



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:25 AM UTC

PDB ID : 1BLB / pdb\_00001blb  
Title : CLOSE PACKING OF AN OLIGOMERIC EYE LENS BETA-CRYSTALLIN INDUCES LOSS OF SYMMETRY AND ORDERING OF SEQUENCE EXTENSIONS  
Authors : Nalini, V.; Bax, B.; Driessen, H.; Moss, D.S.; Lindley, P.F.; Slingsby, C.  
Deposited on : 1993-12-22  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

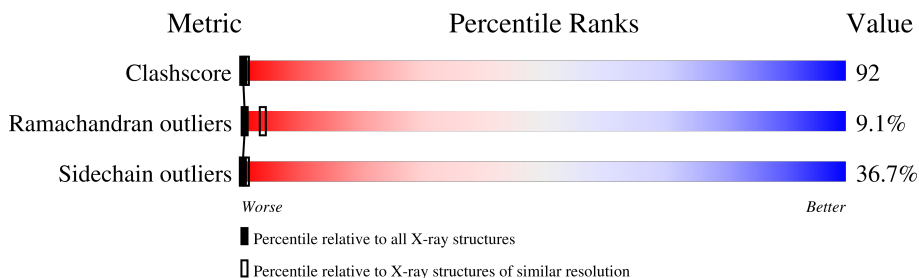
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	204	6% 27% 40% 17% 9%
1	B	204	9% 31% 34% 15% 11%
1	C	204	10% 34% 32% 16% 8%
1	D	204	10% 33% 30% 16% 10%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5941 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 BETA B2-CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	185	Total 1492	C 942	N 261	O 285	S 4	0	0	0
1	B	181	Total 1464	C 924	N 256	O 280	S 4	0	0	0
1	C	187	Total 1505	C 950	N 264	O 287	S 4	0	0	0
1	D	183	Total 1480	C 934	N 259	O 283	S 4	0	0	0

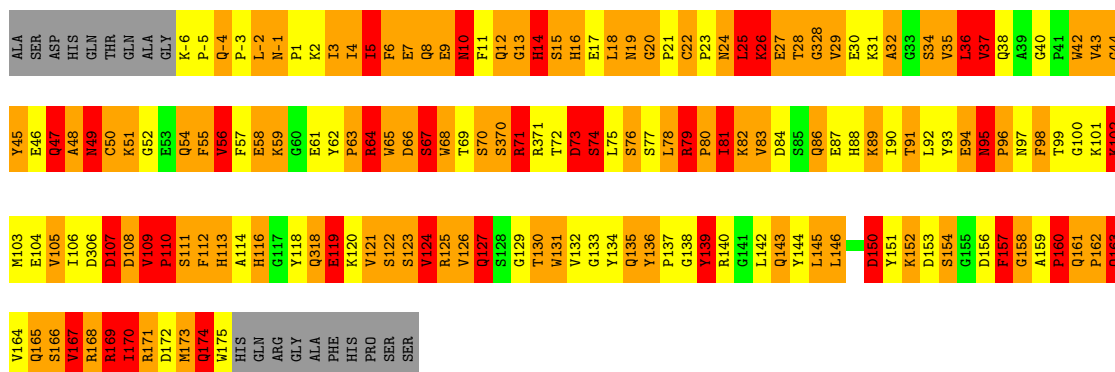
### 3 Residue-property plots [i](#)

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

Note EDS was not executed.

- Molecule 1: BETA B2-CRYSTALLIN

Chain A: 





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.71Å 165.90Å 78.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	RESTRAIN, X-PLOR	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	1.82	49/1535 (3.2%)	2.52	127/2080 (6.1%)
1	B	1.79	46/1505 (3.1%)	2.48	106/2037 (5.2%)
1	C	1.79	40/1548 (2.6%)	2.46	124/2096 (5.9%)
1	D	1.78	44/1522 (2.9%)	2.52	112/2061 (5.4%)
All	All	1.80	179/6110 (2.9%)	2.49	469/8274 (5.7%)

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	2	5
1	B	1	7
1	C	3	5
1	D	5	7
All	All	11	24

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	THR	N-CA	-9.63	1.40	1.46
1	B	74	SER	N-CA	9.37	1.57	1.46
1	D	16	HIS	CE1-NE2	9.26	1.41	1.32
1	A	14	HIS	ND1-CE1	8.97	1.41	1.32
1	A	16	HIS	CE1-NE2	8.74	1.41	1.32
1	C	30	GLU	N-CA	8.69	1.57	1.46
1	A	116	HIS	CE1-NE2	8.55	1.41	1.32
1	A	14	HIS	CE1-NE2	8.46	1.41	1.32
1	B	14	HIS	CE1-NE2	8.16	1.40	1.32
1	C	16	HIS	CE1-NE2	8.11	1.40	1.32
1	D	116	HIS	ND1-CE1	8.05	1.40	1.32
1	C	116	HIS	ND1-CE1	7.98	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	ILE	CA-CB	-7.96	1.44	1.54
1	D	116	HIS	CE1-NE2	7.94	1.40	1.32
1	A	16	HIS	ND1-CE1	7.93	1.40	1.32
1	C	88	HIS	ND1-CE1	7.90	1.40	1.32
1	C	116	HIS	CE1-NE2	7.77	1.40	1.32
1	D	14	HIS	ND1-CE1	7.76	1.40	1.32
1	A	113	HIS	CE1-NE2	7.74	1.40	1.32
1	B	88	HIS	ND1-CE1	7.71	1.40	1.32
1	D	14	HIS	CE1-NE2	7.68	1.40	1.32
1	C	16	HIS	ND1-CE1	7.67	1.40	1.32
1	C	14	HIS	ND1-CE1	7.65	1.40	1.32
1	A	88	HIS	ND1-CE1	7.63	1.40	1.32
1	B	113	HIS	CE1-NE2	7.62	1.40	1.32
1	D	113	HIS	CE1-NE2	7.52	1.40	1.32
1	A	14	HIS	N-CA	-7.51	1.36	1.46
1	B	44	GLY	N-CA	7.44	1.51	1.44
1	D	88	HIS	ND1-CE1	7.39	1.40	1.32
1	B	116	HIS	ND1-CE1	7.30	1.39	1.32
1	A	170	ILE	N-CA	7.24	1.55	1.46
1	D	161	GLN	N-CA	-7.21	1.39	1.46
1	A	88	HIS	CE1-NE2	7.21	1.39	1.32
1	B	86	GLN	CA-CB	-7.20	1.42	1.53
1	A	167	VAL	CA-CB	-7.18	1.44	1.54
1	B	16	HIS	CE1-NE2	7.10	1.39	1.32
1	B	14	HIS	ND1-CE1	7.09	1.39	1.32
1	B	113	HIS	ND1-CE1	6.99	1.39	1.32
1	B	116	HIS	CE1-NE2	6.98	1.39	1.32
1	D	113	HIS	ND1-CE1	6.95	1.39	1.32
1	A	116	HIS	ND1-CE1	6.89	1.39	1.32
1	B	16	HIS	ND1-CE1	6.83	1.39	1.32
1	A	27	GLU	CA-CB	-6.82	1.44	1.52
1	B	8	GLN	CD-OE1	6.80	1.36	1.23
1	C	328	GLY	C-N	-6.77	1.24	1.33
1	B	12	GLN	CD-OE1	6.67	1.36	1.23
1	C	113	HIS	CE1-NE2	6.62	1.39	1.32
1	C	14	HIS	CE1-NE2	6.59	1.39	1.32
1	A	318	GLN	CD-OE1	6.55	1.35	1.23
1	D	88	HIS	CE1-NE2	6.47	1.39	1.32
1	C	113	HIS	ND1-CE1	6.46	1.39	1.32
1	C	318	GLN	CD-OE1	6.44	1.35	1.23
1	D	42	TRP	NE1-CE2	-6.42	1.30	1.37
1	A	8	GLN	CD-OE1	6.41	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	ASP	N-CA	6.39	1.53	1.45
1	B	131	TRP	NE1-CE2	-6.39	1.30	1.37
1	C	71	ARG	CA-C	-6.37	1.44	1.52
1	A	42	TRP	NE1-CE2	-6.32	1.30	1.37
1	D	163	GLN	CD-OE1	6.30	1.35	1.23
1	D	127	GLN	CD-OE1	6.27	1.35	1.23
1	A	74	SER	N-CA	-6.26	1.38	1.46
1	C	132	VAL	CA-CB	-6.24	1.45	1.53
1	C	174	GLN	CA-CB	-6.24	1.44	1.53
