7:ILE:HD13	1.45	1.12
2:D:216:ILE:HG12	2:D:217:LYS:N	1.57	1.12
2:D:75:PRO:CG	2:D:77:ASN:OD1	1.96	1.12
2:B:168:LEU:HD13	2:B:168:LEU:N	1.65	1.12
2:D:137:CYS:O	2:D:139:ASP:OD2	1.65	1.11
2:D:168:LEU:O	2:D:193:PRO:HG2	1.49	1.11
1:A:106:ILE:HD13	1:A:106:ILE:N	1.63	1.11
2:B:133:LEU:HD12	2:B:148:GLY:HA3	1.25	1.11
1:C:106:ILE:HG21	1:C:171:SER:OG	1.51	1.10
1:C:20:ILE:HG13	1:C:74:THR:OG1	1.46	1.10
2:D:19:LYS:CD	2:D:82:GLN:OE1	1.99	1.10
2:B:133:LEU:HD13	2:B:189:LEU:HD11	1.21	1.10
2:D:11:LEU:CD2	2:D:119:ILE:HG22	1.72	1.09
1:C:144:ILE:HG23	1:C:144:ILE:O	1.49	1.09
2:B:103:THR:HG22	2:B:104:ARG:HG3	1.11	1.09
2:B:166:GLY:O	2:B:168:LEU:HD11	1.49	1.09
1:C:166:GLN:HG2	1:C:171:SER:HA	1.24	1.09
1:C:38:GLN:HB3	1:C:85:THR:HG22	1.11	1.08
1:C:49:TYR:CD2	1:C:53:ARG:HB2	1.87	1.08
1:C:86:PHE:HE2	1:C:104:LEU:HD13	1.16	1.08
2:D:74:ASN:O	2:D:77:ASN:HB2	1.54	1.08
2:B:60:TYR:OH	2:B:69:THR:HA	1.54	1.07
1:A:83:ILE:HD12	1:A:106:ILE:HD11	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:TYR:HD2	2:B:150:LEU:HD12	1.11	1.07
2:B:60:TYR:CD2	2:B:65:LYS:HD3	1.89	1.07
2:B:106:LEU:HD23	2:B:108:TYR:HD1	0.94	1.07
1:A:205:ILE:CD1	1:A:205:ILE:C	2.23	1.07
2:B:140:THR:HG22	2:B:141:SER:N	1.67	1.06
1:A:130:ALA:N	1:A:181:LEU:O	1.87	1.06
2:B:217:LYS:HE2	2:B:217:LYS:HA	1.37	1.05
2:D:38:ARG:CZ	2:D:46:GLU:OE2	2.02	1.05
2:D:147:LEU:HD12	2:D:217:LYS:HZ2	0.92	1.05
1:A:130:ALA:O	1:A:181:LEU:N	1.89	1.05
1:C:124:GLN:O	1:C:127:SER:HB2	1.55	1.05
1:C:4:MET:CE	1:C:90:GLN:HG3	1.86	1.05
2:B:203:ILE:HA	2:B:217:LYS:HB2	1.35	1.05
1:C:144:ILE:O	1:C:144:ILE:CG2	1.99	1.05
1:C:12:SER:OG	1:C:105:GLU:HB3	1.54	1.04
2:B:68:PHE:CE2	2:B:83:MET:HG2	1.91	1.04
2:D:19:LYS:HD3	2:D:82:GLN:OE1	1.57	1.04
2:D:88:SER:HA	2:D:120:VAL:CG1	1.87	1.04
2:D:11:LEU:HD23	2:D:119:ILE:CB	1.86	1.04
2:D:99:GLY:O	2:D:110:ASP:HB2	1.56	1.04
2:D:169:SER:HB3	2:D:193:PRO:HD3	1.39	1.04
2:B:17:SER:CB	2:B:83:MET:O	2.05	1.04
2:D:131:TYR:N	2:D:150:LEU:O	1.90	1.03
1:A:155:ARG:HG2	1:A:179:LEU:HD21	1.41	1.03
2:D:179:LEU:C	2:D:179:LEU:HD23	1.79	1.03
1:A:120:PRO:CB	1:A:125:LEU:CD2	2.34	1.03
1:C:15:LEU:CD2	1:C:80:GLU:OE1	2.07	1.02
1:A:15:LEU:HD21	1:A:80:GLU:HB3	1.40	1.02
2:D:11:LEU:HD23	2:D:119:ILE:HB	1.42	1.02
1:C:108:ARG:HG2	1:C:140:TYR:CD1	1.94	1.02
2:D:10:GLY:HA3	2:D:18:ARG:HH12	1.24	1.02
1:A:120:PRO:HB3	1:A:125:LEU:HD21	1.02	1.02
1:A:105:GLU:O	1:A:105:GLU:HG3	1.60	1.02
1:A:108:ARG:CD	1:A:171:SER:HB2	1.90	1.01
2:B:140:THR:OG1	2:B:145:VAL:HA	1.61	1.01
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.42	1.01
1:A:80:GLU:HG2	1:A:81:GLU:OE1	1.59	1.01
2:B:144:SER:HA	2:B:193:PRO:HA	1.03	1.01
1:A:12:SER:HA	1:A:105:GLU:O	1.59	1.00
1:C:166:GLN:HE21	1:C:171:SER:HB3	1.25	1.00
2:D:11:LEU:HD21	2:D:119:ILE:HG21	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LEU:HD22	2:D:178:VAL:HG21	1.42	1.00
1:A:24:ARG:HG3	1:A:70:ASP:OD2	1.59	1.00
1:C:133:VAL:HG21	2:D:133:LEU:HD21	1.38	0.99
2:B:131:TYR:CD2	2:B:150:LEU:HD12	1.98	0.99
1:A:108:ARG:HD2	1:A:171:SER:HB2	1.00	0.99
2:D:2:VAL:HG12	2:D:2:VAL:O	1.60	0.99
1:A:148:TRP:O	1:A:155:ARG:N	1.94	0.99
1:A:8:THR:HG21	1:A:11:LEU:HD13	1.42	0.98
2:B:131:TYR:HD2	2:B:150:LEU:CD1	1.76	0.98
1:C:21:ILE:HB	1:C:73:LEU:HB3	1.44	0.98
1:A:33:LEU:HD13	1:A:71:TYR:CG	1.97	0.98
1:A:19:VAL:CG2	1:A:78:LEU:HD12	1.92	0.98
2:B:144:SER:CA	2:B:193:PRO:HA	1.93	0.98
2:B:133:LEU:HB2	2:B:148:GLY:HA3	1.46	0.98
1:A:12:SER:OG	1:A:107:LYS:CG	2.12	0.98
2:B:171:GLY:O	2:B:190:VAL:HA	1.62	0.98
2:B:133:LEU:HD12	2:B:189:LEU:HD13	1.43	0.97
1:C:2:ILE:O	1:C:3:GLN:HG3	1.64	0.97
2:B:158:PRO:O	2:B:209:PRO:CG	2.11	0.97
1:A:18:ARG:HH21	1:A:74:THR:HG21	1.27	0.97
1:C:49:TYR:N	1:C:53:ARG:O	1.97	0.97
2:D:73:ASP:O	2:D:77:ASN:HB3	1.63	0.97
2:D:125:THR:HG22	2:D:126:THR:N	1.75	0.97
1:A:136:LEU:HD13	1:A:144:ILE:HD12	1.47	0.97
2:D:216:ILE:CG1	2:D:217:LYS:H	1.77	0.97
2:D:11:LEU:CD2	2:D:119:ILE:HG21	1.86	0.96
2:D:104:ARG:O	2:D:105:SER:CB	2.10	0.96
2:B:168:LEU:CD1	2:B:168:LEU:N	2.29	0.96
2:B:154:TYR:OH	2:B:186:LEU:HD23	1.65	0.96
1:A:6:GLN:OE1	1:A:101:GLY:N	1.96	0.96
1:A:13:VAL:CG2	1:A:78:LEU:HD13	1.96	0.96
2:D:216:ILE:HG12	2:D:217:LYS:H	1.19	0.96
1:A:108:ARG:HD2	1:A:171:SER:CB	1.95	0.96
2:D:10:GLY:HA3	2:D:18:ARG:NH1	1.80	0.96
1:A:135:PHE:CE2	1:A:174:SER:HB3	2.01	0.95
2:D:147:LEU:CD1	2:D:217:LYS:NZ	2.28	0.95
2:B:121:SER:OG	2:B:122:SER:N	1.97	0.95
1:C:196:ALA:HB3	1:C:205:ILE:CG2	1.96	0.95
2:D:163:TRP:HD1	2:D:172:VAL:HG21	1.04	0.95
2:B:130:VAL:HG22	2:B:206:VAL:HG21	1.47	0.95
2:D:11:LEU:HD21	2:D:119:ILE:CG2	1.88	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:TYR:O	1:C:52:SER:N	1.99	0.95
1:A:198:HIS:O	1:A:200:THR:N	2.00	0.94
1:C:108:ARG:NH2	1:C:109:ALA:O	2.00	0.94
2:D:34:MET:HE2	2:D:34:MET:HA	1.44	0.94
1:A:41:ASP:N	1:A:41:ASP:OD1	1.96	0.94
2:B:6:GLU:CB	2:B:116:ALA:HB2	1.98	0.94
1:A:149:LYS:HA	1:A:153:SER:O	1.66	0.94
1:C:108:ARG:HG3	1:C:109:ALA:N	1.81	0.94
1:C:86:PHE:CE2	1:C:104:LEU:HD13	2.02	0.94
1:A:27:GLN:O	1:A:29:ILE:HD13	1.65	0.94
1:C:23:CYS:HB2	1:C:35:TRP:HH2	1.32	0.94
2:D:216:ILE:O	2:D:217:LYS:HB2	1.68	0.94
2:D:27:PHE:CD2	2:D:32:PHE:HE1	1.84	0.94
1:A:12:SER:HB3	1:A:107:LYS:NZ	1.82	0.94
2:B:156:PRO:O	2:B:208:HIS:HE1	1.48	0.94
1:A:135:PHE:HE2	1:A:174:SER:HB3	1.32	0.93
2:D:133:LEU:HD12	2:D:148:GLY:HA3	1.50	0.93
1:A:51:THR:OG1	1:A:71:TYR:HE2	1.51	0.93
1:A:122:SER:O	1:A:123:GLU:C	2.03	0.93
2:B:19:LYS:HA	2:B:82:GLN:HA	1.51	0.93
1:A:29:ILE:HG23	1:A:32:PHE:HB2	1.50	0.93
1:C:91:GLY:O	2:D:107:TYR:N	2.00	0.93
1:C:150:ILE:O	1:C:152:GLY:N	2.01	0.93
2:D:216:ILE:CG1	2:D:217:LYS:N	2.25	0.92
2:B:125:THR:HG22	2:B:125:THR:O	1.68	0.92
1:A:12:SER:CB	1:A:107:LYS:HG3	1.97	0.92
1:A:135:PHE:CE1	2:B:189:LEU:HD23	2.04	0.92
2:B:133:LEU:CD1	2:B:148:GLY:HA3	1.98	0.92
2:D:19:LYS:HD2	2:D:82:GLN:OE1	1.66	0.92
1:C:108:ARG:NH2	1:C:108:ARG:HG3	1.79	0.91
2:D:67:ARG:HD2	2:D:85:SER:O	1.70	0.91
2:D:71:SER:O	2:D:79:LEU:HD12	1.70	0.91
2:B:144:SER:HA	2:B:193:PRO:CA	1.98	0.90
2:D:67:ARG:O	2:D:84:THR:HG22	1.70	0.90
2:D:34:MET:HE3	2:D:34:MET:HA	1.51	0.90
2:B:133:LEU:HB2	2:B:148:GLY:N	1.86	0.90
2:B:103:THR:HG22	2:B:104:ARG:CG	2.00	0.90
1:C:2:ILE:HD13	1:C:90:GLN:NE2	1.86	0.90
1:C:61:ARG:NH2	1:C:82:ASP:OD1	2.05	0.90
1:A:12:SER:OG	1:A:140:TYR:OH	1.90	0.90
2:B:87:ARG:NH1	2:B:89:GLU:HB2	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:GLY:O	2:B:101:THR:HB	1.70	0.90
2:B:98:ARG:N	2:B:111:TYR:O	2.05	0.89
2:B:140:THR:CG2	2:B:141:SER:N	2.27	0.89
2:D:1:ASP:O	2:D:2:VAL:HB	1.72	0.89
1:A:31:ASN:HA	1:A:71:TYR:OH	1.72	0.89
2:B:6:GLU:HB3	2:B:116:ALA:HB2	1.52	0.89
1:C:108:ARG:NH2	1:C:109:ALA:HB3	1.86	0.89
1:C:108:ARG:CG	1:C:109:ALA:N	2.27	0.89
2:B:101:THR:O	2:B:101:THR:CG2	2.21	0.89
2:B:204:CYS:SG	2:B:216:ILE:HG22	2.12	0.89
2:B:104:ARG:O	2:B:106:LEU:N	2.05	0.89
2:D:34:MET:HE1	2:D:98:ARG:HA	1.53	0.89
2:D:104:ARG:O	2:D:105:SER:HB2	1.72	0.89
2:B:110:ASP:OD2	2:B:111:TYR:CE2	2.26	0.88
1:C:56:SER:O	1:C:58:VAL:N	2.06	0.88
2:D:6:GLU:OE2	2:D:6:GLU:N	2.04	0.88
1:C:80:GLU:O	1:C:83:ILE:HG22	1.73	0.88
1:C:12:SER:OG	1:C:105:GLU:CB	2.21	0.88
2:D:217:LYS:O	2:D:217:LYS:HE2	1.74	0.88
1:C:190:ASN:HD22	1:C:190:ASN:N	1.69	0.87
1:C:78:LEU:HD12	1:C:79:GLU:N	1.88	0.87
1:A:19:VAL:CG2	1:A:78:LEU:CD1	2.53	0.87
1:A:31:ASN:HD21	1:A:67:SER:HA	1.40	0.87
2:B:106:LEU:CD2	2:B:108:TYR:HD1	1.85	0.87
2:B:97:THR:HG21	2:B:109:PHE:HB3	1.57	0.87
1:C:55:GLN:HG3	1:C:56:SER:N	1.90	0.87
2:B:67:ARG:HG2	2:B:67:ARG:HH21	1.38	0.86
2:B:8:GLY:O	2:B:18:ARG:NH1	2.08	0.86
1:C:23:CYS:HB2	1:C:35:TRP:CH2	2.09	0.86
1:A:120:PRO:HB2	1:A:125:LEU:HD21	1.54	0.86
2:D:128:PRO:O	2:D:128:PRO:HD2	1.75	0.86
1:A:162:SER:HB2	2:B:175:VAL:CG1	2.05	0.86
2:B:87:ARG:HB3	2:B:89:GLU:OE1	1.76	0.86
1:C:169:LYS:HG2	1:C:169:LYS:O	1.74	0.86
1:C:49:TYR:O	1:C:53:ARG:N	2.09	0.86
1:A:4:MET:HA	1:A:4:MET:HE2	1.55	0.86
2:D:196:THR:OG1	2:D:197:TRP:N	2.06	0.86
2:B:167:ALA:CA	2:B:170:SER:OG	2.23	0.85
2:B:87:ARG:NH1	2:B:89:GLU:CB	2.39	0.85