1	D	-4	GLN	CD-OE1	6.22	1.35	1.23
1	C	131	TRP	NE1-CE2	-6.22	1.30	1.37
1	A	12	GLN	CD-OE1	6.20	1.35	1.23
1	D	63	PRO	CA-C	-6.18	1.43	1.52
1	C	-4	GLN	CD-OE1	6.16	1.35	1.23
1	D	68	TRP	NE1-CE2	-6.13	1.30	1.37
1	A	161	GLN	CD-OE1	6.12	1.35	1.23
1	B	17	GLU	CA-CB	-6.12	1.44	1.53
1	D	16	HIS	ND1-CE1	6.12	1.38	1.32
1	D	97	ASN	CA-CB	-6.07	1.44	1.53
1	D	95	ASN	CG-OD1	6.04	1.35	1.23
1	D	131	TRP	NE1-CE2	-6.04	1.30	1.37
1	D	154	SER	N-CA	6.01	1.53	1.46
1	B	42	TRP	NE1-CE2	-6.00	1.30	1.37
1	C	127	GLN	CD-OE1	5.99	1.34	1.23
1	D	47	GLN	CD-OE1	5.99	1.34	1.23
1	C	161	GLN	CD-OE1	5.94	1.34	1.23
1	B	86	GLN	CD-OE1	5.93	1.34	1.23
1	C	68	TRP	NE1-CE2	-5.91	1.30	1.37
1	A	127	GLN	CD-OE1	5.86	1.34	1.23
1	B	161	GLN	CD-OE1	5.85	1.34	1.23
1	C	42	TRP	NE1-CE2	-5.85	1.31	1.37
1	B	88	HIS	CE1-NE2	5.84	1.38	1.32
1	D	156	ASP	CA-CB	-5.83	1.43	1.53
1	A	86	GLN	CD-OE1	5.78	1.34	1.23
1	A	13	GLY	C-N	-5.77	1.25	1.33
1	A	-4	GLN	CD-OE1	5.76	1.34	1.23
1	C	167	VAL	CA-CB	-5.76	1.46	1.54
1	C	8	GLN	CD-OE1	5.75	1.34	1.23
1	B	38	GLN	CD-OE1	5.75	1.34	1.23
1	A	89	LYS	CA-C	-5.74	1.45	1.52
1	C	10	ASN	CG-OD1	5.73	1.34	1.23
1	A	67	SER	N-CA	-5.72	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	GLN	CD-OE1	5.71	1.34	1.23
1	C	88	HIS	CE1-NE2	5.70	1.38	1.32
1	A	102	LYS	C-N	-5.70	1.26	1.33
1	A	170	ILE	CA-CB	-5.69	1.47	1.54
1	C	165	GLN	CD-OE1	5.69	1.34	1.23
1	B	24	ASN	CG-OD1	5.66	1.34	1.23
1	D	8	GLN	CD-OE1	5.66	1.34	1.23
1	B	170	ILE	CA-CB	-5.65	1.47	1.54
1	A	20	GLY	N-CA	5.65	1.52	1.44
1	B	127	GLN	CD-OE1	5.64	1.34	1.23
1	B	54	GLN	CD-OE1	5.63	1.34	1.23
1	C	-4	GLN	N-CA	-5.62	1.38	1.46
1	B	161	GLN	CA-CB	-5.62	1.46	1.53
1	D	12	GLN	CD-OE1	5.62	1.34	1.23
1	D	86	GLN	CD-OE1	5.60	1.34	1.23
1	B	35	VAL	CA-CB	-5.59	1.46	1.54
1	C	37	VAL	N-CA	-5.58	1.39	1.46
1	C	135	GLN	CD-OE1	5.57	1.34	1.23
1	A	113	HIS	ND1-CE1	5.56	1.38	1.32
1	B	23	PRO	N-CA	-5.56	1.40	1.47
1	D	86	GLN	N-CA	-5.55	1.39	1.45
1	D	175	TRP	NE1-CE2	-5.55	1.31	1.37
1	B	47	GLN	CD-OE1	5.54	1.34	1.23
1	C	47	GLN	CD-OE1	5.53	1.34	1.23
1	A	25	LEU	N-CA	5.51	1.51	1.46
1	A	174	GLN	CD-OE1	5.51	1.34	1.23
1	A	131	TRP	NE1-CE2	-5.50	1.31	1.37
1	A	146	LEU	N-CA	5.50	1.54	1.47
1	D	161	GLN	CD-OE1	5.50	1.33	1.23
1	A	97	ASN	CG-OD1	5.48	1.33	1.23
1	A	26	LYS	N-CA	5.47	1.53	1.46
1	D	165	GLN	CD-OE1	5.45	1.33	1.23
1	A	47	GLN	CD-OE1	5.45	1.33	1.23
1	A	10	ASN	CG-OD1	5.44	1.33	1.23
1	D	152	LYS	CA-C	-5.42	1.45	1.52
1	A	38	GLN	CD-OE1	5.42	1.33	1.23
1	B	175	TRP	NE1-CE2	-5.40	1.31	1.37
1	C	104	GLU	N-CA	5.40	1.53	1.46
1	B	173	MET	N-CA	-5.39	1.39	1.46
1	A	165	GLN	CD-OE1	5.38	1.33	1.23
1	A	16	HIS	CG-CD2	5.37	1.41	1.35
1	D	318	GLN	CD-OE1	5.37	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	ASN	CG-OD1	5.33	1.33	1.23
1	A	-1	ASN	CG-OD1	5.33	1.33	1.23
1	A	50	CYS	CA-C	-5.33	1.45	1.52
1	D	54	GLN	CD-OE1	5.31	1.33	1.23
1	B	61	GLU	N-CA	-5.28	1.39	1.46
1	C	37	VAL	CA-CB	-5.28	1.48	1.54
1	B	68	TRP	NE1-CE2	-5.27	1.31	1.37
1	B	22	CYS	N-CA	-5.24	1.38	1.46
1	D	174	GLN	CD-OE1	5.24	1.33	1.23
1	D	38	GLN	CD-OE1	5.23	1.33	1.23
1	B	135	GLN	CD-OE1	5.22	1.33	1.23
1	B	48	ALA	CA-CB	-5.22	1.45	1.53
1	B	53	GLU	N-CA	5.19	1.52	1.46
1	B	95	ASN	CG-OD1	5.19	1.33	1.23
1	B	318	GLN	CD-OE1	5.17	1.33	1.23
1	C	173	MET	N-CA	5.17	1.52	1.46
1	D	19	ASN	CG-OD1	5.17	1.33	1.23
1	A	49	ASN	CG-OD1	5.17	1.33	1.23
1	A	54	GLN	CD-OE1	5.17	1.33	1.23
1	B	143	GLN	CD-OE1	5.16	1.33	1.23
1	B	163	GLN	CD-OE1	5.14	1.33	1.23
1	C	163	GLN	CD-OE1	5.14	1.33	1.23
1	C	11	PHE	CA-C	-5.13	1.45	1.52
1	B	97	ASN	CG-OD1	5.12	1.33	1.23
1	D	-1	ASN	CG-OD1	5.12	1.33	1.23
1	C	65	TRP	NE1-CE2	-5.11	1.31	1.37
1	A	95	ASN	CG-OD1	5.09	1.33	1.23
1	B	10	ASN	CG-OD1	5.09	1.33	1.23
1	D	120	LYS	CA-CB	-5.09	1.45	1.53
1	D	371	ARG	C-N	-5.08	1.28	1.33
1	C	170	ILE	N-CA	5.06	1.52	1.46
1	C	23	PRO	CA-C	-5.06	1.45	1.52
1	B	-1	ASN	N-CA	5.04	1.53	1.46
1	A	37	VAL	CA-CB	-5.04	1.48	1.54
1	C	81	ILE	N-CA	-5.03	1.40	1.46
1	D	10	ASN	CG-OD1	5.03	1.33	1.23
1	A	63	PRO	N-CA	-5.03	1.40	1.47
1	A	86	GLN	CA-C	-5.03	1.46	1.53
1	D	160	PRO	C-N	-5.03	1.28	1.33
1	B	58	GLU	CA-C	-5.02	1.47	1.52
1	C	12	GLN	CD-OE1	5.01	1.33	1.23

All (469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	GLY	CA-C-N	21.19	162.01	121.54
1	A	13	GLY	C-N-CA	21.19	162.01	121.54
1	D	371	ARG	CA-C-N	19.61	144.22	123.04
1	D	371	ARG	C-N-CA	19.61	144.22	123.04
1	D	72	THR	N-CA-C	16.10	121.98	108.78
1	B	22	CYS	CA-C-N	14.49	137.96	119.84
1	B	22	CYS	C-N-CA	14.49	137.96	119.84
1	B	172	ASP	CA-C-N	12.92	140.98	122.77
1	B	172	ASP	C-N-CA	12.92	140.98	122.77
1	A	107	ASP	CA-CB-CG	12.89	125.49	112.60
1	A	81	ILE	N-CA-CB	12.74	124.61	110.72
1	C	66	ASP	CA-C-N	11.87	137.71	120.38
1	C	66	ASP	C-N-CA	11.87	137.71	120.38
1	C	132	VAL	CA-CB-CG2	10.77	128.71	110.40
1	D	80	PRO	N-CA-CB	-10.59	93.44	103.39
1	C	328	GLY	CA-C-N	10.31	140.52	121.97
1	C	328	GLY	C-N-CA	10.31	140.52	121.97
1	B	157	PHE	CA-C-N	10.21	140.58	120.77
1	B	157	PHE	C-N-CA	10.21	140.58	120.77
1	A	167	VAL	CA-CB-CG1	10.17	127.68	110.40
1	A	108	ASP	CA-CB-CG	10.12	122.72	112.60
1	C	167	VAL	CA-CB-CG2	10.00	127.40	110.40
1	A	14	HIS	CA-CB-CG	-9.97	103.83	113.80
1	A	157	PHE	CA-C-N	9.94	135.12	120.11
1	A	157	PHE	C-N-CA	9.94	135.12	120.11
1	C	37	VAL	N-CA-C	9.91	123.40	108.23
1	B	60	GLY	CA-C-N	9.85	134.86	120.87
1	B	60	GLY	C-N-CA	9.85	134.86	120.87
1	D	160	PRO	CA-C-N	9.78	136.04	122.74
1	D	160	PRO	C-N-CA	9.78	136.04	122.74
1	C	38	GLN	CA-C-O	9.74	129.58	118.77
1	D	156	ASP	CA-CB-CG	9.64	122.24	112.60
1	D	72	THR	CA-C-O	9.64	123.53	117.94
1	D	109	VAL	CA-CB-CG2	9.51	126.57	110.40
1	B	121	VAL	CA-CB-CG2	9.42	126.41	110.40
1	C	11	PHE	CA-CB-CG	-9.38	104.42	113.80
1	A	89	LYS	N-CA-C	9.34	124.12	108.90
1	D	154	SER	N-CA-C	-9.08	100.12	111.75
1	B	129	GLY	CA-C-N	9.07	134.63	122.84
1	B	129	GLY	C-N-CA	9.07	134.63	122.84
1	C	51	LYS	CA-C-N	-9.04	114.17	121.86
1	C	51	LYS	C-N-CA	-9.04	114.17	121.86
1	B	83	VAL	N-CA-C	9.01	121.78	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	GLU	N-CA-C	8.97	123.55	110.28
1	C	70	SER	CA-C-N	8.85	133.05	121.90
1	C	70	SER	C-N-CA	8.85	133.05	121.90
1	B	31	LYS	CA-C-N	8.80	135.80	122.77
1	B	31	LYS	C-N-CA	8.80	135.80	122.77
1	C	98	PHE	CA-CB-CG	-8.79	105.02	113.80
1	D	13	GLY	CA-C-N	8.59	137.94	121.54
1	D	13	GLY	C-N-CA	8.59	137.94	121.54
1	D	154	SER	O-C-N	8.56	131.96	122.20
1	D	72	THR	CB-CA-C	-8.42	104.94	117.07
1	D	95	ASN	CA-C-N	8.40	128.91	119.92
1	D	95	ASN	C-N-CA	8.40	128.91	119.92
1	D	172	ASP	CA-C-N	8.38	134.82	123.00
1	D	172	ASP	C-N-CA	8.38	134.82	123.00
1	C	161	GLN	O-C-N	8.34	127.80	121.88
1	D	98	PHE	CA-CB-CG	-8.32	105.48	113.80
1	D	370	SER	CA-C-N	8.28	137.36	121.54
1	D	370	SER	C-N-CA	8.28	137.36	121.54
1	D	112	PHE	CA-CB-CG	-8.20	105.61	113.80
1	A	112	PHE	N-CA-C	-8.16	102.36	111.82
1	C	38	GLN	CA-C-N	-8.15	109.93	121.33
1	C	38	GLN	C-N-CA	-8.15	109.93	121.33
1	D	66	ASP	O-C-N	8.08	130.50	122.09
1	B	86	GLN	N-CA-CB	8.06	123.55	110.41
1	B	111	SER	CA-C-N	8.01	131.01	120.28
1	B	111	SER	C-N-CA	8.01	131.01	120.28
1	C	42	TRP	CA-C-N	-7.91	112.35	123.11
1	C	42	TRP	C-N-CA	-7.91	112.35	123.11
1	B	12	GLN	CA-C-N	7.89	129.34	120.42
1	B	12	GLN	C-N-CA	7.89	129.34	120.42
1	A	62	TYR	CA-C-N	7.88	129.69	119.84
1	A	62	TYR	C-N-CA	7.88	129.69	119.84
1	A	158	GLY	O-C-N	-7.85	116.16	122.51
1	C	37	VAL	CA-CB-CG2	7.82	123.69	110.40
1	C	83	VAL	CA-C-N	7.80	133.41	122.41
1	C	83	VAL	C-N-CA	7.80	133.41	122.41
1	C	161	GLN	CA-C-O	-7.78	112.26	120.28
1	A	165	GLN	OE1-CD-NE2	-7.78	114.82	122.60
1	A	81	ILE	O-C-N	7.76	131.80	122.95
1	C	28	THR	N-CA-C	-7.74	103.97	113.41
1	D	37	VAL	CA-CB-CG2	7.67	123.44	110.40
1	B	105	VAL	CA-CB-CG2	7.66	123.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASN	CA-CB-CG	-7.56	105.04	112.60
1	B	35	VAL	CA-CB-CG2	7.55	123.23	110.40
1	A	35	VAL	CA-CB-CG2	7.55	123.23	110.40
1	A	109	VAL	CA-CB-CG2	7.51	123.17	110.40
1	A	74	SER	CA-C-N	7.50	132.42	122.30
1	A	74	SER	C-N-CA	7.50	132.42	122.30
1	C	19	ASN	O-C-N	7.47	129.55	121.85
1	C	29	VAL	CA-C-N	-7.43	108.20	121.81
1	C	29	VAL	C-N-CA	-7.43	108.20	121.81
1	C	56	VAL	CA-C-N	7.43	133.70	122.93
1	C	56	VAL	C-N-CA	7.43	133.70	122.93
1	C	172	ASP	CA-CB-CG	-7.40	105.20	112.60
1	B	86	GLN	CB-CA-C	7.39	122.14	109.51
1	C	105	VAL	CA-CB-CG2	7.34	122.89	110.40
1	A	71	ARG	CA-C-O	7.34	127.64	119.78
1	C	81	ILE	N-CA-CB	7.29	119.11	110.95
1	C	121	VAL	CA-CB-CG2	7.28	122.78	110.40
1	C	371	ARG	O-C-N	7.25	131.89	122.68
1	C	10	ASN	CA-CB-CG	-7.23	105.37	112.60
1	B	160	PRO	N-CA-CB	-7.19	95.31	103.15
1	C	38	GLN	O-C-N	-7.19	114.44	122.34
1	A	-1	ASN	CA-CB-CG	-7.18	105.42	112.60
1	D	105	VAL	CA-CB-CG2	7.17	122.59	110.40
1	D	165	GLN	CA-C-O	7.17	126.72	118.55
1	A	116	HIS	N-CA-C	-7.16	104.12	112.92
1	B	73	ASP	CA-C-N	-7.14	112.57	122.93
1	B	73	ASP	C-N-CA	-7.14	112.57	122.93
1	D	156	ASP	CB-CA-C	7.13	124.61	110.42
1	B	128	SER	O-C-N	-7.12	114.56	123.17
1	D	152	LYS	CA-C-N	-7.11	110.06	122.64
1	D	152	LYS	C-N-CA	-7.11	110.06	122.64
1	C	6	PHE	CA-C-N	7.10	129.67	120.44
1	C	6	PHE	C-N-CA	7.10	129.67	120.44
1	B	31	LYS	O-C-N	7.09	131.28	122.63
1	A	12	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	D	49	ASN	CA-CB-CG	-7.08	105.53	112.60
1	C	-5	PRO	CA-C-N	7.07	139.04	121.80
1	C	-5	PRO	C-N-CA	7.07	139.04	121.80
1	D	111	SER	N-CA-C	7.04	121.93	107.37
1	B	49	ASN	CA-CB-CG	-7.02	105.58	112.60
1	B	127	GLN	OE1-CD-NE2	-7.01	115.59	122.60
1	D	163	GLN	OE1-CD-NE2	-7.01	115.59	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ASP	CA-C-N	7.00	135.09	122.13
1	B	108	ASP	C-N-CA	7.00	135.09	122.13
1	D	63	PRO	N-CA-C	7.00	126.89	112.47
1	C	113	HIS	CA-CB-CG	-6.98	106.82	113.80
1	B	-1	ASN	CA-CB-CG	-6.94	105.66	112.60
1	D	97	ASN	N-CA-CB	6.94	122.61	112.13
1	B	107	ASP	N-CA-C	6.93	120.64	110.59
1	C	58	GLU	CA-C-O	-6.93	113.75	121.51
1	D	107	ASP	CA-CB-CG	-6.92	105.68	112.60
1	C	43	VAL	CA-CB-CG2	6.92	122.16	110.40
1	C	66	ASP	CA-CB-CG	6.92	119.52	112.60
1	C	35	VAL	CA-CB-CG2	6.91	122.14	110.40
1	B	13	GLY	N-CA-C	6.89	122.66	110.95
1	A	167	VAL	N-CA-CB	6.88	122.72	111.44
1	D	86	GLN	N-CA-C	6.85	120.84	109.95
1	B	124	VAL	CA-CB-CG2	6.85	122.05	110.40
1	A	42	TRP	CA-C-O	-6.83	113.12	121.11
1	D	97	ASN	CB-CA-C	6.83	121.42	111.73
1	A	328	GLY	N-CA-C	-6.81	104.21	113.27
1	A	5	ILE	O-C-N	6.81	129.61	122.67
1	B	126	VAL	CA-CB-CG2	6.77	121.91	110.40
1	C	66	ASP	O-C-N	6.75	129.27	122.12
1	A	86	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	A	76	SER	CA-C-N	-6.73	112.24	122.81
1	A	76	SER	C-N-CA	-6.73	112.24	122.81
1	A	76	SER	CA-C-O	6.73	127.47	119.06
1	D	156	ASP	N-CA-CB	6.71	121.84	110.49
1	B	109	VAL	CA-CB-CG2	6.71	121.81	110.40
1	C	26	LYS	N-CA-C	-6.70	104.05	111.82
1	A	15	SER	N-CA-C	6.69	120.43	109.85