1:A:131:SER:OG	1:A:180:THR:HG23	1.76	0.85
1:A:189:HIS:HB2	1:A:192:TYR:OH	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:HA	2:D:82:GLN:HA	1.58	0.85
1:C:4:MET:HE1	1:C:90:GLN:HG3	1.56	0.85
1:A:65:TRP:CD1	1:A:65:TRP:N	2.43	0.85
2:D:34:MET:CE	2:D:98:ARG:HA	2.05	0.85
1:A:185:GLU:HA	1:A:188:ARG:HG3	1.57	0.85
1:A:8:THR:HG21	1:A:11:LEU:CD1	2.06	0.85
2:D:97:THR:HG22	2:D:112:TRP:HA	1.57	0.85
1:A:135:PHE:CD1	2:B:189:LEU:HD23	2.12	0.84
1:A:7:ILE:HD13	1:A:7:ILE:N	1.91	0.84
1:C:20:ILE:HA	1:C:74:THR:HA	1.60	0.84
1:A:79:GLU:CB	1:A:81:GLU:OE2	2.23	0.84
2:B:106:LEU:CD2	2:B:108:TYR:CD1	2.58	0.84
1:A:120:PRO:CG	1:A:125:LEU:HD21	2.05	0.84
1:A:41:ASP:OD2	1:A:43:SER:OG	1.96	0.84
1:A:60:SER:O	1:C:126:THR:HG23	1.78	0.84
1:C:133:VAL:HG21	2:D:133:LEU:CD2	2.06	0.84
2:B:51:ILE:HG13	2:B:58:ILE:HG12	1.59	0.84
2:B:140:THR:CG2	2:B:141:SER:H	1.78	0.84
1:C:38:GLN:HB3	1:C:85:THR:CG2	2.04	0.84
1:C:89:GLN:HG2	1:C:98:PHE:CE2	2.12	0.84
1:A:83:ILE:HD12	1:A:106:ILE:CD1	2.08	0.84
1:A:49:TYR:CZ	1:A:53:ARG:HB3	2.13	0.84
1:C:83:ILE:HA	1:C:104:LEU:HD22	1.58	0.83
1:C:39:LYS:HB2	1:C:43:SER:HB2	1.60	0.83
1:C:183:LYS:HE2	1:C:187:GLU:OE2	1.78	0.83
2:D:125:THR:CG2	2:D:126:THR:N	2.41	0.83
2:D:88:SER:HA	2:D:120:VAL:HG12	1.58	0.83
2:D:11:LEU:HD11	2:D:155:PHE:HE2	1.43	0.83
2:B:102:GLY:HA3	2:B:108:TYR:OH	1.79	0.83
1:C:83:ILE:HA	1:C:104:LEU:CD2	2.08	0.83
1:C:166:GLN:HG2	1:C:171:SER:CA	2.07	0.83
1:C:36:TYR:CE2	1:C:46:LEU:HD23	2.14	0.83
2:B:134:VAL:HG23	2:B:135:PRO:HD2	1.61	0.83
1:C:4:MET:HE1	1:C:90:GLN:CG	2.09	0.83
2:B:91:THR:HB	2:B:120:VAL:H	1.43	0.83
1:A:142:LYS:HG3	1:A:173:TYR:CE1	2.14	0.82
1:A:19:VAL:HG23	1:A:78:LEU:HD12	1.58	0.82
1:C:49:TYR:CD2	1:C:53:ARG:CB	2.62	0.82
1:C:196:ALA:HB3	1:C:205:ILE:HG22	1.59	0.82
2:B:133:LEU:HB2	2:B:148:GLY:C	1.99	0.82
1:A:39:LYS:HB2	1:A:40:PRO:HD2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:MET:CE	1:C:90:GLN:CG	2.58	0.82
1:A:2:ILE:CD1	1:A:29:ILE:HD11	2.09	0.82
2:D:19:LYS:HD2	2:D:82:GLN:HB2	1.60	0.81
2:D:88:SER:HA	2:D:120:VAL:HG11	1.62	0.81
2:B:144:SER:OG	2:B:193:PRO:HB3	1.78	0.81
2:B:217:LYS:CE	2:B:217:LYS:HA	2.09	0.81
1:C:108:ARG:CG	1:C:108:ARG:HH21	1.88	0.81
1:C:108:ARG:HH22	1:C:109:ALA:HB3	1.42	0.81
1:C:9:SER:HA	1:C:102:THR:HA	1.61	0.81
1:C:4:MET:HE3	1:C:90:GLN:H	1.45	0.81
1:A:36:TYR:HE1	1:A:89:GLN:HG2	1.42	0.81
2:B:107:TYR:HD1	2:B:107:TYR:N	1.73	0.81
2:D:38:ARG:NH1	2:D:46:GLU:OE2	2.12	0.81
1:A:85:THR:HB	1:A:103:LYS:HA	1.61	0.81
2:D:204:CYS:O	2:D:216:ILE:N	2.12	0.81
2:D:140:THR:OG1	2:D:144:SER:HB3	1.81	0.81
2:D:159:VAL:CG2	2:D:208:HIS:HB2	2.11	0.80
2:D:78:THR:HG22	2:D:79:LEU:N	1.93	0.80
2:D:33:GLY:O	2:D:34:MET:HE3	1.81	0.80
2:B:103:THR:CG2	2:B:104:ARG:HG3	2.03	0.80
1:C:2:ILE:HG12	1:C:29:ILE:CD1	2.12	0.80
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.16	0.80
2:D:179:LEU:HB2	2:D:184:TYR:CD1	2.17	0.80
1:A:13:VAL:HG21	1:A:78:LEU:HD13	1.62	0.80
1:C:20:ILE:HD11	1:C:65:TRP:HE1	1.47	0.80
2:D:75:PRO:HG2	2:D:77:ASN:CG	2.02	0.80
1:A:170:ASP:O	1:A:172:THR:N	2.15	0.80
2:D:100:GLY:O	2:D:101:THR:HB	1.80	0.80
1:C:78:LEU:HD11	1:C:79:GLU:O	1.80	0.79
1:A:79:GLU:O	1:A:81:GLU:N	2.15	0.79
2:D:78:THR:CG2	2:D:79:LEU:N	2.45	0.79
2:B:64:VAL:HB	2:B:68:PHE:CD1	2.17	0.79
2:B:139:ASP:C	2:B:145:VAL:HG13	2.03	0.79
2:D:128:PRO:CD	2:D:128:PRO:O	2.28	0.79
2:D:89:GLU:N	2:D:89:GLU:OE2	2.16	0.79
2:D:27:PHE:CD2	2:D:32:PHE:CE1	2.71	0.79
2:B:139:ASP:O	2:B:145:VAL:HG13	1.82	0.79
1:C:143:ASP:OD1	1:C:143:ASP:N	2.07	0.79
1:C:49:TYR:CG	1:C:53:ARG:HB2	2.17	0.79
1:C:71:TYR:N	1:C:71:TYR:CD1	2.51	0.79
1:A:136:LEU:HD22	1:A:144:ILE:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG22	1:A:78:LEU:HD13	1.62	0.79
1:C:135:PHE:CD2	2:D:189:LEU:HG	2.17	0.79
2:B:147:LEU:O	2:B:189:LEU:HD12	1.83	0.78
2:D:128:PRO:HB3	2:D:154:TYR:HB3	1.65	0.78
1:A:15:LEU:HD21	1:A:80:GLU:CB	2.12	0.78
1:A:106:ILE:HD13	1:A:106:ILE:H	1.47	0.78
2:B:203:ILE:CA	2:B:217:LYS:HB2	2.12	0.78
2:B:139:ASP:O	2:B:145:VAL:CG1	2.31	0.78
2:B:138:SER:O	2:B:145:VAL:HG22	1.83	0.78
2:D:34:MET:CE	2:D:34:MET:CA	2.62	0.78
2:D:204:CYS:SG	2:D:216:ILE:HG23	2.24	0.78
2:D:49:ALA:C	2:D:70:ILE:HD11	2.04	0.78
1:C:94:LEU:HD11	1:C:96:TYR:OH	1.83	0.78
2:D:87:ARG:O	2:D:89:GLU:N	2.16	0.78
1:A:135:PHE:CD1	2:B:189:LEU:CD2	2.67	0.78
2:D:179:LEU:CD2	2:D:179:LEU:C	2.50	0.78
2:D:179:LEU:HD23	2:D:180:GLN:N	1.97	0.78
1:C:203:SER:HB2	1:C:204:PRO:HD3	1.64	0.78
2:D:156:PRO:O	2:D:208:HIS:HE1	1.66	0.77
2:B:98:ARG:HG2	2:B:99:GLY:N	1.99	0.77
1:C:4:MET:HE3	1:C:90:GLN:HG3	1.66	0.77
2:D:146:THR:OG1	2:D:191:THR:HG23	1.84	0.77
2:D:145:VAL:O	2:D:191:THR:HA	1.84	0.77
2:B:151:VAL:O	2:B:151:VAL:HG22	1.84	0.77
1:A:48:ILE:HA	1:A:53:ARG:O	1.84	0.77
2:B:34:MET:O	2:B:50:TYR:CD2	2.37	0.77
2:B:22:CYS:O	2:B:79:LEU:N	2.15	0.77
1:C:29:ILE:HG12	1:C:90:GLN:CB	2.14	0.77
2:B:146:THR:HA	2:B:191:THR:HG22	1.67	0.77
2:D:30:SER:O	2:D:53:SER:HB2	1.84	0.77
1:A:106:ILE:N	1:A:106:ILE:CD1	2.41	0.77
2:D:204:CYS:N	2:D:216:ILE:O	2.16	0.77
2:B:97:THR:CG2	2:B:109:PHE:HB3	2.14	0.77
2:B:13:GLN:CA	2:B:121:SER:O	2.29	0.77
2:D:151:VAL:CG1	2:D:186:LEU:HD12	2.14	0.77
1:A:108:ARG:CZ	1:A:172:THR:HG23	2.14	0.77
2:B:156:PRO:O	2:B:208:HIS:CE1	2.36	0.77
1:C:117:ILE:HG23	1:C:117:ILE:O	1.85	0.77
1:C:7:ILE:O	1:C:7:ILE:CD1	2.29	0.77
1:A:31:ASN:OD1	1:A:51:THR:HG21	1.84	0.77
1:C:36:TYR:HE1	1:C:89:GLN:CG	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:MET:SD	2:B:86:LEU:HD21	2.25	0.77
1:C:29:ILE:HG12	1:C:90:GLN:HB3	1.66	0.76
2:B:33:GLY:HA2	2:B:72:ARG:HH22	1.50	0.76
1:A:121:SER:O	1:A:125:LEU:HG	1.84	0.76
2:D:163:TRP:CD1	2:D:172:VAL:HG23	2.20	0.76
1:C:108:ARG:HG3	1:C:109:ALA:O	1.85	0.76
2:B:101:THR:HG22	2:B:101:THR:O	1.83	0.76
2:B:200:GLN:OE1	2:B:200:GLN:N	2.18	0.76
1:A:18:ARG:HH21	1:A:74:THR:CG2	1.97	0.76
1:A:149:LYS:CA	1:A:153:SER:O	2.33	0.76
1:A:51:THR:HG1	1:A:71:TYR:HE2	0.80	0.76
1:A:140:TYR:CD2	1:A:141:PRO:HA	2.21	0.76
2:B:87:ARG:HH11	2:B:89:GLU:HG2	1.50	0.76
2:D:11:LEU:HD11	2:D:155:PHE:CE2	2.20	0.76
2:B:159:VAL:O	2:B:159:VAL:HG12	1.86	0.76
1:C:65:TRP:HZ2	1:C:74:THR:HG1	1.34	0.76
2:B:34:MET:O	2:B:50:TYR:HD2	1.68	0.76
2:D:179:LEU:O	2:D:179:LEU:HD23	1.86	0.75
1:A:32:PHE:HD2	2:B:106:LEU:HD12	1.50	0.75
1:A:23:CYS:O	1:A:71:TYR:N	2.17	0.75
1:A:18:ARG:NH2	1:A:74:THR:HG21	2.00	0.75
1:A:50:TYR:OH	2:B:104:ARG:HD2	1.86	0.75
1:C:190:ASN:O	1:C:192:TYR:CD2	2.39	0.75
2:D:18:ARG:HG3	2:D:118:LEU:HD11	1.67	0.75
1:C:2:ILE:HD13	1:C:90:GLN:CD	2.07	0.75
1:A:102:THR:HG22	1:A:102:THR:O	1.85	0.75
1:C:106:ILE:CG2	1:C:171:SER:OG	2.34	0.75
2:B:17:SER:HB3	2:B:83:MET:O	1.85	0.75
2:D:39:GLN:HA	2:D:44:GLY:O	1.86	0.75
2:D:193:PRO:O	2:D:196:THR:HG22	1.86	0.74
1:A:164:THR:OG1	1:A:174:SER:N	2.20	0.74
2:D:73:ASP:O	2:D:77:ASN:CB	2.36	0.74
1:A:33:LEU:HD13	1:A:71:TYR:CB	2.17	0.74
2:B:60:TYR:CG	2:B:65:LYS:HD3	2.23	0.74
1:C:6:GLN:OE1	1:C:101:GLY:N	2.21	0.74
1:C:70:ASP:C	1:C:71:TYR:CD1	2.61	0.74
1:C:78:LEU:CD1	1:C:79:GLU:O	2.35	0.74
2:B:98:ARG:NH1	2:B:110:ASP:OD1	2.19	0.74
1:A:39:LYS:O	1:A:41:ASP:N	2.21	0.74
2:D:179:LEU:HG	2:D:183:PHE:O	1.87	0.74
2:D:150:LEU:HD13	2:D:152:LYS:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:HG2	1:A:179:LEU:CD2	2.16	0.74
1:C:203:SER:CB	1:C:204:PRO:HD3	2.17	0.74
1:A:56:SER:CB	2:D:212:LYS:HD2	2.10	0.74
2:B:168:LEU:HD13	2:B:168:LEU:H	1.47	0.73
2:D:107:TYR:N	2:D:107:TYR:CD1	2.54	0.73
1:A:13:VAL:HG21	1:A:78:LEU:CD1	2.18	0.73
2:B:133:LEU:CB	2:B:148:GLY:HA3	2.17	0.73
1:A:12:SER:CA	1:A:105:GLU:O	2.35	0.73
1:A:136:LEU:HD11	1:A:146:VAL:HG21	1.71	0.73
1:A:29:ILE:N	1:A:29:ILE:CD1	2.51	0.73
1:A:136:LEU:HD22	1:A:144:ILE:CD1	2.17	0.73
1:C:81:GLU:OE2	1:C:81:GLU:N	2.21	0.73
1:A:135:PHE:CD1	2:B:189:LEU:HG	2.23	0.73
2:B:151:VAL:O	2:B:151:VAL:CG2	2.36	0.73
1:C:79:GLU:O	1:C:82:ASP:HB2	1.88	0.73
2:B:107:TYR:N	2:B:107:TYR:CD1	2.50	0.73
2:B:168:LEU:O	2:B:169:SER:HB3	1.86	0.73
1:C:166:GLN:NE2	1:C:171:SER:HB3	2.00	0.73
1:C:166:GLN:CG	1:C:171:SER:HA	2.14	0.73