1	D	12	GLN	CA-C-N	6.69	134.53	121.41
1	D	12	GLN	C-N-CA	6.69	134.53	121.41
1	C	371	ARG	CA-C-O	-6.69	113.96	120.92
1	B	24	ASN	N-CA-CB	6.69	121.01	111.65
1	A	50	CYS	N-CA-C	6.66	124.99	110.80
1	A	5	ILE	CA-C-O	-6.63	113.44	121.13
1	B	11	PHE	CA-CB-CG	-6.63	107.17	113.80
1	B	123	SER	CA-C-O	-6.61	113.88	121.68
1	D	69	THR	O-C-N	6.61	130.39	122.26
1	D	151	TYR	CA-C-N	6.61	134.16	121.54
1	D	151	TYR	C-N-CA	6.61	134.16	121.54
1	C	63	PRO	N-CA-CB	-6.60	97.63	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	SER	CA-C-N	6.59	131.73	120.72
1	A	70	SER	C-N-CA	6.59	131.73	120.72
1	D	93	TYR	N-CA-C	6.59	119.68	109.07
1	C	318	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	B	37	VAL	CA-CB-CG2	6.56	121.55	110.40
1	C	174	GLN	N-CA-CB	6.53	121.09	111.43
1	A	154	SER	N-CA-C	-6.52	103.44	111.33
1	A	-2	LEU	N-CA-C	-6.52	104.47	112.88
1	C	37	VAL	N-CA-CB	6.51	118.43	111.00
1	D	173	MET	CA-C-N	6.49	129.26	120.44
1	D	173	MET	C-N-CA	6.49	129.26	120.44
1	D	81	ILE	CA-C-N	-6.46	112.91	122.41
1	D	81	ILE	C-N-CA	-6.46	112.91	122.41
1	C	81	ILE	N-CA-C	6.46	118.10	108.54
1	A	8	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	B	11	PHE	CA-C-N	-6.43	112.51	122.87
1	B	11	PHE	C-N-CA	-6.43	112.51	122.87
1	C	113	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	C	109	VAL	C-N-CD	-6.43	98.65	125.00
1	A	27	GLU	N-CA-CB	6.42	120.64	110.49
1	B	22	CYS	N-CA-CB	6.39	121.75	110.37
1	A	89	LYS	O-C-N	-6.39	115.70	123.30
1	D	120	LYS	N-CA-CB	6.37	120.50	110.56
1	D	69	THR	N-CA-C	-6.37	104.82	112.59
1	D	40	GLY	C-N-CD	-6.35	106.64	120.60
1	A	26	LYS	N-CA-C	-6.33	103.64	112.45
1	A	66	ASP	CA-C-N	6.33	133.63	121.54
1	A	66	ASP	C-N-CA	6.33	133.63	121.54
1	C	-4	GLN	N-CA-C	6.33	123.80	109.81
1	C	29	VAL	CA-C-O	-6.32	112.88	120.78
1	D	32	ALA	CA-C-N	6.31	126.82	119.94
1	D	32	ALA	C-N-CA	6.31	126.82	119.94
1	A	63	PRO	N-CA-C	6.30	125.45	112.47
1	D	62	TYR	CA-C-N	6.30	127.72	119.84
1	D	62	TYR	C-N-CA	6.30	127.72	119.84
1	D	85	SER	CA-C-N	6.30	133.01	122.87
1	D	85	SER	C-N-CA	6.30	133.01	122.87
1	C	8	GLN	N-CA-CB	6.28	120.20	110.46
1	A	67	SER	N-CA-CB	6.28	121.10	110.49
1	B	161	GLN	CB-CA-C	6.27	118.28	108.63
1	A	121	VAL	CA-CB-CG2	6.25	121.03	110.40
1	D	14	HIS	CA-CB-CG	-6.21	107.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ARG	CA-C-N	-6.21	114.96	122.90
1	B	169	ARG	C-N-CA	-6.21	114.96	122.90
1	A	73	ASP	CA-C-N	6.20	133.37	121.54
1	A	73	ASP	C-N-CA	6.20	133.37	121.54
1	A	166	SER	N-CA-C	6.16	119.07	109.52
1	B	51	LYS	CA-C-O	-6.16	114.20	121.16
1	A	152	LYS	N-CA-C	6.16	118.07	111.36
1	A	37	VAL	CA-CB-CG2	6.14	120.84	110.40
1	D	66	ASP	CA-C-N	6.14	133.27	121.54
1	D	66	ASP	C-N-CA	6.14	133.27	121.54
1	C	124	VAL	CA-CB-CG2	6.13	120.83	110.40
1	C	63	PRO	CA-C-O	-6.11	114.51	121.97
1	A	80	PRO	N-CA-CB	-6.11	97.39	103.19
1	B	116	HIS	CA-CB-CG	-6.11	107.69	113.80
1	B	31	LYS	CA-C-O	-6.10	114.56	121.39
1	D	89	LYS	CA-C-N	6.08	132.92	121.97
1	D	89	LYS	C-N-CA	6.08	132.92	121.97
1	B	370	SER	CA-C-N	6.08	133.15	121.54
1	B	370	SER	C-N-CA	6.08	133.15	121.54
1	D	12	GLN	N-CA-C	6.07	119.07	109.96
1	C	29	VAL	CA-CB-CG2	6.05	120.69	110.40
1	A	36	LEU	N-CA-CB	6.04	120.08	110.65
1	A	163	GLN	N-CA-C	6.04	119.19	107.71
1	A	132	VAL	CA-C-N	6.03	133.22	121.41
1	A	132	VAL	C-N-CA	6.03	133.22	121.41
1	C	103	MET	CG-SD-CE	6.02	114.15	100.90
1	D	10	ASN	CA-CB-CG	-6.01	106.59	112.60
1	D	62	TYR	CA-C-O	-6.01	114.25	121.22
1	B	120	LYS	CA-C-N	6.00	131.29	122.94
1	B	120	LYS	C-N-CA	6.00	131.29	122.94
1	A	-4	GLN	CA-C-N	5.99	127.33	119.84
1	A	-4	GLN	C-N-CA	5.99	127.33	119.84
1	C	89	LYS	CA-C-N	5.99	131.65	122.25
1	C	89	LYS	C-N-CA	5.99	131.65	122.25
1	A	82	LYS	CA-C-N	5.97	128.57	120.63
1	A	82	LYS	C-N-CA	5.97	128.57	120.63
1	A	169	ARG	CA-C-N	-5.97	112.61	120.91
1	A	169	ARG	C-N-CA	-5.97	112.61	120.91
1	C	3	ILE	CA-C-N	-5.97	114.10	122.75
1	C	3	ILE	C-N-CA	-5.97	114.10	122.75
1	D	174	GLN	CA-C-N	5.96	132.42	121.70
1	D	174	GLN	C-N-CA	5.96	132.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	GLY	O-C-N	-5.96	117.69	123.35
1	D	29	VAL	CA-CB-CG2	5.95	120.51	110.40
1	A	158	GLY	N-CA-C	5.93	122.14	113.48
1	C	105	VAL	CA-C-N	-5.93	115.83	123.19
1	C	105	VAL	C-N-CA	-5.93	115.83	123.19
1	A	124	VAL	CA-CB-CG2	5.92	120.46	110.40
1	C	57	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	132	VAL	CA-CB-CG2	5.91	120.45	110.40
1	B	62	TYR	CA-C-N	5.91	127.23	119.84
1	B	62	TYR	C-N-CA	5.91	127.23	119.84
1	D	33	GLY	CA-C-N	5.90	132.29	121.85
1	D	33	GLY	C-N-CA	5.90	132.29	121.85
1	C	23	PRO	CA-C-N	-5.89	114.49	122.86
1	C	23	PRO	C-N-CA	-5.89	114.49	122.86
1	C	103	MET	CA-C-N	-5.89	115.18	122.84
1	C	103	MET	C-N-CA	-5.89	115.18	122.84
1	D	56	VAL	N-CA-C	5.87	116.58	108.84
1	C	83	VAL	CA-CB-CG2	5.86	120.36	110.40
1	B	111	SER	O-C-N	5.84	130.36	122.59
1	C	84	ASP	CA-CB-CG	-5.84	106.76	112.60
1	D	99	THR	N-CA-C	5.83	117.83	109.14
1	A	119	GLU	N-CA-C	5.83	118.07	110.43
1	A	164	VAL	CA-CB-CG2	5.83	120.31	110.40
1	D	66	ASP	CA-C-O	-5.83	114.67	120.90
1	C	108	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	110	PRO	CA-C-N	-5.82	115.03	122.77
1	A	110	PRO	C-N-CA	-5.82	115.03	122.77
1	C	126	VAL	N-CA-C	5.82	115.69	106.32
1	B	22	CYS	N-CA-C	5.80	122.63	109.81
1	A	102	LYS	O-C-N	5.80	131.23	122.94
1	C	-1	ASN	CA-CB-CG	-5.80	106.80	112.60
1	A	107	ASP	CB-CA-C	5.79	116.93	109.80
1	C	71	ARG	N-CA-C	5.79	123.13	110.80
1	D	145	LEU	CA-C-N	-5.79	113.33	122.76
1	D	145	LEU	C-N-CA	-5.79	113.33	122.76
1	A	98	PHE	CA-CB-CG	-5.77	108.03	113.80
1	C	79	ARG	CB-CA-C	5.77	117.54	108.88
1	B	60	GLY	N-CA-C	-5.77	104.32	111.70
1	D	50	CYS	CA-C-N	5.77	132.06	121.85
1	D	50	CYS	C-N-CA	5.77	132.06	121.85
1	C	146	LEU	CA-C-O	-5.76	114.75	120.98
1	D	126	VAL	CA-CB-CG2	5.76	120.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	GLN	N-CA-CB	5.75	121.14	111.03
1	B	54	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	D	112	PHE	N-CA-C	-5.73	105.12	111.71
1	B	83	VAL	CA-CB-CG2	5.73	120.14	110.40
1	C	24	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	27	GLU	O-C-N	5.71	130.15	122.61
1	B	50	CYS	N-CA-CB	-5.70	103.45	112.63
1	D	76	SER	CB-CA-C	5.70	116.52	109.16
1	B	116	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	A	102	LYS	CA-C-N	5.70	131.15	122.95
1	A	102	LYS	C-N-CA	5.70	131.15	122.95
1	C	71	ARG	CA-C-N	-5.68	114.06	122.41
1	C	71	ARG	C-N-CA	-5.68	114.06	122.41
1	D	63	PRO	O-C-N	-5.68	114.98	122.64
1	B	14	HIS	O-C-N	-5.67	115.05	122.59
1	C	173	MET	CA-C-O	-5.67	113.74	120.43
1	D	62	TYR	CB-CA-C	-5.66	101.81	111.15
1	C	63	PRO	N-CA-C	5.66	120.12	112.48