2:B:146:THR:CA	2:B:191:THR:HG22	2.19	0.73
1:A:196:ALA:O	1:A:205:ILE:HG22	1.89	0.72
1:A:56:SER:HB2	2:D:212:LYS:CD	2.10	0.72
1:C:12:SER:HB3	1:C:107:LYS:HB2	1.71	0.72
2:B:61:ALA:O	2:B:63:THR:N	2.20	0.72
1:A:150:ILE:N	1:A:153:SER:O	2.22	0.72
2:B:172:VAL:HA	2:B:189:LEU:O	1.88	0.72
2:B:87:ARG:HH11	2:B:89:GLU:CG	2.02	0.72
1:A:21:ILE:O	1:A:72:SER:HA	1.88	0.72
2:D:147:LEU:CD1	2:D:217:LYS:HZ3	2.02	0.72
2:D:93:ILE:HA	2:D:117:THR:HA	1.69	0.72
1:A:88:CYS:O	1:A:99:GLY:N	2.16	0.72
1:C:124:GLN:HG2	1:C:129:GLY:C	2.09	0.72
2:B:68:PHE:CZ	2:B:83:MET:HG2	2.23	0.72
1:A:135:PHE:HD1	2:B:189:LEU:CD2	2.02	0.72
2:D:159:VAL:HG23	2:D:208:HIS:HB2	1.71	0.72
2:D:216:ILE:O	2:D:217:LYS:CB	2.38	0.72
2:D:112:TRP:N	2:D:112:TRP:CD1	2.57	0.72
1:A:37:GLN:HB2	1:A:47:LEU:CD1	2.19	0.72
1:C:127:SER:OG	2:D:131:TYR:OH	1.60	0.72
2:D:17:SER:HB3	2:D:84:THR:HA	1.70	0.72
1:A:12:SER:HB3	1:A:107:LYS:HZ2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HD13	1:A:7:ILE:H	1.52	0.72
2:B:167:ALA:C	2:B:168:LEU:CD1	2.58	0.72
1:C:75:ILE:HG22	1:C:76:SER:N	2.03	0.71
2:B:17:SER:HB3	2:B:84:THR:HA	1.72	0.71
1:A:162:SER:HB2	2:B:175:VAL:HG12	1.71	0.71
2:B:148:GLY:HA3	2:B:189:LEU:CD1	2.21	0.71
1:A:12:SER:HB3	1:A:107:LYS:HZ1	1.54	0.71
1:C:124:GLN:OE1	1:C:131:SER:N	2.20	0.71
2:D:130:VAL:HG11	2:D:216:ILE:HG22	1.72	0.71
2:B:134:VAL:CG2	2:B:135:PRO:HD2	2.20	0.71
2:B:166:GLY:O	2:B:168:LEU:HD13	1.88	0.71
2:D:68:PHE:CD2	2:D:81:LEU:HD21	2.26	0.71
1:C:92:LYS:HG3	1:C:93:THR:HG1	1.53	0.71
2:B:152:LYS:HG2	2:B:185:SER:HG	1.55	0.71
2:B:68:PHE:CE2	2:B:83:MET:CG	2.71	0.71
2:D:212:LYS:HE3	2:D:214:ASP:OD1	1.91	0.70
2:D:30:SER:HA	2:D:74:ASN:ND2	2.06	0.70
2:B:88:SER:O	2:B:91:THR:CG2	2.34	0.70
1:C:158:GLY:O	1:C:179:LEU:HA	1.91	0.70
2:B:91:THR:O	2:B:92:ALA:HB2	1.89	0.70
2:B:17:SER:CA	2:B:83:MET:O	2.40	0.70
1:A:184:ASP:O	1:A:188:ARG:HG3	1.91	0.70
1:A:124:GLN:O	1:A:127:SER:N	2.24	0.70
1:A:21:ILE:N	1:A:73:LEU:O	2.21	0.70
2:B:133:LEU:CB	2:B:148:GLY:CA	2.58	0.70
2:D:34:MET:CA	2:D:34:MET:HE3	2.20	0.70
1:C:80:GLU:O	1:C:82:ASP:N	2.25	0.70
1:C:33:LEU:HD23	1:C:34:ASN:N	2.07	0.70
1:C:2:ILE:CD1	1:C:90:GLN:NE2	2.55	0.70
1:A:8:THR:CG2	1:A:11:LEU:HD13	2.21	0.70
1:A:144:ILE:HG22	1:A:144:ILE:O	1.92	0.69
2:D:67:ARG:CD	2:D:85:SER:O	2.39	0.69
2:D:204:CYS:SG	2:D:216:ILE:CG2	2.80	0.69
2:B:87:ARG:HB3	2:B:89:GLU:CD	2.12	0.69
2:B:49:ALA:HB1	2:B:70:ILE:HG13	1.72	0.69
2:B:148:GLY:HA3	2:B:189:LEU:HD13	1.74	0.69
2:D:137:CYS:HA	2:D:197:TRP:CH2	2.27	0.69
1:C:55:GLN:HG3	1:C:56:SER:H	1.56	0.69
1:A:32:PHE:HD2	2:B:106:LEU:CD1	2.04	0.69
1:A:150:ILE:CG2	1:A:189:HIS:CD2	2.70	0.69
2:D:34:MET:O	2:D:50:TYR:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLN:O	1:C:127:SER:CB	2.38	0.69
1:C:36:TYR:HE1	1:C:89:GLN:HG2	1.58	0.69
1:C:64:GLY:HA2	1:C:72:SER:O	1.92	0.69
1:C:4:MET:HE3	1:C:90:GLN:N	2.07	0.69
2:D:49:ALA:HB1	2:D:70:ILE:HD11	1.75	0.69
2:B:167:ALA:HA	2:B:170:SER:HG	1.58	0.69
1:C:146:VAL:O	1:C:147:LYS:HB2	1.93	0.69
1:C:183:LYS:CE	1:C:187:GLU:OE2	2.41	0.69
2:B:143:SER:C	2:B:194:SER:OG	2.31	0.69
1:A:164:THR:HG1	1:A:174:SER:H	1.37	0.68
1:A:143:ASP:O	1:A:198:HIS:CD2	2.46	0.68
2:D:168:LEU:O	2:D:169:SER:HB2	1.91	0.68
2:B:89:GLU:H	2:B:89:GLU:CD	1.96	0.68
2:B:2:VAL:HG12	2:B:2:VAL:O	1.93	0.68
2:B:6:GLU:HB3	2:B:116:ALA:CB	2.23	0.68
1:C:38:GLN:CB	1:C:85:THR:HG22	2.06	0.68
2:D:130:VAL:HG21	2:D:214:ASP:HB3	1.76	0.68
1:C:10:SER:HA	1:C:103:LYS:O	1.93	0.68
1:C:108:ARG:HG3	1:C:109:ALA:H	1.54	0.68
2:B:4:LEU:O	2:B:114:GLN:NE2	2.26	0.68
1:A:123:GLU:O	1:A:124:GLN:C	2.29	0.68
1:A:49:TYR:CZ	1:A:53:ARG:CB	2.76	0.68
2:D:168:LEU:O	2:D:193:PRO:CG	2.37	0.68
2:B:197:TRP:CD1	2:B:198:PRO:HA	2.28	0.68
1:A:51:THR:OG1	1:A:71:TYR:CE2	2.33	0.68
2:D:67:ARG:O	2:D:84:THR:CG2	2.42	0.68
1:A:33:LEU:HD13	1:A:71:TYR:HB2	1.76	0.68
1:A:201:SER:OG	1:A:203:SER:N	2.27	0.68
1:A:83:ILE:CD1	1:A:106:ILE:HD11	2.20	0.68
2:B:106:LEU:C	2:B:107:TYR:HD1	1.98	0.68
1:A:108:ARG:HH21	1:A:108:ARG:HG2	1.60	0.67
2:D:146:THR:HA	2:D:190:VAL:O	1.94	0.67
2:B:87:ARG:HH11	2:B:89:GLU:CB	2.07	0.67
1:A:39:LYS:H	1:A:43:SER:HB2	1.59	0.67
1:C:155:ARG:HG2	1:C:179:LEU:HD21	1.75	0.67
1:A:2:ILE:HD13	1:A:29:ILE:HD11	1.75	0.67
1:C:108:ARG:CG	1:C:109:ALA:O	2.42	0.67
1:A:48:ILE:HG12	1:A:54:LEU:HD12	1.74	0.67
2:D:169:SER:HB2	2:D:193:PRO:CG	2.24	0.67
1:C:91:GLY:O	2:D:106:LEU:HD12	1.94	0.67
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:HD3	1:C:140:TYR:CG	2.30	0.67
2:B:17:SER:HB2	2:B:83:MET:O	1.94	0.67
2:B:22:CYS:O	2:B:78:THR:HA	1.95	0.67
2:D:134:VAL:HG22	2:D:135:PRO:O	1.94	0.67
2:B:164:ASN:ND2	2:B:164:ASN:O	2.28	0.67
1:C:93:THR:C	1:C:94:LEU:HD12	2.14	0.67
1:C:115:VAL:HG21	1:C:205:ILE:CG2	2.25	0.67
1:A:108:ARG:NH2	1:A:108:ARG:HG2	2.08	0.67
1:A:167:ASP:O	1:A:171:SER:N	2.25	0.67
1:C:67:SER:O	1:C:69:THR:N	2.27	0.67
2:B:217:LYS:HE2	2:B:217:LYS:CA	2.21	0.67
2:D:139:ASP:HA	2:D:142:GLY:O	1.95	0.67
2:B:67:ARG:HG2	2:B:67:ARG:NH2	2.10	0.67
1:C:155:ARG:HH12	1:C:185:GLU:CD	1.98	0.67
2:B:42:GLU:OE2	2:B:43:LYS:HG3	1.95	0.67
2:D:180:GLN:O	2:D:181:SER:HB2	1.93	0.67
1:C:153:SER:OG	1:C:154:GLU:N	2.28	0.67
2:B:203:ILE:HA	2:B:217:LYS:CB	2.20	0.66
2:D:196:THR:HG1	2:D:197:TRP:H	1.42	0.66
1:A:136:LEU:HD13	1:A:144:ILE:CD1	2.24	0.66
1:A:24:ARG:NE	1:A:70:ASP:OD2	2.28	0.66
2:B:167:ALA:C	2:B:168:LEU:HD12	2.16	0.66
2:D:151:VAL:CG1	2:D:186:LEU:CD1	2.73	0.66
1:C:108:ARG:O	1:C:140:TYR:CE1	2.48	0.66
1:A:183:LYS:HE2	1:A:187:GLU:OE2	1.96	0.66
2:D:159:VAL:HG22	2:D:208:HIS:HB2	1.77	0.66
1:A:27:GLN:O	1:A:29:ILE:CD1	2.42	0.66
1:A:31:ASN:OD1	1:A:66:GLY:O	2.14	0.66
2:D:89:GLU:H	2:D:89:GLU:CD	1.99	0.66
1:A:86:PHE:O	1:A:101:GLY:HA2	1.95	0.66
1:A:29:ILE:CG2	1:A:32:PHE:HB2	2.22	0.66
1:C:108:ARG:CG	1:C:109:ALA:H	2.09	0.66
2:D:140:THR:N	2:D:142:GLY:O	2.28	0.66
1:C:108:ARG:O	1:C:140:TYR:HE1	1.77	0.66
1:C:19:VAL:O	1:C:74:THR:HA	1.97	0.65
1:C:20:ILE:CG1	1:C:74:THR:OG1	2.36	0.65
1:C:78:LEU:HD12	1:C:79:GLU:CA	2.25	0.65
1:A:29:ILE:HD13	1:A:29:ILE:N	2.12	0.65
1:A:89:GLN:HB3	1:A:98:PHE:CE2	2.31	0.65
1:C:160:LEU:HD13	2:D:178:VAL:HG13	1.77	0.65
1:A:21:ILE:O	1:A:73:LEU:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ASN:N	1:C:190:ASN:ND2	2.40	0.65
2:B:73:ASP:O	2:B:74:ASN:C	2.31	0.65
1:C:66:GLY:HA3	1:C:71:TYR:CD2	2.32	0.65
1:C:89:GLN:HB3	1:C:98:PHE:CD2	2.31	0.65
1:C:125:LEU:C	1:C:128:GLY:H	1.99	0.64
2:B:64:VAL:HB	2:B:68:PHE:CG	2.32	0.64
2:D:1:ASP:O	2:D:2:VAL:CB	2.40	0.64
2:D:169:SER:HB3	2:D:193:PRO:CD	2.22	0.64
2:D:169:SER:CB	2:D:193:PRO:HD3	2.23	0.64
2:B:140:THR:HG22	2:B:141:SER:H	1.42	0.64
1:A:203:SER:C	1:A:204:PRO:O	2.30	0.64
2:D:158:PRO:O	2:D:208:HIS:ND1	2.23	0.64
1:A:18:ARG:CG	1:A:74:THR:HG23	2.26	0.64
1:C:78:LEU:CD1	1:C:79:GLU:N	2.53	0.64
1:A:2:ILE:HG23	1:A:27:GLN:N	2.13	0.64
1:C:2:ILE:HG12	1:C:29:ILE:HD13	1.79	0.64
2:D:50:TYR:N	2:D:70:ILE:HD11	2.13	0.63
1:C:49:TYR:HE1	1:C:55:GLN:HA	1.61	0.63
1:C:55:GLN:O	1:C:58:VAL:HB	1.98	0.63
1:A:89:GLN:HB3	1:A:98:PHE:CD2	2.33	0.63
1:C:115:VAL:HG21	1:C:205:ILE:HG23	1.79	0.63
1:C:196:ALA:CB	1:C:205:ILE:HG22	2.26	0.63
2:B:202:VAL:O	2:B:203:ILE:HG13	1.98	0.63
2:B:124:THR:HG23	2:B:124:THR:O	1.97	0.63
1:C:46:LEU:HD11	1:C:49:TYR:HB3	1.81	0.63
1:C:15:LEU:HD23	1:C:80:GLU:OE1	1.99	0.63
2:B:202:VAL:O	2:B:217:LYS:HB3	1.99	0.63
1:A:134:CYS:HB2	1:A:148:TRP:CZ2	2.33	0.63
1:C:160:LEU:HD13	2:D:178:VAL:CG1	2.29	0.63
1:C:155:ARG:NH1	1:C:185:GLU:OE2	2.31	0.63
1:A:24:ARG:CG	1:A:70:ASP:OD2	2.42	0.63
1:A:54:LEU:HD11	1:A:62:PHE:O	1.99	0.63
2:B:131:TYR:O	2:B:149:CYS:HA	1.98	0.63
2:B:131:TYR:CD2	2:B:150:LEU:CD1	2.69	0.63
1:C:144:ILE:HG22	1:C:144:ILE:O	1.95	0.63
2:D:139:ASP:O	2:D:145:VAL:HA	1.99	0.62
2:B:130:VAL:HG23	2:B:214:ASP:CB	2.28	0.62
1:A:47:LEU:O	1:A:48:ILE:HG13	1.98	0.62
1:A:134:CYS:HB2	1:A:148:TRP:CH2	2.34	0.62
2:D:169:SER:HB3	2:D:191:THR:O	1.98	0.62
1:A:80:GLU:HG2	1:A:81:GLU:CD	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ILE:HD13	1:C:90:GLN:HE21	1.65	0.62
1:C:2:ILE:HG12	1:C:29:ILE:HD11	1.82	0.62
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.79	0.62
1:C:108:ARG:HG2	1:C:140:TYR:CE1	2.33	0.62
2:B:133:LEU:CB	2:B:148:GLY:C	2.68	0.62
1:C:85:THR:HG23	1:C:87:PHE:CE1	2.35	0.62
1:A:205:ILE:CD1	1:A:206:VAL:N	2.46	0.62
1:C:3:GLN:N	1:C:26:SER:OG	2.31	0.62
1:C:139:PHE:CE1	1:C:141:PRO:O	2.53	0.62
2:D:163:TRP:NE1	2:D:188:SER:OG	1.91	0.62
1:C:123:GLU:O	1:C:126:THR:HG22	2.00	0.62
1:A:7:ILE:CD1	1:A:7:ILE:H	2.10	0.62
2:B:29:PHE:O	2:B:31:ASN:N	2.33	0.62
1:A:135:PHE:HE1	2:B:189:LEU:HD23	1.61	0.61
1:A:18:ARG:HG3	1:A:74:THR:HG23	1.82	0.61
2:D:72:ARG:HG2	2:D:74:ASN:OD1	2.01	0.61
2:D:93:ILE:HG13	2:D:117:THR:HB	1.82	0.61
2:D:92:ALA:O	2:D:117:THR:OG1	2.18	0.61
1:C:78:LEU:HD13	1:C:78:LEU:C	2.12	0.61
1:C:2:ILE:HD13	1:C:90:GLN:CG	2.30	0.61
1:A:17:ASP:OD2	1:A:78:LEU:HB3	2.00	0.61
1:A:30:GLY:O	1:A:32:PHE:CD1	2.53	0.61
2:D:72:ARG:HE	2:D:74:ASN:HD21	1.49	0.61
1:C:135:PHE:CE2	2:D:189:LEU:HG	2.36	0.61
2:D:130:VAL:HG11	2:D:216:ILE:CG2	2.31	0.61
2:B:20:LEU:HD21	2:B:94:TYR:CB	2.31	0.61
2:B:69:THR:O	2:B:81:LEU:HA	2.00	0.61
1:A:120:PRO:HB2	1:A:125:LEU:HD11	1.82	0.61
2:B:148:GLY:CA	2:B:189:LEU:HD13	2.30	0.61
2:D:156:PRO:O	2:D:156:PRO:HG2	2.01	0.61
1:A:198:HIS:O	1:A:199:LYS:C	2.36	0.61
2:D:49:ALA:HB1	2:D:70:ILE:CD1	2.31	0.61
2:B:4:LEU:HD23	2:B:4:LEU:N	2.16	0.61
2:D:179:LEU:HD23	2:D:180:GLN:CA	2.30	0.61
1:A:153:SER:OG	1:A:154:GLU:N	2.34	0.61
1:C:17:ASP:N	1:C:17:ASP:OD1	2.33	0.61
1:C:183:LYS:HZ3	1:C:187:GLU:CD	2.04	0.61
1:A:135:PHE:CD1	2:B:189:LEU:CG	2.84	0.60
2:D:144:SER:HA	2:D:192:VAL:O	2.02	0.60
2:D:212:LYS:HE3	2:D:214:ASP:HB2	1.82	0.60
1:C:94:LEU:HD12	1:C:94:LEU:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:PRO:HD3	2:B:208:HIS:CD2	2.36	0.60
1:A:173:TYR:HD2	1:A:173:TYR:N	1.99	0.60
1:A:12:SER:HA	1:A:105:GLU:HG3	1.82	0.60
1:C:4:MET:HE3	1:C:90:GLN:CG	2.29	0.60
2:B:18:ARG:N	2:B:83:MET:O	2.30	0.60
1:C:35:TRP:CE3	1:C:73:LEU:HD22	2.37	0.60
1:A:122:SER:O	1:A:123:GLU:O	2.19	0.60
2:B:49:ALA:HB1	2:B:70:ILE:CG1	2.31	0.60
1:A:132:VAL:O	1:A:178:THR:HA	2.02	0.60
2:D:151:VAL:HG11	2:D:186:LEU:CD1	2.31	0.60
2:D:132:PRO:O	2:D:132:PRO:HG2	2.00	0.60
1:A:19:VAL:HG22	1:A:78:LEU:CD1	2.31	0.60
2:B:162:LYS:O	2:B:205:ASN:N	2.23	0.60
2:D:13:GLN:HG2	2:D:14:PRO:CD	2.30	0.60
1:A:29:ILE:HG22	1:A:32:PHE:H	1.66	0.60
2:D:58:ILE:HG22	2:D:60:TYR:CE2	2.37	0.60
2:B:98:ARG:HH11	2:B:110:ASP:CG	2.05	0.60
2:B:128:PRO:HG2	2:B:212:LYS:HD3	1.83	0.60
1:C:117:ILE:CG2	1:C:117:ILE:O	2.49	0.60
1:A:31:ASN:ND2	1:A:67:SER:HA	2.12	0.60
1:A:92:LYS:HG3	1:A:93:THR:OG1	2.02	0.60
2:D:91:THR:HA	2:D:118:LEU:O	2.00	0.60
1:A:146:VAL:HG22	1:A:196:ALA:HB2	1.84	0.60
2:D:212:LYS:CE	2:D:214:ASP:HB2	2.31	0.60
1:A:12:SER:HB3	1:A:107:LYS:HG3	1.84	0.59
1:A:143:ASP:O	1:A:198:HIS:HD2	1.84	0.59
1:A:17:ASP:OD2	1:A:17:ASP:N	2.28	0.59
1:A:37:GLN:HE21	1:A:84:ALA:HB3	1.66	0.59
2:D:151:VAL:HG11	2:D:186:LEU:HD11	1.84	0.59
1:C:24:ARG:NH1	1:C:69:THR:HB	2.17	0.59
2:B:174:THR:HG23	2:B:188:SER:HB2	1.84	0.59
1:C:54:LEU:HD21	1:C:58:VAL:O	2.02	0.59
1:A:138:ASN:OD1	1:A:138:ASN:N	2.24	0.59
1:C:80:GLU:H	1:C:80:GLU:CD	2.06	0.59
1:A:85:THR:HG22	1:A:103:LYS:HG2	1.84	0.59
1:C:81:GLU:CD	1:C:81:GLU:N	2.56	0.59
2:B:64:VAL:HA	2:B:67:ARG:HH11	1.67	0.59
2:D:11:LEU:HA	2:D:119:ILE:HB	1.83	0.59
1:A:18:ARG:HD3	1:A:74:THR:HG23	1.84	0.59
1:A:26:SER:OG	1:A:27:GLN:N	2.35	0.59
1:C:125:LEU:O	1:C:128:GLY:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:TYR:CD2	2:D:51:ILE:N	2.71	0.59
2:D:103:THR:HG22	2:D:104:ARG:HG3	1.85	0.59
2:D:58:ILE:CG2	2:D:60:TYR:CE2	2.86	0.59
2:B:101:THR:O	2:B:101:THR:HG23	2.03	0.59
2:D:119:ILE:HD13	2:D:156:PRO:HB2	1.85	0.59
1:A:49:TYR:CE1	1:A:53:ARG:CB	2.85	0.59
1:C:24:ARG:NH1	1:C:69:THR:CB	2.66	0.59
1:C:89:GLN:HA	1:C:97:THR:O	2.03	0.59
1:A:21:ILE:O	1:A:72:SER:CA	2.51	0.59
1:A:17:ASP:OD2	1:A:78:LEU:CB	2.50	0.58
2:B:98:ARG:O	2:B:109:PHE:HA	2.03	0.58
2:B:98:ARG:HG2	2:B:99:GLY:H	1.66	0.58
2:D:133:LEU:HD12	2:D:148:GLY:CA	2.30	0.58
1:A:163:TRP:CE3	1:A:163:TRP:N	2.71	0.58
1:C:152:GLY:O	1:C:153:SER:CB	2.46	0.58
1:C:196:ALA:HB3	1:C:205:ILE:HG21	1.81	0.58
2:B:19:LYS:HD3	2:B:80:PHE:CD1	2.38	0.58
2:D:154:TYR:CE2	2:D:184:TYR:HB2	2.38	0.58
1:A:136:LEU:HD12	1:A:175:MET:SD	2.44	0.58
1:A:110:ASP:O	1:A:111:ALA:HB2	2.03	0.58
1:A:4:MET:CE	1:A:4:MET:HA	2.31	0.58
1:A:173:TYR:CD2	1:A:173:TYR:N	2.72	0.58
2:B:174:THR:HA	2:B:188:SER:HA	1.86	0.58
1:A:49:TYR:CD1	1:A:49:TYR:N	2.72	0.58
2:D:146:THR:CG2	2:D:189:LEU:HB3	2.34	0.58
1:A:156:GLN:HA	1:A:156:GLN:OE1	2.03	0.58
2:B:128:PRO:CG	2:B:212:LYS:HD3	2.34	0.58
1:A:163:TRP:HE3	1:A:163:TRP:N	2.02	0.58
2:B:168:LEU:O	2:B:169:SER:CB	2.52	0.58
2:B:139:ASP:OD1	2:B:145:VAL:HG11	2.03	0.58
1:C:65:TRP:HZ2	1:C:74:THR:OG1	1.86	0.58
1:A:12:SER:CB	1:A:107:LYS:HZ1	2.17	0.58
2:D:179:LEU:HA	2:D:184:TYR:HA	1.86	0.57
2:B:130:VAL:HG22	2:B:206:VAL:CG2	2.27	0.57
2:B:65:LYS:HD2	2:B:66:GLY:H	1.69	0.57
1:A:22:SER:HA	1:A:72:SER:HA	1.86	0.57
1:A:4:MET:CA	1:A:4:MET:HE2	2.30	0.57
1:A:49:TYR:CD1	1:A:53:ARG:HB2	2.39	0.57
1:C:35:TRP:CD2	1:C:73:LEU:HD22	2.40	0.57
2:D:29:PHE:O	2:D:72:ARG:NH1	2.35	0.57
1:A:34:ASN:HD21	2:B:106:LEU:HD21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:SER:O	2:B:54:GLY:C	2.42	0.57
2:D:49:ALA:HB1	2:D:70:ILE:CG1	2.35	0.57
1:C:170:ASP:O	1:C:172:THR:HG23	2.05	0.57
2:B:133:LEU:CG	2:B:148:GLY:HA3	2.35	0.57
1:A:18:ARG:CD	1:A:74:THR:HG23	2.35	0.57
2:B:87:ARG:NE	2:B:89:GLU:OE1	2.33	0.57
1:C:137:ASN:O	1:C:138:ASN:HB2	2.05	0.57
2:D:145:VAL:HG23	2:D:192:VAL:O	2.05	0.57
2:B:166:GLY:C	2:B:168:LEU:CD1	2.69	0.57
1:C:124:GLN:NE2	1:C:131:SER:N	2.53	0.57
1:A:148:TRP:HA	1:A:193:THR:O	2.05	0.57
2:B:146:THR:HG23	2:B:191:THR:HG23	1.86	0.57
1:C:167:ASP:O	1:C:171:SER:N	2.38	0.57
1:C:183:LYS:NZ	1:C:187:GLU:OE2	2.37	0.57
1:C:203:SER:HB2	1:C:204:PRO:CD	2.31	0.57
1:C:49:TYR:O	1:C:53:ARG:HG2	2.04	0.56
2:B:68:PHE:HD2	2:B:81:LEU:HD11	1.69	0.56
1:C:35:TRP:CE3	1:C:73:LEU:CD2	2.88	0.56
1:A:185:GLU:HA	1:A:188:ARG:CG	2.31	0.56
2:D:60:TYR:HH	2:D:69:THR:HA	1.66	0.56
1:A:39:LYS:O	1:A:41:ASP:OD1	2.21	0.56
2:D:74:ASN:C	2:D:77:ASN:HB2	2.25	0.56
1:A:107:LYS:HA	1:A:140:TYR:OH	2.05	0.56
1:A:144:ILE:O	1:A:144:ILE:CG2	2.49	0.56
2:D:84:THR:O	2:D:85:SER:C	2.39	0.56
2:D:74:ASN:O	2:D:77:ASN:CB	2.43	0.56
1:C:164:THR:HG22	2:D:175:VAL:HA	1.86	0.56
1:A:108:ARG:NE	1:A:170:ASP:O	2.36	0.56
2:B:180:GLN:O	2:B:181:SER:CB	2.52	0.56
2:D:68:PHE:CE2	2:D:81:LEU:HD21	2.39	0.56
2:D:93:ILE:HG22	2:D:115:GLY:HA3	1.87	0.56
1:A:85:THR:CG2	1:A:103:LYS:HG2	2.36	0.56
2:D:74:ASN:N	2:D:75:PRO:HD2	2.21	0.56
2:B:203:ILE:HG21	2:B:215:LEU:HD11	1.87	0.56
1:C:183:LYS:O	1:C:183:LYS:HG2	2.06	0.56
1:C:61:ARG:NH2	1:C:82:ASP:CG	2.58	0.56
1:A:17:ASP:O	1:A:78:LEU:HB2	2.06	0.56
1:C:2:ILE:HD13	1:C:90:GLN:HG2	1.88	0.56
2:D:34:MET:HB3	2:D:79:LEU:HD22	1.87	0.56
2:B:102:GLY:C	2:B:103:THR:OG1	2.42	0.56
1:C:12:SER:HA	1:C:105:GLU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:CD1	1:A:175:MET:SD	2.94	0.55
1:A:33:LEU:CD1	1:A:71:TYR:HB2	2.36	0.55
1:A:90:GLN:HG3	1:A:97:THR:H	1.71	0.55
1:A:147:LYS:CE	1:A:154:GLU:OE2	2.55	0.55
2:D:49:ALA:CB	2:D:70:ILE:HD11	2.35	0.55
2:D:91:THR:O	2:D:92:ALA:HB2	2.05	0.55
2:B:128:PRO:HD2	2:B:212:LYS:HD3	1.87	0.55
1:A:197:THR:O	1:A:198:HIS:HB2	2.06	0.55
2:D:215:LEU:O	2:D:216:ILE:HB	2.07	0.55
2:D:10:GLY:CA	2:D:18:ARG:NH1	2.64	0.55
1:C:139:PHE:N	1:C:173:TYR:O	2.38	0.55
1:A:120:PRO:HB3	1:A:125:LEU:CG	2.37	0.55
1:A:115:VAL:HG21	1:A:205:ILE:HD12	1.88	0.55
1:C:107:LYS:HA	1:C:140:TYR:OH	2.06	0.55
1:A:39:LYS:CB	1:A:40:PRO:HD2	2.30	0.55
1:A:197:THR:HG22	1:A:198:HIS:N	2.22	0.55
1:C:182:THR:O	1:C:184:ASP:N	2.39	0.55
2:B:179:LEU:HG	2:B:184:TYR:CZ	2.42	0.55
1:C:4:MET:HE3	1:C:90:GLN:CB	2.37	0.55
2:B:110:ASP:OD2	2:B:111:TYR:HE2	1.87	0.55
1:C:196:ALA:CB	1:C:205:ILE:CG2	2.79	0.55
1:C:49:TYR:CE2	1:C:53:ARG:CB	2.89	0.55
2:D:4:LEU:HD12	2:D:96:CYS:O	2.07	0.55
1:C:148:TRP:HA	1:C:193:THR:O	2.06	0.55