1	C	90	ILE	CA-C-N	-5.63	115.06	123.00
1	C	90	ILE	C-N-CA	-5.63	115.06	123.00
1	B	41	PRO	N-CA-CB	-5.63	96.41	102.60
1	D	152	LYS	O-C-N	-5.61	115.12	122.59
1	B	29	VAL	CA-CB-CG2	5.61	119.93	110.40
1	A	24	ASN	CA-C-N	-5.60	111.54	120.17
1	A	24	ASN	C-N-CA	-5.60	111.54	120.17
1	B	50	CYS	CA-C-O	5.60	126.56	120.12
1	A	160	PRO	N-CA-CB	-5.60	97.37	103.25
1	D	56	VAL	CA-CB-CG2	5.60	119.92	110.40
1	A	24	ASN	O-C-N	-5.59	115.16	122.59
1	A	5	ILE	CB-CA-C	-5.56	102.53	111.59
1	B	60	GLY	CA-C-O	-5.56	116.75	122.26
1	C	35	VAL	O-C-N	-5.55	117.53	122.69
1	A	14	HIS	N-CA-C	5.55	122.62	110.80
1	B	30	GLU	N-CA-C	-5.55	107.15	114.31
1	C	28	THR	O-C-N	5.55	130.24	122.36
1	C	125	ARG	CA-C-N	5.55	128.69	122.59
1	C	125	ARG	C-N-CA	5.55	128.69	122.59
1	A	108	ASP	N-CA-CB	5.53	118.70	110.29
1	A	44	GLY	CA-C-N	5.53	133.14	121.91
1	A	44	GLY	C-N-CA	5.53	133.14	121.91
1	C	318	GLN	CB-CG-CD	5.52	121.99	112.60
1	A	121	VAL	O-C-N	-5.52	117.09	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	ASN	CA-C-N	5.52	130.53	121.87
1	C	19	ASN	C-N-CA	5.52	130.53	121.87
1	C	144	TYR	N-CA-CB	5.52	119.22	110.84
1	B	132	VAL	CA-CB-CG2	5.51	119.77	110.40
1	A	152	LYS	N-CA-CB	5.51	118.31	110.16
1	A	66	ASP	O-C-N	5.50	127.95	122.12
1	C	66	ASP	N-CA-CB	5.50	118.31	110.06
1	B	170	ILE	CA-C-N	5.50	129.79	120.88
1	B	170	ILE	C-N-CA	5.50	129.79	120.88
1	A	50	CYS	CA-C-N	-5.49	113.20	123.03
1	A	50	CYS	C-N-CA	-5.49	113.20	123.03
1	B	29	VAL	N-CA-C	5.49	116.38	106.61
1	C	109	VAL	CA-CB-CG2	5.48	119.72	110.40
1	C	137	PRO	N-CA-CB	-5.47	97.50	103.25
1	A	6	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	97	ASN	CA-C-N	5.47	129.89	122.07
1	A	97	ASN	C-N-CA	5.47	129.89	122.07
1	B	50	CYS	CA-CB-SG	-5.46	101.83	114.40
1	D	64	ARG	CA-C-N	5.46	131.97	121.54
1	D	64	ARG	C-N-CA	5.46	131.97	121.54
1	B	138	GLY	N-CA-C	-5.46	107.67	115.64
1	C	12	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	D	164	VAL	CA-CB-CG2	5.46	119.68	110.40
1	C	51	LYS	O-C-N	-5.46	116.09	122.96
1	D	70	SER	N-CA-CB	5.45	119.71	110.49
1	D	83	VAL	CA-CB-CG2	5.45	119.67	110.40
1	A	150	ASP	CA-C-O	-5.44	115.21	121.47
1	B	12	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	C	118	TYR	O-C-N	5.43	130.23	123.01
1	B	123	SER	CA-C-N	5.43	131.74	121.97
1	B	123	SER	C-N-CA	5.43	131.74	121.97
1	A	105	VAL	CA-CB-CG2	5.43	119.62	110.40
1	D	84	ASP	CB-CA-C	-5.42	104.05	112.07
1	B	328	GLY	CA-C-N	-5.41	116.25	123.17
1	B	328	GLY	C-N-CA	-5.41	116.25	123.17
1	A	102	LYS	CA-C-O	-5.41	115.30	121.68
1	B	128	SER	N-CA-C	5.40	117.39	109.24
1	D	152	LYS	N-CA-C	5.40	122.30	110.80
1	D	95	ASN	CB-CA-C	5.39	116.15	108.76
1	D	41	PRO	N-CD-CG	-5.39	97.33	103.80
1	A	71	ARG	CA-C-N	-5.38	115.36	122.85
1	A	71	ARG	C-N-CA	-5.38	115.36	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ILE	CA-C-O	-5.38	114.22	121.32
1	C	107	ASP	N-CA-C	5.38	117.47	110.53
1	D	12	GLN	N-CA-CB	5.36	117.84	109.85
1	B	138	GLY	CA-C-N	5.36	131.67	123.47
1	B	138	GLY	C-N-CA	5.36	131.67	123.47
1	D	54	GLN	O-C-N	-5.36	116.94	123.10
1	D	162	PRO	N-CA-CB	-5.35	97.63	103.25
1	A	86	GLN	N-CA-C	5.35	118.16	107.62
1	A	19	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	B	306	ASP	CA-CB-CG	-5.34	107.26	112.60
1	D	35	VAL	CA-CB-CG2	5.34	119.48	110.40
1	C	24	ASN	N-CA-C	5.34	117.52	108.02
1	A	50	CYS	O-C-N	-5.33	115.50	122.59
1	C	136	TYR	C-N-CD	-5.33	103.14	125.00
1	A	27	GLU	CA-C-N	5.33	131.86	121.63
1	A	27	GLU	C-N-CA	5.33	131.86	121.63
1	A	126	VAL	CA-CB-CG2	5.33	119.45	110.40
1	D	328	GLY	CA-C-N	-5.33	115.87	123.11
1	D	328	GLY	C-N-CA	-5.33	115.87	123.11
1	C	96	PRO	CA-C-N	-5.32	114.97	122.63
1	C	96	PRO	C-N-CA	-5.32	114.97	122.63
1	B	104	GLU	CA-C-O	-5.31	114.68	120.36
1	B	17	GLU	CA-C-O	-5.31	115.14	121.89
1	B	56	VAL	CA-CB-CG2	5.30	119.41	110.40
1	C	104	GLU	CB-CA-C	5.29	119.25	110.78
1	A	89	LYS	CA-C-O	5.29	126.08	120.36
1	D	41	PRO	CA-C-N	5.29	130.88	122.94
1	D	41	PRO	C-N-CA	5.29	130.88	122.94
1	A	70	SER	N-CA-C	-5.29	106.67	113.01
1	C	318	GLN	CG-CD-NE2	5.27	124.31	116.40
1	B	145	LEU	O-C-N	5.27	129.01	123.11
1	A	110	PRO	O-C-N	-5.26	115.55	122.64
1	B	121	VAL	N-CA-CB	5.25	120.05	111.44
1	D	174	GLN	O-C-N	5.25	127.75	122.09
1	C	84	ASP	CB-CA-C	-5.24	104.09	112.05
1	A	67	SER	N-CA-C	5.23	121.93	110.80
1	A	171	ARG	N-CA-CB	-5.23	103.95	110.90
1	B	172	ASP	O-C-N	5.22	128.79	122.94
1	D	72	THR	CA-CB-OG1	-5.21	101.78	109.60
1	C	98	PHE	CA-C-N	-5.21	113.77	122.21
1	C	98	PHE	C-N-CA	-5.21	113.77	122.21
1	B	58	GLU	O-C-N	-5.20	115.38	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	TYR	N-CA-C	5.20	116.42	108.42
1	A	43	VAL	CA-CB-CG2	5.18	119.21	110.40
1	D	159	ALA	N-CA-C	5.18	118.39	108.97
1	D	47	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	C	134	TYR	CA-C-N	5.17	127.47	120.65
1	C	134	TYR	C-N-CA	5.17	127.47	120.65
1	B	168	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	A	143	GLN	CA-C-N	5.16	130.26	122.99
1	A	143	GLN	C-N-CA	5.16	130.26	122.99
1	A	28	THR	O-C-N	5.15	129.25	123.48
1	C	11	PHE	O-C-N	-5.15	115.74	122.59
1	D	103	MET	CG-SD-CE	5.15	112.23	100.90
1	B	44	GLY	CA-C-O	-5.15	114.07	122.56
1	C	23	PRO	O-C-N	-5.15	115.69	122.64
1	D	106	ILE	CA-C-N	5.14	131.37	121.54
1	D	106	ILE	C-N-CA	5.14	131.37	121.54
1	D	121	VAL	CA-CB-CG2	5.14	119.14	110.40
1	A	27	GLU	N-CA-C	-5.14	102.74	110.70
1	C	11	PHE	N-CA-C	5.13	121.74	110.80
1	A	14	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	171	ARG	N-CA-C	5.12	117.84	111.24
1	C	105	VAL	O-C-N	-5.12	116.21	122.97
1	B	46	GLU	N-CA-C	-5.12	104.67	112.04
1	C	98	PHE	O-C-N	-5.11	115.79	122.59
1	A	168	ARG	CD-NE-CZ	-5.11	117.24	124.40
1	B	74	SER	CA-C-O	-5.10	115.30	120.71
1	C	73	ASP	N-CA-C	-5.10	105.31	112.25
1	B	164	VAL	O-C-N	5.10	128.94	122.57
1	D	124	VAL	CA-CB-CG2	5.10	119.07	110.40
1	C	-5	PRO	N-CA-CB	-5.10	97.90	103.25
1	B	31	LYS	N-CA-CB	5.08	118.97	110.53
1	D	128	SER	N-CA-CB	-5.08	103.64	111.46
1	B	117	GLY	N-CA-C	-5.07	108.33	114.92
1	A	145	LEU	CA-C-N	-5.07	112.60	121.87
1	A	145	LEU	C-N-CA	-5.07	112.60	121.87
1	C	328	GLY	O-C-N	5.07	129.29	122.70
1	A	154	SER	O-C-N	5.06	127.49	122.12
1	B	62	TYR	CA-C-O	-5.05	116.14	121.29
1	A	170	ILE	CA-C-N	-5.05	114.31	122.24
1	A	170	ILE	C-N-CA	-5.05	114.31	122.24
1	A	79	ARG	CB-CA-C	5.05	115.68	108.76
1	B	14	HIS	CA-C-N	-5.04	115.76	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	HIS	C-N-CA	-5.04	115.76	122.72
1	C	74	SER	O-C-N	-5.04	115.88	122.59
1	C	56	VAL	CA-CB-CG2	5.04	118.96	110.40
1	A	68	TRP	O-C-N	5.03	128.93	122.19
1	B	23	PRO	N-CA-C	5.02	122.81	112.47
1	A	56	VAL	CA-CB-CG2	5.00	118.91	110.40