1:A:135:PHE:CE1	2:B:189:LEU:HB2	2.41	0.55
1:A:135:PHE:HE1	2:B:189:LEU:HB2	1.72	0.55
1:C:170:ASP:O	1:C:171:SER:C	2.44	0.55
2:D:19:LYS:HD2	2:D:82:GLN:CD	2.27	0.55
1:C:182:THR:C	1:C:184:ASP:N	2.59	0.55
2:D:38:ARG:O	2:D:45:LEU:HA	2.07	0.55
2:B:201:THR:HG22	2:B:202:VAL:O	2.07	0.55
1:A:70:ASP:C	1:A:71:TYR:CD1	2.80	0.55
2:B:99:GLY:O	2:B:110:ASP:HB3	2.07	0.55
2:B:67:ARG:N	2:B:67:ARG:HD3	2.22	0.55
1:C:67:SER:O	1:C:68:GLY:C	2.45	0.55
2:B:180:GLN:O	2:B:181:SER:HB2	2.07	0.55
1:A:48:ILE:CG1	1:A:54:LEU:HD12	2.37	0.54
2:D:13:GLN:CG	2:D:14:PRO:HD2	2.36	0.54
1:A:2:ILE:HD12	1:A:29:ILE:HD11	1.88	0.54
1:A:49:TYR:CE1	1:A:53:ARG:HB2	2.42	0.54
2:D:169:SER:HB2	2:D:193:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:ARG:O	2:D:88:SER:C	2.42	0.54
1:A:7:ILE:CD1	1:A:7:ILE:N	2.60	0.54
2:B:143:SER:CA	2:B:194:SER:OG	2.55	0.54
2:B:164:ASN:ND2	2:B:164:ASN:C	2.61	0.54
1:A:135:PHE:CE1	2:B:189:LEU:CD2	2.83	0.54
1:C:85:THR:CG2	1:C:87:PHE:CE1	2.91	0.54
2:D:91:THR:HG22	2:D:91:THR:O	2.06	0.54
1:A:39:LYS:HG3	1:A:43:SER:CB	2.37	0.54
1:A:15:LEU:CD2	1:A:80:GLU:HB3	2.25	0.54
1:A:48:ILE:HD11	1:A:54:LEU:CD1	2.38	0.54
2:B:30:SER:HB3	2:B:74:ASN:HD22	1.71	0.54
2:D:179:LEU:O	2:D:179:LEU:CD2	2.53	0.54
2:B:167:ALA:C	2:B:168:LEU:HD13	2.21	0.54
2:B:159:VAL:O	2:B:159:VAL:CG1	2.36	0.54
2:B:130:VAL:CG2	2:B:206:VAL:HG21	2.31	0.54
1:C:147:LYS:HE2	1:C:154:GLU:OE2	2.08	0.54
1:C:57:GLY:O	1:C:58:VAL:C	2.44	0.54
1:A:137:ASN:O	1:A:139:PHE:HD2	1.90	0.54
1:A:18:ARG:NH2	1:A:74:THR:CG2	2.66	0.54
1:C:2:ILE:C	1:C:3:GLN:HG3	2.28	0.54
2:B:140:THR:HG1	2:B:145:VAL:HA	1.70	0.54
2:B:100:GLY:O	2:B:101:THR:CB	2.40	0.54
2:D:167:ALA:C	2:D:170:SER:OG	2.47	0.54
1:C:29:ILE:HG12	1:C:90:GLN:HB2	1.89	0.54
2:D:93:ILE:CG2	2:D:115:GLY:HA3	2.38	0.54
2:D:179:LEU:HD12	2:D:184:TYR:CE2	2.43	0.54
2:B:51:ILE:HG21	2:B:72:ARG:HD2	1.89	0.54
1:A:4:MET:CE	1:A:4:MET:CA	2.86	0.54
2:B:133:LEU:HD13	2:B:189:LEU:CD1	2.10	0.54
1:C:83:ILE:HG13	1:C:104:LEU:O	2.08	0.54
2:D:168:LEU:N	2:D:170:SER:OG	2.40	0.54
1:C:37:GLN:HG3	1:C:86:PHE:CE1	2.42	0.53
1:A:46:LEU:HD22	1:A:47:LEU:H	1.73	0.53
2:B:87:ARG:O	2:B:120:VAL:HG11	2.08	0.53
1:C:136:LEU:HD23	1:C:144:ILE:HD11	1.90	0.53
2:D:41:PRO:HA	2:D:43:LYS:O	2.07	0.53
2:B:134:VAL:CG2	2:B:135:PRO:CD	2.86	0.53
2:D:79:LEU:HD12	2:D:80:PHE:H	1.73	0.53
2:B:216:ILE:HG23	2:B:217:LYS:N	2.22	0.53
2:B:63:THR:O	2:B:64:VAL:CG1	2.56	0.53
1:C:93:THR:HG22	1:C:94:LEU:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:TYR:HH	2:B:186:LEU:HD23	1.71	0.53
1:C:41:ASP:O	1:C:41:ASP:CG	2.47	0.53
1:C:78:LEU:O	1:C:78:LEU:CD1	2.30	0.53
2:D:33:GLY:C	2:D:34:MET:HE3	2.28	0.53
1:C:166:GLN:O	1:C:167:ASP:C	2.44	0.53
1:C:146:VAL:O	1:C:147:LYS:CB	2.50	0.53
2:D:13:GLN:CD	2:D:14:PRO:HD2	2.29	0.53
1:A:105:GLU:O	1:A:105:GLU:CG	2.46	0.53
1:C:34:ASN:OD1	2:D:106:LEU:HD21	2.08	0.53
2:B:51:ILE:HB	2:B:70:ILE:HG22	1.91	0.53
1:C:39:LYS:C	1:C:41:ASP:H	2.11	0.53
1:C:85:THR:CG2	1:C:87:PHE:CZ	2.91	0.53
1:A:2:ILE:HG23	1:A:27:GLN:H	1.73	0.53
1:C:152:GLY:O	1:C:153:SER:HB2	2.08	0.53
1:C:108:ARG:HD3	1:C:140:TYR:CB	2.39	0.53
1:C:89:GLN:HB3	1:C:98:PHE:HA	1.91	0.53
1:C:83:ILE:CG1	1:C:104:LEU:O	2.57	0.53
1:A:62:PHE:CE2	1:A:75:ILE:HD13	2.44	0.53
1:A:34:ASN:ND2	2:B:108:TYR:HB3	2.23	0.53
2:B:88:SER:N	2:B:89:GLU:OE2	2.42	0.53
2:D:9:GLY:O	2:D:18:ARG:CZ	2.58	0.53
1:A:139:PHE:O	1:A:173:TYR:N	2.42	0.52
1:A:19:VAL:O	1:A:75:ILE:N	2.42	0.52
1:A:49:TYR:CE1	1:A:53:ARG:HB3	2.43	0.52
2:B:87:ARG:CB	2:B:89:GLU:OE1	2.53	0.52
1:C:189:HIS:C	1:C:190:ASN:HD22	2.12	0.52
2:B:61:ALA:O	2:B:62:ASP:C	2.46	0.52
1:C:20:ILE:CD1	1:C:72:SER:HB2	2.40	0.52
1:A:66:GLY:HA3	1:A:71:TYR:CG	2.43	0.52
1:C:31:ASN:HD21	1:C:67:SER:HA	1.74	0.52
2:D:13:GLN:CG	2:D:14:PRO:CD	2.87	0.52
1:C:136:LEU:HD23	1:C:144:ILE:CD1	2.40	0.52
1:C:89:GLN:HG2	1:C:98:PHE:CD2	2.45	0.52
2:B:63:THR:O	2:B:64:VAL:HG12	2.10	0.52
1:C:71:TYR:N	1:C:71:TYR:HD1	2.03	0.52
1:A:77:ASN:O	1:A:78:LEU:C	2.45	0.52
2:D:199:SER:HB2	2:D:200:GLN:OE1	2.10	0.52
2:D:34:MET:HE2	2:D:98:ARG:HA	1.86	0.52
2:B:9:GLY:C	2:B:18:ARG:HH12	2.13	0.52
2:B:32:PHE:O	2:B:72:ARG:NH1	2.42	0.52
2:B:143:SER:HB3	2:B:194:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:ALA:HB2	2:D:92:ALA:HB2	1.91	0.52
2:B:98:ARG:HD2	2:B:111:TYR:HD2	1.75	0.52
1:C:32:PHE:HB3	2:D:106:LEU:CD1	2.40	0.52
2:B:150:LEU:HD13	2:B:152:LYS:HB2	1.91	0.52
2:B:144:SER:OG	2:B:193:PRO:CB	2.55	0.52
2:B:147:LEU:O	2:B:189:LEU:CD1	2.53	0.52
2:B:130:VAL:CG2	2:B:214:ASP:CB	2.88	0.52
2:D:100:GLY:O	2:D:101:THR:C	2.42	0.52
2:B:65:LYS:HD2	2:B:66:GLY:N	2.24	0.52
1:A:43:SER:O	1:A:44:LEU:C	2.47	0.52
2:D:13:GLN:HG2	2:D:14:PRO:HD3	1.90	0.52
1:C:78:LEU:CD1	1:C:79:GLU:C	2.77	0.52
2:D:126:THR:C	2:D:127:ALA:O	2.46	0.52
2:D:179:LEU:HD21	2:D:182:GLY:H	1.75	0.52
1:A:57:GLY:O	1:A:58:VAL:C	2.44	0.52
1:C:75:ILE:CG2	1:C:76:SER:N	2.71	0.52
2:D:192:VAL:HG23	2:D:192:VAL:O	2.07	0.52
1:C:150:ILE:C	1:C:152:GLY:H	2.10	0.52
2:B:20:LEU:N	2:B:81:LEU:O	2.42	0.52
1:C:125:LEU:CD2	1:C:130:ALA:HB2	2.41	0.51
1:A:39:LYS:CB	1:A:40:PRO:CD	2.88	0.51
1:A:141:PRO:HD2	1:A:198:HIS:CE1	2.45	0.51
1:A:54:LEU:HD23	1:A:58:VAL:O	2.10	0.51
1:C:36:TYR:CE1	1:C:89:GLN:HG2	2.42	0.51
1:A:108:ARG:CZ	1:A:172:THR:CG2	2.86	0.51
1:C:9:SER:OG	1:C:10:SER:N	2.43	0.51
2:B:33:GLY:HA2	2:B:72:ARG:NH2	2.23	0.51
2:B:60:TYR:CD2	2:B:65:LYS:CD	2.79	0.51
1:A:163:TRP:CE2	1:A:175:MET:HG3	2.45	0.51
1:A:62:PHE:CE2	1:A:75:ILE:CD1	2.94	0.51
1:C:160:LEU:HD22	2:D:178:VAL:CG2	2.27	0.51
2:B:28:THR:O	2:B:29:PHE:C	2.49	0.51
1:C:164:THR:CG2	2:D:175:VAL:HG23	2.40	0.51
1:C:83:ILE:O	1:C:84:ALA:HB2	2.09	0.51
1:C:32:PHE:HB3	2:D:106:LEU:HD13	1.91	0.51
2:D:125:THR:CG2	2:D:126:THR:H	2.20	0.51
2:D:34:MET:CB	2:D:79:LEU:HD22	2.40	0.51
1:C:21:ILE:HG22	1:C:22:SER:N	2.21	0.51
1:A:39:LYS:HG3	1:A:43:SER:HB3	1.93	0.51
1:C:38:GLN:O	1:C:84:ALA:HB1	2.10	0.51
2:D:30:SER:HA	2:D:74:ASN:HD22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HA	1:A:140:TYR:HH	1.76	0.51
1:A:34:ASN:OD1	1:A:49:TYR:HA	2.11	0.51
2:B:2:VAL:HG11	2:B:111:TYR:CE1	2.46	0.51
2:D:177:SER:HA	2:D:185:SER:O	2.11	0.51
1:A:111:ALA:N	1:A:200:THR:HG21	2.25	0.51
1:A:136:LEU:HD21	1:A:146:VAL:CG2	2.41	0.51
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.93	0.51
2:D:130:VAL:CG1	2:D:216:ILE:CG2	2.88	0.51
2:D:130:VAL:HG12	2:D:216:ILE:HG21	1.93	0.51
1:C:118:PHE:CE1	2:D:135:PRO:HD3	2.46	0.51
1:A:136:LEU:HD21	1:A:146:VAL:HG21	1.93	0.51
2:D:169:SER:CB	2:D:193:PRO:CD	2.87	0.51
2:D:146:THR:OG1	2:D:191:THR:CG2	2.56	0.51
1:A:150:ILE:HG21	1:A:189:HIS:CG	2.38	0.51
1:C:182:THR:O	1:C:183:LYS:C	2.46	0.51
1:A:80:GLU:O	1:A:83:ILE:CG2	2.58	0.50
1:A:25:ALA:HB1	1:A:27:GLN:O	2.11	0.50
1:A:31:ASN:CA	1:A:71:TYR:OH	2.53	0.50
2:B:58:ILE:HG23	2:B:70:ILE:HB	1.93	0.50
1:A:156:GLN:O	1:A:157:ASN:C	2.47	0.50
2:B:22:CYS:HB3	2:B:79:LEU:HB3	1.92	0.50
1:A:18:ARG:CA	1:A:75:ILE:O	2.37	0.50
1:C:139:PHE:N	1:C:139:PHE:CD2	2.78	0.50
2:D:100:GLY:O	2:D:101:THR:CB	2.41	0.50
1:C:159:VAL:HA	1:C:178:THR:O	2.10	0.50
1:C:85:THR:HG21	1:C:87:PHE:CZ	2.46	0.50
2:B:17:SER:HA	2:B:83:MET:O	2.11	0.50
2:D:75:PRO:CD	2:D:77:ASN:OD1	2.58	0.50
1:C:166:GLN:CG	1:C:171:SER:CA	2.83	0.50
2:D:73:ASP:OD1	2:D:77:ASN:OD1	2.29	0.50
2:D:41:PRO:O	2:D:42:GLU:HB3	2.11	0.50
1:C:90:GLN:OE1	1:C:92:LYS:HB3	2.11	0.50
2:B:91:THR:HA	2:B:118:LEU:O	2.11	0.50
1:C:49:TYR:CE2	1:C:53:ARG:HB3	2.46	0.50
1:A:130:ALA:CA	1:A:181:LEU:O	2.59	0.50
1:A:108:ARG:NE	1:A:172:THR:HG23	2.26	0.50
1:C:81:GLU:H	1:C:81:GLU:CD	2.14	0.50
2:D:13:GLN:HG2	2:D:14:PRO:HD2	1.93	0.50
1:C:120:PRO:HG3	1:C:132:VAL:HG22	1.94	0.50
1:A:19:VAL:O	1:A:74:THR:HA	2.12	0.50
2:B:52:SER:O	2:B:72:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PHE:HE1	1:C:141:PRO:O	1.93	0.50
2:D:174:THR:HG22	2:D:175:VAL:O	2.12	0.50
2:D:42:GLU:HG2	2:D:42:GLU:O	2.12	0.50
1:C:78:LEU:HD12	1:C:79:GLU:C	2.32	0.50
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.94	0.50
2:D:169:SER:CB	2:D:193:PRO:CG	2.90	0.50
2:B:159:VAL:HG13	2:B:160:THR:N	2.12	0.50