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	-6	LYS	CA
1	A	67	SER	CA
1	B	86	GLN	CA
1	C	-5	PRO	CA
1	C	37	VAL	CA
1	C	74	SER	CA
1	D	371	ARG	CA
1	D	86	GLN	CA
1	D	97	ASN	CA
1	D	152	LYS	CA
1	D	156	ASP	CA

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Sidechain
1	A	168	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	71	ARG	Sidechain
1	A	79	ARG	Sidechain
1	B	125	ARG	Sidechain
1	B	140	ARG	Sidechain
1	B	168	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	371	ARG	Sidechain
1	B	64	ARG	Sidechain
1	B	79	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	140	ARG	Sidechain
1	C	171	ARG	Sidechain
1	C	371	ARG	Sidechain
1	C	64	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	125	ARG	Sidechain
1	D	140	ARG	Sidechain
1	D	171	ARG	Sidechain
1	D	371	ARG	Sidechain
1	D	64	ARG	Sidechain
1	D	71	ARG	Sidechain
1	D	79	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	1492	0	1416	279	2
1	B	1464	0	1393	285	0
1	C	1505	0	1435	290	1
1	D	1480	0	1408	275	1
All	All	5941	0	5652	1071	3

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 92.

All (1071) 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:D:41:PRO:HB2	1:D:81:ILE:CD1	1.47	1.43
1:C:43:VAL:HG12	1:C:81:ILE:CD1	1.50	1.39
1:D:154:SER:HB2	1:D:159:ALA:CB	1.51	1.39
1:D:41:PRO:CB	1:D:81:ILE:HD11	1.55	1.36
1:C:94:GLU:C	1:C:95:ASN:HD22	1.32	1.33
1:D:154:SER:CB	1:D:159:ALA:HB3	1.61	1.31
1:C:86:GLN:O	1:C:86:GLN:NE2	1.64	1.30
1:B:151:TYR:CD2	1:B:157:PHE:HB3	1.65	1.28
1:A:7:GLU:CD	1:A:8:GLN:H	1.42	1.26
1:A:7:GLU:CG	1:A:8:GLN:H	1.50	1.24
1:A:109:VAL:HG23	1:A:116:HIS:CE1	1.71	1.24
1:D:154:SER:HA	1:D:157:PHE:CZ	1.73	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:PHE:CE1	1:D:159:ALA:HB2	1.74	1.22
1:D:69:THR:HB	1:D:371:ARG:N	1.55	1.21
1:D:69:THR:CG2	1:D:371:ARG:HA	1.69	1.21
1:A:24:ASN:O	1:A:25:LEU:HD23	1.03	1.20
1:B:157:PHE:HD1	1:B:157:PHE:O	1.24	1.20
1:D:7:GLU:O	1:D:33:GLY:HA3	1.42	1.16
1:B:2:LYS:NZ	1:B:38:GLN:OE1	1.77	1.15
1:C:43:VAL:HG12	1:C:81:ILE:HD11	1.26	1.15
1:A:10:ASN:HB3	1:A:12:GLN:NE2	1.60	1.14
1:B:144:TYR:O	1:B:146:LEU:HD13	1.46	1.14
1:A:72:THR:O	1:A:73:ASP:OD1	1.64	1.14
1:D:16:HIS:ND1	1:D:29:VAL:HG13	1.65	1.12
1:A:32:ALA:HB3	1:A:74:SER:HB3	1.11	1.11
1:D:94:GLU:HA	1:D:120:LYS:O	1.48	1.11
1:A:64:ARG:HG2	1:A:64:ARG:NH1	1.50	1.11
1:A:92:LEU:HD22	1:A:112:PHE:CE2	1.84	1.11
1:C:9:GLU:OE1	1:C:64:ARG:NH1	1.82	1.11
1:D:16:HIS:CE1	1:D:29:VAL:HG13	1.85	1.11
1:A:10:ASN:CB	1:A:12:GLN:HE21	1.63	1.09
1:A:64:ARG:HH11	1:A:64:ARG:CG	1.65	1.09
1:C:94:GLU:C	1:C:95:ASN:ND2	2.09	1.09
1:A:24:ASN:O	1:A:25:LEU:CD2	1.99	1.09
1:C:173:MET:CE	1:D:83:VAL:H	1.66	1.09
1:A:28:THR:HG22	1:A:29:VAL:H	1.06	1.09
1:C:43:VAL:HG12	1:C:81:ILE:HD13	1.24	1.09
1:D:69:THR:HG22	1:D:371:ARG:HA	1.12	1.09
1:C:173:MET:HE2	1:D:83:VAL:N	1.68	1.08
1:C:175:TRP:HA	1:D:-1:ASN:HB3	1.35	1.08
1:C:136:TYR:HB3	1:C:137:PRO:HD2	1.32	1.08
1:B:157:PHE:O	1:B:157:PHE:CD1	2.07	1.07
1:C:173:MET:HE2	1:D:83:VAL:HB	1.30	1.07
1:A:7:GLU:HG2	1:A:8:GLN:N	1.68	1.07
1:C:94:GLU:HG3	1:C:95:ASN:ND2	1.70	1.06
1:B:18:LEU:HD12	1:B:19:ASN:H	1.18	1.06
1:C:173:MET:HE2	1:D:83:VAL:CB	1.87	1.05
1:A:7:GLU:OE1	1:A:8:GLN:N	1.89	1.04
1:B:7:GLU:HA	1:B:14:HIS:NE2	1.72	1.04
1:C:137:PRO:HD3	1:C:165:GLN:NE2	1.72	1.04
1:D:41:PRO:CB	1:D:81:ILE:CD1	2.23	1.04
1:A:10:ASN:HB3	1:A:12:GLN:HE21	0.92	1.04
1:B:151:TYR:HD2	1:B:157:PHE:HB3	0.90	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ALA:HB2	1:A:75:LEU:HB2	1.36	1.03
1:D:135:GLN:HG2	1:D:142:LEU:H	1.23	1.02
1:C:173:MET:HE2	1:D:83:VAL:H	1.20	1.02
1:A:65:TRP:CE3	1:A:72:THR:HB	1.95	1.01
1:B:92:LEU:HD13	1:B:124:VAL:HG22	1.37	1.01
1:C:86:GLN:CD	1:C:86:GLN:H	1.67	1.01
1:B:18:LEU:HD12	1:B:19:ASN:N	1.75	1.01
1:B:58:GLU:O	1:B:59:LYS:HB2	1.58	1.00
1:C:79:ARG:HG3	1:C:79:ARG:HH11	1.23	1.00
1:C:121:VAL:HB	1:C:164:VAL:HG23	1.42	1.00
1:D:145:LEU:C	1:D:146:LEU:HD12	1.86	1.00
1:C:94:GLU:O	1:C:95:ASN:ND2	1.95	1.00
1:B:94:GLU:HG3	1:B:95:ASN:N	1.71	0.99
1:C:43:VAL:CG1	1:C:81:ILE:HD13	1.92	0.98
1:B:48:ALA:HB2	1:B:76:SER:HB3	1.45	0.98
1:D:7:GLU:O	1:D:33:GLY:CA	2.10	0.98
1:D:154:SER:HB2	1:D:159:ALA:HB3	1.07	0.98
1:A:92:LEU:HD22	1:A:112:PHE:HE2	1.14	0.98
1:D:157:PHE:HE1	1:D:159:ALA:HB2	1.20	0.97
1:B:151:TYR:CD2	1:B:157:PHE:CB	2.46	0.97
1:A:106:ILE:O	1:A:107:ASP:N	1.96	0.97
1:C:43:VAL:CG1	1:C:81:ILE:CD1	2.44	0.96
1:C:151:TYR:CD2	1:C:157:PHE:HB3	2.01	0.96
1:A:7:GLU:CD	1:A:8:GLN:N	2.19	0.95
1:D:69:THR:CB	1:D:371:ARG:N	2.29	0.95
1:A:109:VAL:HG23	1:A:116:HIS:ND1	1.81	0.95
1:D:-2:LEU:O	1:D:-1:ASN:C	2.07	0.95
1:A:90:ILE:HD11	1:A:146:LEU:HD23	1.49	0.95
1:A:7:GLU:HG2	1:A:8:GLN:H	1.26	0.95
1:A:18:LEU:HD21	1:A:22:CYS:HB2	1.45	0.95
1:D:8:GLN:OE1	1:D:14:HIS:NE2	2.00	0.94
1:A:28:THR:HG22	1:A:29:VAL:N	1.83	0.94
1:B:151:TYR:HD2	1:B:157:PHE:CB	1.80	0.94
1:C:132:VAL:O	1:C:134:TYR:CE1	2.21	0.93
1:C:173:MET:HE2	1:D:83:VAL:CA	1.95	0.93
1:D:14:HIS:ND1	1:D:14:HIS:N	2.14	0.93
1:C:370:SER:O	1:C:71:ARG:HB2	1.67	0.93
1:D:3:ILE:HG23	1:D:3:ILE:O	1.65	0.93
1:C:91:THR:HG23	1:C:104:GLU:HB2	1.51	0.93
1:B:42:TRP:O	1:B:81:ILE:HD11	1.69	0.92
1:C:30:GLU:OE1	1:C:31:LYS:HE3	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:HD21	1:C:22:CYS:HB2	1.51	0.92
1:C:146:LEU:HD13	1:C:146:LEU:N	1.83	0.92
1:C:79:ARG:HG3	1:C:79:ARG:NH1	1.80	0.92
1:C:51:LYS:HG2	1:C:52:GLY:N	1.81	0.92
1:A:7:GLU:CG	1:A:8:GLN:N	2.14	0.91
1:D:154:SER:HB2	1:D:159:ALA:HB1	1.51	0.91
1:B:55:PHE:HE2	1:B:72:THR:HG21	1.34	0.91
1:B:25:LEU:HG	1:B:29:VAL:HG23	1.53	0.91
1:B:8:GLN:O	1:B:9:GLU:O	1.87	0.91
1:B:109:VAL:HG12	1:B:109:VAL:O	1.70	0.91
1:A:72:THR:C	1:A:73:ASP:OD1	2.13	0.91
1:C:173:MET:CE	1:D:83:VAL:HB	2.01	0.90
1:C:47:GLN:HG2	1:C:51:LYS:HD3	1.54	0.90
1:B:55:PHE:CE2	1:B:72:THR:HG21	2.06	0.90
1:A:130:THR:HG22	1:A:170:ILE:HB	1.54	0.89
1:C:136:TYR:HB3	1:C:137:PRO:CD	2.02	0.89
1:D:9:GLU:HG2	1:D:10:ASN:N	1.85	0.89
1:B:7:GLU:HG2	1:B:31:LYS:NZ	1.88	0.89
1:C:64:ARG:O	1:C:67:SER:HB2	1.73	0.89
1:A:10:ASN:CB	1:A:12:GLN:NE2	2.28	0.89
1:D:86:GLN:HA	1:D:86:GLN:OE1	1.73	0.89
1:D:98:PHE:CD1	1:D:98:PHE:N	2.38	0.89
1:B:34:SER:O	1:B:35:VAL:HG23	1.74	0.88
1:D:86:GLN:OE1	1:D:86:GLN:N	2.06	0.88
1:B:153:ASP:H	1:B:156:ASP:CB	1.87	0.88
1:A:18:LEU:HD11	1:A:22:CYS:SG	2.13	0.88
1:C:18:LEU:HD21	1:C:22:CYS:CB	2.03	0.88
1:B:158:GLY:O	1:B:160:PRO:HD3	1.74	0.87
1:B:-2:LEU:N	1:B:-2:LEU:CD2	2.37	0.87
1:C:86:GLN:CD	1:C:86:GLN:N	2.26	0.87
1:A:32:ALA:HB3	1:A:74:SER:CB	2.01	0.87
1:A:110:PRO:O	1:A:166:SER:HB3	1.75	0.86
1:B:-2:LEU:HD23	1:B:-2:LEU:H3	1.39	0.86
1:C:25:LEU:O	1:C:28:THR:HB	1.75	0.86
1:D:69:THR:CG2	1:D:371:ARG:CA	2.54	0.86
1:B:26:LYS:HE3	1:B:74:SER:HB2	1.56	0.86
1:D:-1:ASN:O	1:D:39:ALA:HB3	1.74	0.86
1:A:32:ALA:CB	1:A:74:SER:HB3	2.04	0.86
1:B:27:GLU:C	1:B:27:GLU:OE1	2.19	0.86
1:C:6:PHE:HD1	1:C:6:PHE:N	1.69	0.86
1:C:22:CYS:SG	1:C:25:LEU:HD23	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLN:HB2	1:C:142:LEU:H	1.38	0.85
1:B:49:ASN:C	1:B:50:CYS:SG	2.59	0.85
1:B:69:THR:C	1:B:370:SER:H	1.83	0.85
1:A:86:GLN:HB2	1:B:88:HIS:HE1	1.41	0.84
1:B:7:GLU:HG2	1:B:31:LYS:HZ2	1.40	0.84
1:A:5:ILE:O	1:A:5:ILE:HG22	1.77	0.84
1:D:69:THR:HG22	1:D:371:ARG:CA	2.04	0.84
1:C:5:ILE:HD13	1:C:5:ILE:O	1.77	0.84
1:D:89:LYS:HB3	1:D:127:GLN:HG3	1.60	0.83
1:C:5:ILE:CD1	1:C:16:HIS:O	2.25	0.83
1:B:153:ASP:H	1:B:156:ASP:HB2	1.42	0.83
1:A:18:LEU:HD21	1:A:22:CYS:CB	2.09	0.83
1:A:145:LEU:O	1:A:146:LEU:HD12	1.76	0.83
1:B:7:GLU:HB2	1:B:14:HIS:CG	2.13	0.83
1:D:69:THR:HB	1:D:371:ARG:H	1.41	0.83
1:A:7:GLU:OE2	1:A:14:HIS:N	2.11	0.83
1:C:94:GLU:CG	1:C:95:ASN:ND2	2.40	0.83
1:D:16:HIS:ND1	1:D:29:VAL:CG1	2.41	0.83
1:C:6:PHE:N	1:C:6:PHE:CD1	2.40	0.82
1:D:167:VAL:O	1:D:167:VAL:CG1	2.27	0.82
1:A:7:GLU:HB3	1:A:14:HIS:O	1.79	0.82
1:A:44:GLY:O	1:A:45:TYR:CG	2.32	0.82
1:D:69:THR:HB	1:D:71:ARG:C	2.04	0.82
1:B:65:TRP:HA	1:B:68:TRP:CH2	2.14	0.81
1:A:40:GLY:H	1:B:174:GLN:HG3	1.44	0.81
1:C:47:GLN:HB3	1:C:51:LYS:O	1.80	0.81
1:B:103:MET:HB2	1:B:118:TYR:CD2	2.16	0.81
1:A:5:ILE:HD11	1:A:75:LEU:HD13	1.63	0.81
1:B:44:GLY:O	1:B:45:TYR:CD1	2.34	0.81
1:C:53:GLU:OE2	1:C:55:PHE:HE1	1.64	0.81
1:B:135:GLN:HG2	1:B:136:TYR:CE1	2.16	0.80
1:D:69:THR:CB	1:D:371:ARG:H	1.91	0.80
1:D:98:PHE:N	1:D:98:PHE:HD1	1.75	0.80
1:B:8:GLN:HG2	1:B:31:LYS:HZ1	1.43	0.80
1:B:144:TYR:O	1:B:145:LEU:C	2.22	0.80
1:D:167:VAL:O	1:D:167:VAL:HG13	1.80	0.80
1:B:8:GLN:CG	1:B:31:LYS:HZ1	1.94	0.80
1:C:5:ILE:C	1:C:6:PHE:HD1	1.89	0.80
1:C:5:ILE:CD1	1:C:5:ILE:H	1.94	0.79
1:C:86:GLN:NE2	1:C:86:GLN:C	2.39	0.79
1:C:95:ASN:HD22	1:C:95:ASN:N	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:ASN:HB2	1:A:1:PRO:CD	2.12	0.79
1:A:18:LEU:HD11	1:A:22:CYS:CB	2.13	0.79
1:A:47:GLN:HB2	1:A:51:LYS:O	1.83	0.78
1:B:72:THR:HG22	1:B:73:ASP:H	1.48	0.78
1:A:28:THR:HG21	1:A:29:VAL:HG12	1.65	0.78
1:A:37:VAL:HG12	1:A:59:LYS:HA	1.65	0.78
1:A:7:GLU:OE2	1:A:13:GLY:HA3	1.83	0.78
1:D:155:GLY:O	1:D:156:ASP:C	2.23	0.78
1:A:136:TYR:C	1:A:165:GLN:HB2	2.08	0.78
1:D:23:PRO:O	1:D:24:ASN:HB2	1.83	0.78
1:D:26:LYS:HD3	1:D:29:VAL:O	1.84	0.78
1:A:109:VAL:CG2	1:A:116:HIS:ND1	2.47	0.78
1:C:58:GLU:OE2	1:D:168:ARG:NH2	2.17	0.77
1:C:125:ARG:HH11	1:C:125:ARG:HG2	1.48	0.77
1:A:44:GLY:O	1:A:45:TYR:CD1	2.37	0.77
1:B:152:LYS:N	1:B:156:ASP:OD2	2.18	0.77
1:D:86:GLN:OE1	1:D:86:GLN:CA	2.33	0.77
1:D:41:PRO:CG	1:D:81:ILE:CD1	2.62	0.77
1:D:159:ALA:O	1:D:162:PRO:HD3	1.85	0.77
1:D:98:PHE:HD1	1:D:98:PHE:H	1.33	0.77
1:C:136:TYR:CB	1:C:137:PRO:CD	2.60	0.76
1:D:42:TRP:CE3	1:D:80:PRO:HD3	2.20	0.76
1:B:144:TYR:CE2	1:B:157:PHE:HE1	2.04	0.76
1:A:4:ILE:O	1:A:6:PHE:CD1	2.38	0.76
1:C:173:MET:HE1	1:D:83:VAL:H	1.51	0.76
1:C:175:TRP:HA	1:D:-1:ASN:CB	2.15	0.76
1:D:132:VAL:CG2	1:D:170:ILE:HD11	2.16	0.76
1:C:4:ILE:HG22	1:C:6:PHE:CE1	2.21	0.76
1:C:173:MET:CE	1:D:83:VAL:N	2.34	0.76
1:D:-2:LEU:O	1:D:1:PRO:C	2.29	0.76
1:D:3:ILE:O	1:D:3:ILE:CG2	2.34	0.76
1:A:4:ILE:O	1:A:6:PHE:HD1	1.69	0.75
1:B:-2:LEU:N	1:B:-2:LEU:HD23	2.01	0.75
1:C:44:GLY:HA2	1:C:78:LEU:HD23	1.68	0.75
1:B:93:TYR:HB2	1:B:123:SER:HB2	1.67	0.75
1:B:175:TRP:H	1:B:175:TRP:CD1	2.04	0.74
1:D:28:THR:C	1:D:29:VAL:H	1.93	0.74
1:D:95:ASN:C	1:D:95:ASN:HD22	1.95	0.74
1:A:109:VAL:CG2	1:A:116:HIS:CE1	2.63	0.74
1:C:37:VAL:HG12	1:C:59:LYS:HA	1.67	0.74
1:A:65:TRP:CZ3	1:A:72:THR:HB	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:PHE:N	1:B:98:PHE:CD1	2.53	0.74
1:D:154:SER:CA	1:D:157:PHE:CZ	2.64	0.74
1:A:7:GLU:HG3	1:A:14:HIS:HB3	1.69	0.74
1:C:-7:GLY:C	1:C:-6:LYS:HG2	2.11	0.74
1:C:50:CYS:SG	1:C:79:ARG:HD3	2.28	0.74
1:D:146:LEU:HD12	1:D:146:LEU:N	2.01	0.74
1:C:91:THR:HG23	1:C:104:GLU:CB	2.18	0.73
1:D:5:ILE:O	1:D:5:ILE:CG1	2.34	0.73
1:A:-1:ASN:HB2	1:A:1:PRO:HD2	1.68	0.73
1:B:46:GLU:O	1:B:73:ASP:HB2	1.88	0.73
1:D:96:PRO:HA	1:D:123:SER:OG	1.88	0.73
1:C:70:SER:HB3	1:D:140:ARG:HG2	1.69	0.73
1:D:154:SER:HA	1:D:157:PHE:CE2	2.22	0.73
1:B:109:VAL:HG11	1:B:112:PHE:CE1	2.22	0.73
1:D:88:HIS:HA	1:D:128:SER:OG	1.88	0.73
1:D:153:ASP:OD2	1:D:155:GLY:HA3	1.87	0.73
1:A:5:ILE:HD11	1:A:75:LEU:CD1	2.18	0.73
1:B:27:GLU:OE1	1:B:28:THR:N	2.22	0.73
1:B:88:HIS:CD2	1:B:169:ARG:CZ	2.72	0.73
1:C:53:GLU:CD	1:C:55:PHE:HE1	1.96	0.73
1:B:92:LEU:CD1	1:B:124:VAL:HG22	2.15	0.73
1:A:98:PHE:CD1	1:A:123:SER:HB3	2.23	0.72
1:B:7:GLU:HA	1:B:14:HIS:CD2	2.23	0.72
1:B:37:VAL:HB	1:B:59:LYS:HA	1.69	0.72
1:C:136:TYR:HA	1:C:165:GLN:HE21	1.54	0.72
1:C:5:ILE:HD13	1:C:5:ILE:H	1.52	0.72
1:A:93:TYR:CE2	1:A:98:PHE:HB3	2.25	0.72
1:B:143:GLN:O	1:B:144:TYR:HD1	1.73	0.72
1:D:-2:LEU:O	1:D:1:PRO:O	2.07	0.72
1:C:47:GLN:HG2	1:C:51:LYS:CD	2.18	0.72
1:C:94:GLU:HG2	1:C:101:LYS:N	2.05	0.72
1:B:3:ILE:CG2	1:B:18:LEU:HB3	2.20	0.72
1:C:-4:GLN:O	1:C:-3:PRO:O	2.07	0.72
1:C:121:VAL:CB	1:C:164:VAL:HG23	2.18	0.71
1:D:53:GLU:HB3	1:D:55:PHE:HE1	1.53	0.71
1:D:69:THR:CG2	1:D:371:ARG:N	2.53	0.71
1:A:59:LYS:HD2	1:B:174:GLN:NE2	2.03	0.71