1:A:49:TYR:CG	1:A:53:ARG:HB2	2.47	0.49
2:B:2:VAL:CG1	2:B:111:TYR:CD1	2.95	0.49
1:A:133:VAL:HG12	1:A:134:CYS:N	2.26	0.49
1:C:5:THR:HB	1:C:24:ARG:HG2	1.93	0.49
1:A:13:VAL:HG21	1:A:19:VAL:HG22	1.94	0.49
1:C:146:VAL:HG21	1:C:175:MET:HE1	1.93	0.49
1:C:21:ILE:CG2	1:C:22:SER:N	2.72	0.49
1:A:19:VAL:HG21	1:A:78:LEU:CD1	2.41	0.49
1:A:135:PHE:HZ	2:B:173:ARG:HB2	1.76	0.49
1:C:8:THR:HG21	1:C:11:LEU:HD22	1.94	0.49
1:A:46:LEU:HD22	1:A:47:LEU:N	2.28	0.49
2:B:164:ASN:HD22	2:B:165:TYR:C	2.14	0.49
2:D:151:VAL:HG13	2:D:186:LEU:HD12	1.92	0.49
1:C:166:GLN:NE2	1:C:171:SER:CB	2.74	0.49
1:C:136:LEU:HD21	1:C:196:ALA:HB2	1.94	0.49
2:B:128:PRO:CD	2:B:212:LYS:HD3	2.42	0.49
1:A:90:GLN:NE2	1:A:93:THR:O	2.44	0.49
2:B:103:THR:O	2:B:106:LEU:CB	2.61	0.49
1:C:32:PHE:HD1	1:C:92:LYS:HD3	1.78	0.49
2:B:130:VAL:CG2	2:B:214:ASP:HB3	2.42	0.49
2:B:130:VAL:HG23	2:B:214:ASP:HB2	1.94	0.49
1:A:135:PHE:HD1	2:B:189:LEU:HG	1.71	0.49
1:C:13:VAL:HG21	1:C:19:VAL:HG22	1.95	0.49
1:C:66:GLY:HA3	1:C:71:TYR:CB	2.42	0.49
2:D:137:CYS:HA	2:D:197:TRP:HH2	1.77	0.49
2:D:146:THR:HG22	2:D:189:LEU:HB3	1.95	0.49
2:B:87:ARG:CZ	2:B:89:GLU:HB2	2.42	0.49
2:B:134:VAL:HG22	2:B:135:PRO:N	2.26	0.49
1:C:37:GLN:HG3	1:C:86:PHE:HE1	1.78	0.49
1:A:48:ILE:CD1	1:A:54:LEU:HD12	2.43	0.49
2:D:11:LEU:HD22	2:D:119:ILE:HG22	1.81	0.49
2:D:104:ARG:O	2:D:105:SER:HB3	2.07	0.49
2:B:29:PHE:HB2	2:B:77:ASN:ND2	2.27	0.49
1:C:20:ILE:HD11	1:C:72:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:LEU:HD21	2:D:119:ILE:HG22	1.68	0.48
2:B:52:SER:CB	2:B:57:SER:H	2.25	0.48
2:B:27:PHE:HD2	2:B:28:THR:H	1.59	0.48
2:B:104:ARG:C	2:B:106:LEU:H	2.16	0.48
2:D:166:GLY:O	2:D:170:SER:OG	2.31	0.48
2:D:132:PRO:O	2:D:132:PRO:CG	2.61	0.48
2:D:162:LYS:N	2:D:205:ASN:O	2.38	0.48
1:A:2:ILE:HA	1:A:26:SER:OG	2.12	0.48
1:C:133:VAL:CG2	2:D:133:LEU:CD2	2.86	0.48
2:D:168:LEU:O	2:D:169:SER:CB	2.60	0.48
2:D:112:TRP:HD1	2:D:112:TRP:H	1.62	0.48
2:D:163:TRP:HE1	2:D:188:SER:HG	0.50	0.48
1:A:89:GLN:HA	1:A:97:THR:O	2.13	0.48
1:C:32:PHE:CD1	1:C:92:LYS:HD3	2.48	0.48
1:C:29:ILE:CG1	1:C:90:GLN:HB2	2.43	0.48
1:A:79:GLU:O	1:A:80:GLU:C	2.52	0.48
2:B:14:PRO:HD3	2:B:121:SER:O	2.13	0.48
2:B:135:PRO:HD3	2:B:147:LEU:HD12	1.96	0.48
1:C:66:GLY:HA3	1:C:71:TYR:CG	2.49	0.48
2:D:147:LEU:N	2:D:190:VAL:O	2.43	0.48
1:C:183:LYS:O	1:C:187:GLU:HG3	2.13	0.48
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.46	0.48
1:A:34:ASN:HD21	2:B:108:TYR:HB3	1.79	0.48
2:B:90:ASP:O	2:B:91:THR:C	2.47	0.48
1:C:81:GLU:HG2	1:C:81:GLU:O	2.13	0.48
1:A:105:GLU:C	1:A:106:ILE:HD13	2.29	0.48
1:A:110:ASP:HB3	1:A:200:THR:CG2	2.44	0.48
2:D:17:SER:HA	2:D:86:LEU:CD1	2.44	0.48
1:A:125:LEU:O	1:A:126:THR:C	2.51	0.48
1:A:135:PHE:HZ	2:B:173:ARG:HG3	1.79	0.48
1:A:24:ARG:HA	1:A:69:THR:O	2.13	0.48
1:C:124:GLN:CD	1:C:130:ALA:HA	2.34	0.48
1:C:150:ILE:HG23	1:C:192:TYR:CE1	2.48	0.48
1:C:59:PRO:O	1:C:62:PHE:HD1	1.97	0.48
2:B:73:ASP:OD1	2:B:76:LYS:HB2	2.14	0.48
1:A:36:TYR:CE1	1:A:89:GLN:HG2	2.34	0.48
2:D:73:ASP:O	2:D:77:ASN:CG	2.52	0.47
2:D:130:VAL:CG1	2:D:216:ILE:HG21	2.43	0.47
1:C:125:LEU:HD23	1:C:129:GLY:O	2.13	0.47
1:C:32:PHE:CD2	2:D:106:LEU:HD13	2.49	0.47
2:D:34:MET:N	2:D:51:ILE:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:SER:C	1:C:58:VAL:N	2.67	0.47
1:C:94:LEU:CD1	1:C:94:LEU:N	2.77	0.47
1:C:93:THR:O	1:C:96:TYR:CE2	2.67	0.47
1:C:71:TYR:C	1:C:72:SER:OG	2.34	0.47
1:A:115:VAL:HG21	1:A:205:ILE:CD1	2.43	0.47
1:A:50:TYR:CZ	2:B:104:ARG:HD2	2.49	0.47
2:D:19:LYS:CD	2:D:82:GLN:HB2	2.37	0.47
1:C:54:LEU:HD11	1:C:58:VAL:HG12	1.96	0.47
1:C:83:ILE:HA	1:C:104:LEU:HD23	1.95	0.47
2:D:11:LEU:HD23	2:D:119:ILE:HG22	1.52	0.47
2:B:217:LYS:CE	2:B:217:LYS:CA	2.87	0.47
1:C:32:PHE:HE1	1:C:92:LYS:HZ3	1.58	0.47
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.95	0.47
2:B:148:GLY:CA	2:B:189:LEU:CD1	2.90	0.47
1:C:116:SER:N	1:C:135:PHE:O	2.44	0.47
2:B:2:VAL:HG11	2:B:111:TYR:CZ	2.49	0.47
2:B:152:LYS:C	2:B:152:LYS:HD3	2.34	0.47
1:C:167:ASP:OD2	1:C:168:SER:N	2.48	0.47
1:C:47:LEU:O	1:C:58:VAL:HG21	2.15	0.47
2:D:147:LEU:HA	2:D:147:LEU:HD13	1.45	0.47
1:C:9:SER:O	1:C:103:LYS:O	2.33	0.47
2:D:179:LEU:HD11	2:D:182:GLY:O	2.15	0.47
1:A:81:GLU:CD	1:A:81:GLU:N	2.67	0.47
2:D:123:ALA:HB3	2:D:155:PHE:CE2	2.50	0.47
1:A:136:LEU:CD1	1:A:146:VAL:HG21	2.42	0.47
1:A:29:ILE:HD12	1:A:29:ILE:HA	1.32	0.47
2:D:49:ALA:HB1	2:D:70:ILE:HG12	1.97	0.47
1:C:139:PHE:CD1	1:C:141:PRO:O	2.68	0.47
1:C:118:PHE:CD1	2:D:135:PRO:HD3	2.49	0.47
1:C:163:TRP:CH2	1:C:175:MET:HE2	2.50	0.46
2:D:9:GLY:O	2:D:18:ARG:NH1	2.48	0.46
1:A:65:TRP:HD1	1:A:72:SER:O	1.97	0.46
1:A:116:SER:HB3	1:A:118:PHE:CE2	2.50	0.46
1:A:57:GLY:HA2	2:D:214:ASP:OD1	2.15	0.46
1:C:144:ILE:HG13	1:C:198:HIS:HD2	1.80	0.46
1:C:36:TYR:HE2	1:C:46:LEU:HD23	1.72	0.46
2:B:67:ARG:CG	2:B:67:ARG:NH2	2.72	0.46
2:D:53:SER:HA	2:D:72:ARG:CZ	2.45	0.46
1:C:33:LEU:HD23	1:C:33:LEU:C	2.36	0.46
2:B:130:VAL:HG12	2:B:131:TYR:N	2.30	0.46
2:B:17:SER:HA	2:B:86:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLY:O	2:D:18:ARG:HD2	2.15	0.46
1:C:39:LYS:O	1:C:41:ASP:N	2.49	0.46
2:D:155:PHE:CD2	2:D:156:PRO:N	2.83	0.46
1:A:115:VAL:CG1	1:A:116:SER:N	2.79	0.46
2:D:168:LEU:HA	2:D:168:LEU:HD12	1.60	0.46
1:A:73:LEU:CD2	1:A:86:PHE:CD1	2.98	0.46
2:B:3:GLN:N	2:B:25:SER:O	2.43	0.46
1:C:24:ARG:NH1	1:C:69:THR:OG1	2.47	0.46
2:B:133:LEU:HD12	2:B:148:GLY:CA	2.18	0.46
1:A:25:ALA:HB3	1:A:69:THR:HB	1.98	0.46
1:C:4:MET:HE1	1:C:90:GLN:HG2	1.91	0.46
2:D:92:ALA:O	2:D:117:THR:HA	2.15	0.46
2:B:6:GLU:HB2	2:B:116:ALA:HB2	1.91	0.46
2:B:29:PHE:O	2:B:30:SER:C	2.52	0.46
1:A:33:LEU:O	1:A:51:THR:N	2.49	0.46
1:A:48:ILE:HD11	1:A:54:LEU:HD11	1.98	0.46
2:B:91:THR:O	2:B:92:ALA:CB	2.58	0.46
2:B:64:VAL:O	2:B:67:ARG:N	2.46	0.46
2:D:6:GLU:OE2	2:D:114:GLN:OE1	2.33	0.46
1:C:119:PRO:HA	1:C:120:PRO:HD3	1.87	0.46
1:A:174:SER:OG	2:B:173:ARG:HD2	2.15	0.46
1:C:61:ARG:HD3	1:C:77:ASN:O	2.16	0.46
1:C:126:THR:C	1:C:128:GLY:N	2.69	0.46
1:C:124:GLN:CD	1:C:131:SER:N	2.68	0.46
2:B:146:THR:HA	2:B:191:THR:CG2	2.40	0.46
1:C:149:LYS:O	1:C:193:THR:N	2.39	0.46
1:A:123:GLU:O	1:A:126:THR:HB	2.14	0.46
1:A:135:PHE:CE1	2:B:189:LEU:CG	2.99	0.46
2:D:38:ARG:HD3	2:D:48:VAL:HG21	1.98	0.46
1:A:205:ILE:HD12	1:A:205:ILE:HG23	1.71	0.46
1:A:17:ASP:OD2	1:A:78:LEU:HB2	2.15	0.46
1:A:29:ILE:O	1:A:32:PHE:HD1	1.98	0.46
1:C:58:VAL:HA	1:C:59:PRO:HD3	1.63	0.46
2:B:68:PHE:CD1	2:B:68:PHE:N	2.84	0.46
2:B:74:ASN:HB2	2:B:75:PRO:CD	2.46	0.46
1:C:16:GLY:O	1:C:77:ASN:HA	2.15	0.46
1:A:28:ASP:C	1:A:29:ILE:CD1	2.84	0.46
1:C:108:ARG:C	1:C:140:TYR:CE1	2.90	0.46
2:D:19:LYS:HD2	2:D:82:GLN:CB	2.38	0.46
2:B:61:ALA:O	2:B:64:VAL:N	2.39	0.46
2:B:64:VAL:HG23	2:B:68:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:OD2	1:A:172:THR:OG1	2.28	0.46
2:D:216:ILE:HG12	2:D:217:LYS:CA	2.41	0.45
1:A:147:LYS:HE2	1:A:147:LYS:HB3	1.28	0.45
1:A:38:GLN:HB2	1:A:44:LEU:HG	1.98	0.45
2:D:52:SER:O	2:D:53:SER:C	2.50	0.45
1:C:54:LEU:HG	1:C:58:VAL:HB	1.98	0.45
2:B:63:THR:C	2:B:64:VAL:HG13	2.37	0.45
1:A:186:TYR:O	1:A:187:GLU:C	2.52	0.45
1:A:137:ASN:HB3	1:A:138:ASN:OD1	2.15	0.45
1:A:79:GLU:C	1:A:81:GLU:H	2.20	0.45
1:A:48:ILE:HG12	1:A:54:LEU:HA	1.99	0.45
1:C:126:THR:O	1:C:127:SER:C	2.51	0.45
1:C:150:ILE:C	1:C:152:GLY:N	2.66	0.45
1:C:98:PHE:CZ	2:D:109:PHE:HE2	2.34	0.45
1:A:108:ARG:CG	1:A:108:ARG:HH21	2.21	0.45
1:A:195:GLU:HG3	1:A:204:PRO:HB3	1.98	0.45
2:B:17:SER:CB	2:B:84:THR:HA	2.44	0.45
2:D:18:ARG:HG3	2:D:118:LEU:CD1	2.42	0.45
1:C:13:VAL:HG23	1:C:17:ASP:OD2	2.16	0.45
2:B:41:PRO:C	2:B:43:LYS:N	2.62	0.45
1:C:12:SER:HB3	1:C:107:LYS:CB	2.43	0.45
2:D:98:ARG:HD3	2:D:110:ASP:HB3	1.99	0.45
2:B:212:LYS:HE3	2:B:213:THR:C	2.37	0.45
2:B:146:THR:OG1	2:B:191:THR:HG22	2.17	0.45
1:C:130:ALA:O	1:C:180:THR:HG23	2.17	0.45
1:C:92:LYS:CG	1:C:93:THR:OG1	2.36	0.45
2:B:117:THR:OG1	2:B:118:LEU:N	2.49	0.45
1:A:155:ARG:HD2	1:A:155:ARG:HA	1.54	0.45
2:B:146:THR:OG1	2:B:191:THR:CG2	2.65	0.45
2:D:39:GLN:O	2:D:39:GLN:CG	2.64	0.45
1:A:33:LEU:HD13	1:A:71:TYR:CD2	2.47	0.45
1:A:60:SER:O	1:C:126:THR:CG2	2.56	0.45
1:C:94:LEU:HD21	2:D:59:ASN:HB3	1.98	0.45
1:C:108:ARG:N	1:C:140:TYR:OH	2.45	0.45
2:B:52:SER:HB2	2:B:57:SER:H	1.82	0.45
1:A:131:SER:HG	1:A:180:THR:HG23	1.80	0.45
2:D:97:THR:CG2	2:D:112:TRP:HA	2.38	0.45
1:C:108:ARG:HG2	1:C:140:TYR:CG	2.46	0.45
1:C:50:TYR:CE2	2:D:104:ARG:NH1	2.84	0.45
2:D:17:SER:HB2	2:D:83:MET:O	2.17	0.45
2:B:212:LYS:O	2:B:212:LYS:HG3	2.11	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ASN:O	2:B:77:ASN:N	2.45	0.45
1:A:135:PHE:HZ	2:B:173:ARG:CB	2.30	0.45
2:D:24:ALA:HB3	2:D:77:ASN:O	2.17	0.45
2:D:204:CYS:SG	2:D:216:ILE:HG22	2.55	0.45
1:C:106:ILE:HG21	1:C:171:SER:HG	1.75	0.45
2:D:209:PRO:O	2:D:211:SER:N	2.40	0.45
1:C:85:THR:HA	1:C:102:THR:O	2.16	0.44
1:A:111:ALA:O	1:A:200:THR:HG21	2.17	0.44
1:C:12:SER:OG	1:C:105:GLU:HB2	2.09	0.44
1:C:59:PRO:O	1:C:62:PHE:HB2	2.18	0.44
1:C:19:VAL:HG21	1:C:78:LEU:HD22	1.99	0.44
1:A:144:ILE:HG23	1:A:144:ILE:HD13	1.61	0.44
1:A:32:PHE:CD2	2:B:106:LEU:HD12	2.40	0.44
2:D:137:CYS:HA	2:D:197:TRP:CZ3	2.52	0.44
2:D:147:LEU:HD11	2:D:217:LYS:HZ3	1.82	0.44
1:C:9:SER:CA	1:C:102:THR:HA	2.42	0.44
2:B:106:LEU:HA	2:B:106:LEU:HD12	1.75	0.44
2:B:2:VAL:HG12	2:B:111:TYR:CD1	2.52	0.44
2:B:130:VAL:CG2	2:B:214:ASP:HB2	2.47	0.44
2:D:6:GLU:CD	2:D:115:GLY:H	2.21	0.44
1:A:7:ILE:O	1:A:8:THR:CB	2.65	0.44
2:D:97:THR:HG22	2:D:111:TYR:O	2.17	0.44
1:C:39:LYS:C	1:C:41:ASP:N	2.71	0.44
2:B:146:THR:CB	2:B:191:THR:HG22	2.47	0.44
2:B:162:LYS:HA	2:B:162:LYS:HD2	1.26	0.44
2:B:108:TYR:C	2:B:109:PHE:CD1	2.90	0.44
1:C:32:PHE:CB	2:D:106:LEU:HD13	2.47	0.44
2:D:58:ILE:HG21	2:D:60:TYR:CE2	2.52	0.44
1:C:98:PHE:HZ	2:D:109:PHE:HE2	1.64	0.44
2:B:143:SER:CB	2:B:194:SER:OG	2.65	0.44
1:A:57:GLY:CA	2:D:214:ASP:OD1	2.65	0.44
2:D:50:TYR:N	2:D:70:ILE:CD1	2.81	0.44
1:A:47:LEU:HD23	1:A:58:VAL:HG21	2.00	0.44
2:B:2:VAL:CG1	2:B:2:VAL:O	2.63	0.44
2:D:145:VAL:HG11	2:D:197:TRP:CZ3	2.52	0.44
2:B:61:ALA:C	2:B:63:THR:N	2.70	0.44
2:B:138:SER:O	2:B:145:VAL:CG2	2.61	0.44
2:B:48:VAL:CG2	2:B:64:VAL:HG11	2.48	0.44
2:B:139:ASP:O	2:B:145:VAL:HG12	2.17	0.44
2:D:165:TYR:C	2:D:165:TYR:HD1	2.21	0.44
2:D:126:THR:HG21	2:D:183:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HD12	1:A:144:ILE:HG21	1.60	0.44
2:D:33:GLY:HA3	2:D:50:TYR:HE2	1.83	0.44
1:A:28:ASP:C	1:A:29:ILE:HD12	2.38	0.44
1:A:112:ALA:HB1	1:A:113:PRO:HD2	1.99	0.44
2:D:70:ILE:HD13	2:D:70:ILE:HG21	1.37	0.43
1:C:167:ASP:O	1:C:168:SER:C	2.56	0.43
1:C:190:ASN:O	1:C:192:TYR:HD2	1.94	0.43
1:C:85:THR:HG23	1:C:87:PHE:CZ	2.52	0.43
2:B:217:LYS:HD3	2:B:217:LYS:O	2.18	0.43
2:B:17:SER:HB3	2:B:84:THR:CA	2.45	0.43
2:B:51:ILE:HB	2:B:70:ILE:CG2	2.48	0.43
2:D:20:LEU:HD13	2:D:83:MET:CE	2.48	0.43
2:B:104:ARG:O	2:B:105:SER:C	2.52	0.43
2:B:110:ASP:OD2	2:B:111:TYR:CD2	2.68	0.43
2:D:146:THR:HA	2:D:191:THR:HA	1.99	0.43
2:B:11:LEU:HD23	2:B:12:VAL:N	2.33	0.43
1:C:169:LYS:NZ	1:C:170:ASP:HB3	2.33	0.43
1:A:148:TRP:CZ2	1:A:194:CYS:HB2	2.53	0.43
2:D:20:LEU:N	2:D:81:LEU:O	2.35	0.43
2:D:94:TYR:O	2:D:115:GLY:HA2	2.19	0.43
1:C:65:TRP:HZ2	1:C:74:THR:CB	2.30	0.43
1:C:61:ARG:HB3	1:C:75:ILE:HG23	1.99	0.43
2:B:2:VAL:HG11	2:B:111:TYR:CD1	2.54	0.43
2:B:68:PHE:CD2	2:B:83:MET:HG2	2.48	0.43
1:A:7:ILE:O	1:A:8:THR:HB	2.19	0.43
1:A:182:THR:HG22	1:A:184:ASP:N	2.33	0.43
1:C:41:ASP:O	1:C:41:ASP:OD1	2.35	0.43
1:A:135:PHE:HD1	2:B:189:LEU:CG	2.25	0.43
2:B:130:VAL:HG23	2:B:214:ASP:HB3	1.98	0.43
1:C:56:SER:O	1:C:57:GLY:C	2.49	0.43
1:C:182:THR:HG22	1:C:184:ASP:H	1.83	0.43
1:A:151:ASP:OD2	1:A:191:SER:N	2.43	0.43
2:D:45:LEU:HA	2:D:45:LEU:HD23	1.56	0.43
2:D:197:TRP:C	2:D:199:SER:H	2.21	0.43
1:C:144:ILE:CG2	1:C:175:MET:HE3	2.48	0.43
1:A:22:SER:HA	1:A:72:SER:CA	2.48	0.43
2:D:100:GLY:HA3	2:D:108:TYR:CZ	2.54	0.43
2:B:209:PRO:O	2:B:211:SER:N	2.42	0.43
2:D:129:SER:O	2:D:152:LYS:N	2.48	0.43
2:B:63:THR:C	2:B:64:VAL:CG1	2.86	0.43
2:D:100:GLY:C	2:D:102:GLY:N	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:CG2	1:A:189:HIS:CG	2.99	0.43
1:C:106:ILE:HB	1:C:166:GLN:CD	2.38	0.43
1:C:184:ASP:O	1:C:185:GLU:C	2.54	0.43
2:D:194:SER:C	2:D:196:THR:N	2.71	0.43
1:C:90:GLN:OE1	1:C:90:GLN:C	2.58	0.43
1:A:135:PHE:CZ	2:B:173:ARG:HG3	2.54	0.42
2:D:150:LEU:CD1	2:D:152:LYS:HB2	2.44	0.42
2:D:13:GLN:HA	2:D:14:PRO:HD3	1.66	0.42
1:C:199:LYS:HG2	1:C:199:LYS:O	2.16	0.42
1:A:125:LEU:HA	1:A:129:GLY:O	2.19	0.42
2:B:2:VAL:CG1	2:B:111:TYR:CE1	3.02	0.42
1:C:91:GLY:CA	2:D:107:TYR:HB2	2.49	0.42
1:A:59:PRO:HD2	1:A:59:PRO:O	2.18	0.42
1:C:181:LEU:HD12	1:C:186:TYR:HD2	1.84	0.42
1:A:47:LEU:HD23	1:A:58:VAL:CG2	2.49	0.42
2:D:202:VAL:O	2:D:203:ILE:HG13	2.19	0.42
2:D:212:LYS:HE3	2:D:214:ASP:CB	2.49	0.42
2:B:22:CYS:O	2:B:78:THR:CA	2.66	0.42
2:B:203:ILE:CG2	2:B:215:LEU:HD11	2.47	0.42
2:B:70:ILE:HG23	2:B:70:ILE:HD13	1.19	0.42
2:D:1:ASP:O	2:D:1:ASP:OD1	2.37	0.42
1:C:110:ASP:OD2	1:C:199:LYS:CE	2.67	0.42
2:B:45:LEU:HA	2:B:45:LEU:HD23	1.75	0.42
1:A:107:LYS:HA	1:A:140:TYR:CZ	2.55	0.42
2:B:166:GLY:O	2:B:168:LEU:HD12	2.05	0.42
2:B:177:SER:HG	2:B:184:TYR:HD1	1.67	0.42
2:B:38:ARG:O	2:B:46:GLU:N	2.44	0.42
2:D:194:SER:O	2:D:195:SER:C	2.53	0.42
2:B:60:TYR:HH	2:B:69:THR:HA	1.74	0.42
1:A:156:GLN:HB3	1:A:157:ASN:H	1.67	0.42
2:B:166:GLY:C	2:B:168:LEU:HD12	2.40	0.42
2:B:91:THR:CB	2:B:120:VAL:H	2.22	0.42
2:D:17:SER:CB	2:D:83:MET:O	2.68	0.42
2:D:17:SER:HA	2:D:86:LEU:HD11	2.02	0.42
2:B:3:GLN:C	2:B:4:LEU:HD23	2.40	0.42
1:A:173:TYR:H	1:A:173:TYR:HD2	1.67	0.42
2:B:163:TRP:CE3	2:B:203:ILE:O	2.72	0.42
1:A:34:ASN:HD22	1:A:89:GLN:HE21	1.67	0.42
2:D:171:GLY:O	2:D:190:VAL:HG23	2.20	0.42
1:C:29:ILE:CG1	1:C:90:GLN:CB	2.93	0.42
1:C:136:LEU:O	1:C:175:MET:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TRP:CH2	1:A:194:CYS:HB2	2.54	0.42
2:D:101:THR:HG22	2:D:101:THR:O	2.20	0.42
2:D:125:THR:HG23	2:D:155:PHE:O	2.19	0.42
1:A:49:TYR:CE2	1:A:53:ARG:CB	3.03	0.42
2:D:196:THR:HA	2:D:200:GLN:OE1	2.20	0.42
2:D:51:ILE:O	2:D:51:ILE:HG23	2.19	0.42
2:B:60:TYR:OH	2:B:70:ILE:N	2.44	0.42
2:D:92:ALA:O	2:D:117:THR:CA	2.68	0.42
1:A:162:SER:C	1:A:163:TRP:CE3	2.93	0.42
1:C:46:LEU:CD1	1:C:49:TYR:HD1	2.33	0.42
2:B:20:LEU:HD21	2:B:94:TYR:CG	2.55	0.42
1:A:155:ARG:NE	1:A:157:ASN:O	2.53	0.42
2:D:27:PHE:CE2	2:D:32:PHE:CE1	3.08	0.42
2:B:37:VAL:HG11	2:B:112:TRP:HH2	1.84	0.42
1:A:197:THR:O	1:A:198:HIS:CB	2.65	0.41
2:B:174:THR:O	2:B:175:VAL:C	2.56	0.41
2:B:17:SER:CA	2:B:86:LEU:HD12	2.50	0.41
1:A:6:GLN:NE2	1:A:86:PHE:O	2.48	0.41
1:C:39:LYS:HB2	1:C:41:ASP:O	2.20	0.41
1:A:121:SER:O	1:A:125:LEU:CG	2.63	0.41
1:C:93:THR:O	1:C:94:LEU:HD12	2.19	0.41
1:C:93:THR:O	1:C:96:TYR:CD2	2.73	0.41
1:C:53:ARG:HD3	1:C:53:ARG:HA	1.81	0.41
2:B:50:TYR:HD1	2:B:59:ASN:HB3	1.85	0.41
2:B:164:ASN:HD22	2:B:164:ASN:C	2.24	0.41
2:D:72:ARG:CD	2:D:74:ASN:OD1	2.68	0.41
1:A:3:GLN:H	1:A:26:SER:HB3	1.85	0.41
2:B:70:ILE:HD12	2:B:70:ILE:HG21	1.41	0.41
1:C:7:ILE:O	1:C:8:THR:CB	2.68	0.41
1:A:149:LYS:C	1:A:153:SER:O	2.59	0.41
1:A:88:CYS:SG	1:A:99:GLY:HA3	2.60	0.41
1:C:66:GLY:HA3	1:C:71:TYR:HB3	2.03	0.41
2:D:148:GLY:HA3	2:D:189:LEU:HD13	2.03	0.41
2:D:192:VAL:HA	2:D:193:PRO:HD3	1.59	0.41
2:D:203:ILE:HG23	2:D:215:LEU:HG	2.03	0.41
1:A:65:TRP:CD1	1:A:72:SER:O	2.74	0.41
1:A:42:GLY:O	1:A:43:SER:C	2.58	0.41
1:A:31:ASN:HA	1:A:71:TYR:CZ	2.54	0.41
1:C:29:ILE:HD12	1:C:29:ILE:HA	1.38	0.41
1:C:196:ALA:H	1:C:205:ILE:HG22	1.86	0.41
1:C:115:VAL:CG2	1:C:205:ILE:CG2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLN:HB3	1:C:98:PHE:CG	2.56	0.41
2:B:51:ILE:HG12	2:B:52:SER:N	2.36	0.41
2:D:67:ARG:NH2	2:D:90:ASP:OD1	2.49	0.41
2:D:192:VAL:CG2	2:D:192:VAL:O	2.65	0.41
1:C:147:LYS:O	1:C:195:GLU:N	2.51	0.41
2:D:10:GLY:CA	2:D:18:ARG:HH12	2.12	0.41
2:D:165:TYR:CD1	2:D:165:TYR:C	2.93	0.41
2:D:123:ALA:HB3	2:D:155:PHE:CZ	2.56	0.41
2:D:39:GLN:HB2	2:D:45:LEU:CD2	2.51	0.41
2:D:93:ILE:CG1	2:D:117:THR:HB	2.47	0.41
2:B:128:PRO:HD2	2:B:212:LYS:HG2	2.02	0.41
1:A:131:SER:OG	1:A:180:THR:HA	2.21	0.41
2:D:111:TYR:CE1	2:D:112:TRP:O	2.73	0.41
1:C:183:LYS:CG	1:C:183:LYS:O	2.68	0.41
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.54	0.41
2:B:39:GLN:O	2:B:93:ILE:HD12	2.20	0.41
1:C:61:ARG:CB	1:C:75:ILE:HG23	2.51	0.41
2:D:179:LEU:HD23	2:D:180:GLN:HA	2.03	0.41
1:A:175:MET:SD	1:A:175:MET:C	2.99	0.41
1:A:48:ILE:HD11	1:A:54:LEU:HD12	2.03	0.41
1:C:91:GLY:C	2:D:106:LEU:HD12	2.40	0.41
1:C:106:ILE:HG22	1:C:166:GLN:NE2	2.34	0.41
1:C:106:ILE:HB	1:C:166:GLN:NE2	2.36	0.41
2:B:21:SER:HA	2:B:80:PHE:HA	2.02	0.41
2:B:20:LEU:O	2:B:80:PHE:HA	2.20	0.41
2:B:19:LYS:HA	2:B:81:LEU:O	2.21	0.41
1:A:133:VAL:CG1	1:A:134:CYS:N	2.84	0.41
2:B:154:TYR:N	2:B:154:TYR:CD1	2.88	0.41
1:A:112:ALA:CB	1:A:113:PRO:HD2	2.49	0.41
2:D:126:THR:HG22	2:D:127:ALA:O	2.21	0.41
1:C:106:ILE:HB	1:C:166:GLN:OE1	2.21	0.41
1:C:166:GLN:O	1:C:168:SER:N	2.54	0.41
1:C:35:TRP:CE3	1:C:73:LEU:HD23	2.56	0.41
2:B:98:ARG:NH1	2:B:111:TYR:CE2	2.90	0.40
2:B:65:LYS:HA	2:B:65:LYS:HD2	1.61	0.40
2:B:71:SER:HB2	2:B:80:PHE:HB2	2.02	0.40
2:D:17:SER:HB3	2:D:84:THR:CA	2.47	0.40
1:C:10:SER:CA	1:C:103:LYS:O	2.67	0.40
2:D:129:SER:O	2:D:151:VAL:HA	2.21	0.40
2:D:86:LEU:HD22	2:D:118:LEU:CD2	2.50	0.40
1:C:41:ASP:O	1:C:42:GLY:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:HB3	2:B:79:LEU:HD22	2.04	0.40
1:A:137:ASN:OD1	2:B:173:ARG:HG3	2.22	0.40
1:C:11:LEU:O	1:C:104:LEU:HA	2.21	0.40
1:A:79:GLU:C	1:A:81:GLU:N	2.71	0.40
2:D:136:GLY:O	2:D:137:CYS:SG	2.80	0.40
1:C:92:LYS:C	1:C:93:THR:OG1	2.58	0.40
2:B:64:VAL:O	2:B:68:PHE:N	2.35	0.40
1:A:134:CYS:CB	1:A:148:TRP:CZ2	3.01	0.40
1:A:111:ALA:CA	1:A:200:THR:HG21	2.52	0.40
1:C:96:TYR:CZ	2:D:107:TYR:CG	3.10	0.40
2:B:130:VAL:CG2	2:B:206:VAL:CG2	2.96	0.40
1:C:50:TYR:C	1:C:52:SER:N	2.70	0.40
1:C:55:GLN:HG3	1:C:56:SER:OG	2.20	0.40
2:B:36:TRP:HB3	2:B:48:VAL:HG12	2.03	0.40
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.66	0.40
1:C:164:THR:HG22	2:D:175:VAL:HG23	2.04	0.40
1:A:16:GLY:HA2	1:A:77:ASN:OD1	2.21	0.40
2:D:60:TYR:OH	2:D:69:THR:CA	2.40	0.40
2:B:12:VAL:O	2:B:120:VAL:HA	2.22	0.40
1:C:50:TYR:HD2	1:C:53:ARG:NH2	2.19	0.40
1:C:54:LEU:HD11	1:C:58:VAL:CG1	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:ASP:N	1:C:77:ASN:OD1[2_656]	2.01	0.19
2:B:124:THR:CG2	1:C:156:GLN:NE2[1_565]	2.04	0.16

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/206 (99%)	166 (81%)	26 (13%)	12 (6%)	2	12
1	C	204/206 (99%)	162 (79%)	24 (12%)	18 (9%)	1	5
2	B	215/217 (99%)	163 (76%)	26 (12%)	26 (12%)	0	2
2	D	215/217 (99%)	169 (79%)	25 (12%)	21 (10%)	1	4
All	All	838/846 (99%)	660 (79%)	101 (12%)	77 (9%)	1	4

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	51	THR
1	A	80	GLU
1	A	199	LYS
2	B	42	GLU
2	B	105	SER
2	B	170	SER
2	B	194	SER
2	B	209	PRO
2	B	211	SER
1	C	8	THR
1	C	31	ASN
1	C	51	THR
1	C	78	LEU
1	C	81	GLU
1	C	151	ASP
2	D	42	GLU
2	D	75	PRO
2	D	88	SER
2	D	123	ALA
2	D	128	PRO
2	D	137	CYS
2	D	138	SER
2	D	167	ALA
2	D	169	SER
2	D	170	SER
2	D	197	TRP
2	D	216	ILE
1	A	8	THR
1	A	26	SER
1	A	123	GLU
1	A	171	SER
1	A	188	ARG

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Mol	Chain	Res	Type
1	A	198	HIS
2	B	2	VAL
2	B	54	GLY
2	B	62	ASP
2	B	73	ASP
2	B	89	GLU
2	B	100	GLY
2	B	125	THR
2	B	139	ASP
1	C	40	PRO
1	C	42	GLY
1	C	57	GLY
1	C	68	GLY
1	C	199	LYS
2	D	48	VAL
1	A	138	ASN
2	B	7	SER
2	B	30	SER
2	B	104	ARG
2	B	135	PRO
2	B	210	ALA
1	C	43	SER
1	C	80	GLU
1	C	113	PRO
2	B	169	SER
2	B	199	SER
1	C	84	ALA
2	D	211	SER
1	C	141	PRO
2	D	2	VAL
2	D	41	PRO
2	D	127	ALA
2	B	144	SER
2	D	100	GLY
2	D	144	SER
1	A	100	GLY
2	D	16	GLY
2	D	99	GLY
2	B	166	GLY
1	C	144	ILE
2	B	197	TRP
2	B	216	ILE

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Mol	Chain	Res	Type
1	C	30	GLY
2	B	74	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/184 (100%)	135 (73%)	49 (27%)	0	1
1	C	184/184 (100%)	138 (75%)	46 (25%)	1	2
2	B	181/181 (100%)	130 (72%)	51 (28%)	0	1
2	D	181/181 (100%)	126 (70%)	55 (30%)	0	1
All	All	730/730 (100%)	529 (72%)	201 (28%)	0	1

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	7	ILE
1	A	10	SER
1	A	13	VAL
1	A	15	LEU
1	A	17	ASP
1	A	27	GLN
1	A	29	ILE
1	A	39	LYS
1	A	40	PRO
1	A	41	ASP
1	A	43	SER
1	A	44	LEU
1	A	46	LEU
1	A	49	TYR
1	A	54	LEU
1	A	55	GLN
1	A	65	TRP

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Mol	Chain	Res	Type
1	A	71	TYR
1	A	76	SER
1	A	77	ASN
1	A	78	LEU
1	A	83	ILE
1	A	85	THR
1	A	92	LYS
1	A	106	ILE
1	A	114	THR
1	A	119	PRO
1	A	120	PRO
1	A	122	SER
1	A	135	PHE
1	A	136	LEU
1	A	142	LYS
1	A	144	ILE
1	A	147	LYS
1	A	154	GLU
1	A	160	LEU
1	A	162	SER
1	A	163	TRP
1	A	164	THR
1	A	168	SER
1	A	171	SER
1	A	173	TYR
1	A	175	MET
1	A	179	LEU
1	A	184	ASP
1	A	194	CYS
1	A	205	ILE
2	B	7	SER
2	B	13	GLN
2	B	17	SER
2	B	18	ARG
2	B	20	LEU
2	B	27	PHE
2	B	28	THR
2	B	31	ASN
2	B	37	VAL
2	B	48	VAL
2	B	56	SER
2	B	59	ASN

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Mol	Chain	Res	Type
2	B	63	THR
2	B	67	ARG
2	B	77	ASN
2	B	84	THR
2	B	85	SER
2	B	89	GLU
2	B	98	ARG
2	B	101	THR
2	B	103	THR
2	B	114	GLN
2	B	117	THR
2	B	126	THR
2	B	135	PRO
2	B	144	SER
2	B	145	VAL
2	B	150	LEU
2	B	152	LYS
2	B	154	TYR
2	B	158	PRO
2	B	164	ASN
2	B	165	TYR
2	B	168	LEU
2	B	170	SER
2	B	172	VAL
2	B	178	VAL
2	B	180	GLN
2	B	185	SER
2	B	192	VAL
2	B	194	SER
2	B	195	SER
2	B	196	THR
2	B	199	SER
2	B	202	VAL
2	B	204	CYS
2	B	205	ASN
2	B	212	LYS
2	B	213	THR
2	B	216	ILE
2	B	217	LYS
1	C	4	MET
1	C	7	ILE
1	C	10	SER

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Mol	Chain	Res	Type
1	C	12	SER
1	C	15	LEU
1	C	17	ASP
1	C	20	ILE
1	C	22	SER
1	C	24	ARG
1	C	27	GLN
1	C	40	PRO
1	C	44	LEU
1	C	48	ILE
1	C	60	SER
1	C	65	TRP
1	C	67	SER
1	C	71	TYR
1	C	72	SER
1	C	78	LEU
1	C	79	GLU
1	C	80	GLU
1	C	81	GLU
1	C	83	ILE
1	C	89	GLN
1	C	95	PRO
1	C	103	LYS
1	C	105	GLU
1	C	107	LYS
1	C	108	ARG
1	C	114	THR
1	C	126	THR
1	C	131	SER
1	C	141	PRO
1	C	142	LYS
1	C	143	ASP
1	C	169	LYS
1	C	172	THR
1	C	175	MET
1	C	178	THR
1	C	179	LEU
1	C	190	ASN
1	C	193	THR
1	C	197	THR
1	C	200	THR
1	C	202	THR

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Mol	Chain	Res	Type
1	C	205	ILE
2	D	3	GLN
2	D	11	LEU
2	D	13	GLN
2	D	17	SER
2	D	18	ARG
2	D	20	LEU
2	D	30	SER
2	D	34	MET
2	D	39	GLN
2	D	48	VAL
2	D	50	TYR
2	D	56	SER
2	D	59	ASN
2	D	65	LYS
2	D	69	THR
2	D	71	SER
2	D	85	SER
2	D	87	ARG
2	D	91	THR
2	D	93	ILE
2	D	103	THR
2	D	105	SER
2	D	108	TYR
2	D	114	GLN
2	D	122	SER
2	D	128	PRO
2	D	132	PRO
2	D	135	PRO
2	D	139	ASP
2	D	144	SER
2	D	145	VAL
2	D	147	LEU
2	D	149	CYS
2	D	151	VAL
2	D	152	LYS
2	D	156	PRO
2	D	159	VAL
2	D	165	TYR
2	D	168	LEU
2	D	170	SER
2	D	173	ARG

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Mol	Chain	Res	Type
2	D	175	VAL
2	D	180	GLN
2	D	184	TYR
2	D	189	LEU
2	D	191	THR
2	D	194	SER
2	D	195	SER
2	D	199	SER
2	D	200	GLN
2	D	201	THR
2	D	202	VAL
2	D	205	ASN
2	D	215	LEU
2	D	217	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	37	GLN
1	A	190	ASN
2	B	59	ASN
2	B	77	ASN
2	B	164	ASN
2	B	180	GLN
2	B	208	HIS
1	C	27	GLN
1	C	31	ASN
1	C	77	ASN
1	C	89	GLN
1	C	161	ASN
1	C	190	ASN
2	D	3	GLN
2	D	59	ASN

### 5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	206/206 (100%)	-0.27	0 100 100	28, 28, 28, 28	0
1	C	206/206 (100%)	-0.28	0 100 100	28, 28, 28, 28	0
2	B	217/217 (100%)	-0.18	11 (5%) 32 13	28, 28, 28, 28	0
2	D	217/217 (100%)	-0.08	12 (5%) 29 12	28, 28, 28, 28	0
All	All	846/846 (100%)	-0.20	23 (2%) 58 34	28, 28, 28, 28	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	137	CYS	5.4
2	D	142	GLY	5.0
2	B	139	ASP	5.0
2	B	140	THR	4.6
2	D	169	SER	4.2
2	D	166	GLY	4.2
2	D	141	SER	4.0
2	D	140	THR	3.7
2	B	166	GLY	3.6
2	D	167	ALA	3.6
2	B	138	SER	3.6
2	B	137	CYS	3.5
2	B	169	SER	3.4
2	B	141	SER	3.1
2	D	139	ASP	3.1
2	B	136	GLY	2.9
2	D	168	LEU	2.8
2	D	136	GLY	2.8
2	B	42	GLU	2.8
2	D	138	SER	2.7
2	B	167	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	42	GLU	2.2
2	B	165	TYR	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.