1:B:103:MET:HE1	1:B:112:PHE:HD1	1.55	0.71
1:A:9:GLU:HA	1:A:34:SER:OG	1.90	0.71
1:A:18:LEU:HD11	1:A:22:CYS:HB3	1.71	0.71
1:D:24:ASN:OD1	1:D:26:LYS:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TRP:HD1	1:B:40:GLY:O	1.72	0.71
1:D:119:GLU:CD	1:D:119:GLU:H	1.98	0.71
1:B:137:PRO:HA	1:B:166:SER:OG	1.91	0.71
1:A:40:GLY:N	1:B:174:GLN:HG3	2.05	0.71
1:A:90:ILE:HD11	1:A:146:LEU:CD2	2.20	0.71
1:B:155:GLY:C	1:B:157:PHE:H	1.99	0.70
1:D:144:TYR:O	1:D:146:LEU:CD1	2.38	0.70
1:A:3:ILE:HG23	1:A:3:ILE:O	1.91	0.70
1:B:26:LYS:HE2	1:B:74:SER:O	1.91	0.70
1:C:146:LEU:N	1:C:146:LEU:CD1	2.54	0.70
1:D:112:PHE:N	1:D:165:GLN:O	2.21	0.70
1:D:155:GLY:O	1:D:158:GLY:N	2.24	0.70
1:C:9:GLU:HA	1:C:33:GLY:O	1.90	0.70
1:D:5:ILE:O	1:D:5:ILE:HG12	1.91	0.70
1:C:36:LEU:HD23	1:C:36:LEU:C	2.17	0.70
1:D:-2:LEU:HA	1:D:19:ASN:HD22	1.56	0.70
1:B:-2:LEU:H1	1:B:-2:LEU:HD22	1.57	0.70
1:C:370:SER:O	1:C:71:ARG:CB	2.33	0.70
1:A:154:SER:HA	1:A:157:PHE:CD1	2.25	0.70
1:B:94:GLU:CG	1:B:95:ASN:N	2.48	0.70
1:B:65:TRP:HA	1:B:68:TRP:CZ3	2.27	0.70
1:D:22:CYS:SG	1:D:25:LEU:HD23	2.32	0.69
1:D:26:LYS:HZ2	1:D:30:GLU:C	2.00	0.69
1:D:154:SER:CA	1:D:159:ALA:HB3	2.21	0.69
1:A:25:LEU:O	1:A:28:THR:HB	1.92	0.69
1:B:7:GLU:CG	1:B:31:LYS:HZ2	2.05	0.69
1:A:174:GLN:NE2	1:B:59:LYS:HD2	2.07	0.69
1:B:8:GLN:HB3	1:B:31:LYS:NZ	2.07	0.69
1:B:144:TYR:CD2	1:B:157:PHE:CE1	2.80	0.69
1:B:135:GLN:HG2	1:B:136:TYR:CZ	2.28	0.69
1:C:91:THR:CG2	1:C:104:GLU:HB2	2.22	0.69
1:C:153:ASP:O	1:C:156:ASP:HB2	1.92	0.69
1:D:135:GLN:HG2	1:D:142:LEU:N	2.03	0.69
1:A:59:LYS:HD2	1:B:174:GLN:HE22	1.56	0.69
1:B:7:GLU:CA	1:B:14:HIS:CD2	2.76	0.69
1:B:18:LEU:HD21	1:B:20:GLY:O	1.93	0.69
1:B:98:PHE:N	1:B:98:PHE:HD1	1.89	0.69
1:C:91:THR:HG23	1:C:104:GLU:HA	1.74	0.69
1:C:5:ILE:O	1:C:5:ILE:CD1	2.40	0.69
1:D:7:GLU:HA	1:D:31:LYS:O	1.91	0.69
1:D:88:HIS:O	1:D:131:TRP:HZ2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASP:HB3	1:C:168:ARG:HA	1.75	0.69
1:A:7:GLU:OE1	1:A:12:GLN:O	2.09	0.68
1:A:8:GLN:HB2	1:A:12:GLN:O	1.92	0.68
1:D:-2:LEU:CD1	1:D:2:LYS:HB2	2.23	0.68
1:C:20:GLY:O	1:C:21:PRO:O	2.11	0.68
1:C:136:TYR:CB	1:C:137:PRO:HD2	2.14	0.68
1:B:157:PHE:CD1	1:B:157:PHE:C	2.71	0.68
1:C:137:PRO:O	1:C:138:GLY:C	2.36	0.68
1:D:41:PRO:HD2	1:D:81:ILE:HD12	1.74	0.68
1:C:45:TYR:HB2	1:C:77:SER:HB2	1.75	0.68
1:C:44:GLY:CA	1:C:78:LEU:HD23	2.24	0.68
1:A:124:VAL:HG23	1:A:151:TYR:HB2	1.76	0.68
1:B:143:GLN:C	1:B:144:TYR:HD1	2.02	0.68
1:A:130:THR:CG2	1:A:170:ILE:HB	2.22	0.68
1:A:136:TYR:HA	1:A:165:GLN:HG3	1.73	0.68
1:C:92:LEU:HD22	1:C:112:PHE:CZ	2.29	0.68
1:C:132:VAL:O	1:C:134:TYR:HE1	1.72	0.68
1:C:89:LYS:HD2	1:C:127:GLN:HE21	1.59	0.67
1:C:70:SER:HA	1:C:71:ARG:NH2	2.10	0.67
1:D:28:THR:O	1:D:29:VAL:N	2.27	0.67
1:D:161:GLN:O	1:D:163:GLN:N	2.26	0.67
1:A:84:ASP:OD2	1:A:86:GLN:NE2	2.27	0.67
1:C:79:ARG:NH1	1:C:79:ARG:CG	2.52	0.67
1:D:8:GLN:HB3	1:D:12:GLN:HB3	1.75	0.67
1:D:154:SER:CB	1:D:159:ALA:CB	2.36	0.67
1:A:86:GLN:HB2	1:B:88:HIS:CE1	2.26	0.67
1:C:125:ARG:HG2	1:C:125:ARG:NH1	2.06	0.67
1:A:90:ILE:HD12	1:A:126:VAL:HG22	1.77	0.67
1:B:142:LEU:HB3	1:B:144:TYR:HE1	1.60	0.67
1:A:154:SER:HA	1:A:157:PHE:HD1	1.60	0.67
1:B:23:PRO:O	1:B:48:ALA:HB1	1.95	0.67
1:C:90:ILE:CG2	1:C:90:ILE:O	2.43	0.67
1:B:91:THR:HG23	1:B:104:GLU:HG3	1.75	0.67
1:C:151:TYR:CE2	1:C:157:PHE:HB3	2.31	0.67
1:C:135:GLN:HB2	1:C:142:LEU:N	2.07	0.66
1:C:137:PRO:HD3	1:C:165:GLN:HE21	1.58	0.66
1:B:3:ILE:HG22	1:B:18:LEU:HB3	1.77	0.66
1:C:106:ILE:O	1:C:107:ASP:N	2.23	0.66
1:B:-2:LEU:CD2	1:B:-2:LEU:H1	2.08	0.66
1:B:91:THR:CG2	1:B:104:GLU:HG3	2.25	0.66
1:A:44:GLY:O	1:A:45:TYR:CD2	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:CYS:SG	1:C:22:CYS:O	2.53	0.66
1:A:83:VAL:HG13	1:B:173:MET:SD	2.35	0.66
1:B:47:GLN:O	1:B:76:SER:HB2	1.96	0.66
1:B:109:VAL:HG11	1:B:112:PHE:CD1	2.29	0.66
1:A:61:GLU:C	1:A:63:PRO:HD3	2.20	0.66
1:D:-3:PRO:O	1:D:-2:LEU:C	2.39	0.66
1:D:-2:LEU:HD12	1:D:19:ASN:ND2	2.11	0.66
1:D:41:PRO:C	1:D:81:ILE:HD11	2.21	0.66
1:A:7:GLU:CG	1:A:14:HIS:HB3	2.27	0.65
1:A:32:ALA:CB	1:A:75:LEU:HB2	2.19	0.65
1:A:24:ASN:C	1:A:25:LEU:HD23	2.12	0.65
1:A:28:THR:CG2	1:A:29:VAL:HG12	2.26	0.65
1:C:25:LEU:C	1:C:28:THR:HB	2.20	0.65
1:D:25:LEU:O	1:D:29:VAL:HG23	1.97	0.65
1:B:109:VAL:O	1:B:109:VAL:CG1	2.42	0.65
1:A:95:ASN:HD21	1:A:99:THR:HB	1.61	0.65
1:B:144:TYR:O	1:B:146:LEU:CD1	2.34	0.65
1:A:49:ASN:O	1:A:50:CYS:HB2	1.95	0.65
1:A:72:THR:O	1:A:73:ASP:CG	2.39	0.65
1:B:44:GLY:C	1:B:45:TYR:CD1	2.75	0.65
1:D:26:LYS:NZ	1:D:30:GLU:C	2.55	0.65
1:B:34:SER:O	1:B:35:VAL:CG2	2.44	0.65
1:C:5:ILE:HD13	1:C:5:ILE:N	2.11	0.65
1:D:69:THR:CG2	1:D:371:ARG:H	2.10	0.65
1:B:26:LYS:CE	1:B:74:SER:HB2	2.28	0.64
1:D:-2:LEU:C	1:D:1:PRO:HD2	2.22	0.64
1:A:92:LEU:HD22	1:A:112:PHE:CZ	2.30	0.64
1:A:-6:LYS:CB	1:A:-5:PRO:CD	2.75	0.64
1:B:26:LYS:HG2	1:B:76:SER:HA	1.78	0.64
1:B:103:MET:HE1	1:B:112:PHE:CD1	2.32	0.64
1:A:120:LYS:HZ1	1:A:162:PRO:HG2	1.63	0.64
1:A:64:ARG:O	1:A:66:ASP:N	2.31	0.64
1:B:-1:ASN:HB2	1:B:1:PRO:HD2	1.79	0.64
1:D:-2:LEU:HD11	1:D:2:LYS:HB2	1.80	0.64
1:B:153:ASP:OD1	1:B:154:SER:N	2.30	0.64
1:D:131:TRP:CH2	1:D:169:ARG:HD3	2.33	0.64
1:C:92:LEU:HD22	1:C:112:PHE:HZ	1.60	0.64
1:D:42:TRP:CZ3	1:D:80:PRO:HD3	2.32	0.64
1:A:7:GLU:OE2	1:A:13:GLY:CA	2.46	0.63
1:B:49:ASN:N	1:B:49:ASN:HD22	1.96	0.63
1:B:144:TYR:CE2	1:B:159:ALA:HB2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:C	1:B:146:LEU:HD13	2.23	0.63
1:B:157:PHE:CE1	1:B:159:ALA:HB2	2.33	0.63
1:D:134:TYR:CD2	1:D:139:TYR:C	2.76	0.63
1:B:21:PRO:O	1:B:22:CYS:HB2	1.97	0.63
1:A:6:PHE:CD2	1:A:11:PHE:HA	2.32	0.63
1:A:120:LYS:NZ	1:A:162:PRO:HG2	2.12	0.63
1:C:96:PRO:O	1:C:97:ASN:HB2	1.99	0.63
1:D:136:TYR:HB3	1:D:137:PRO:HD2	1.79	0.63
1:D:132:VAL:HG23	1:D:170:ILE:HG12	1.80	0.63
1:D:153:ASP:C	1:D:155:GLY:N	2.50	0.63
1:B:8:GLN:CG	1:B:31:LYS:NZ	2.62	0.63
1:D:26:LYS:CD	1:D:29:VAL:O	2.47	0.63
1:D:159:ALA:HB1	1:D:162:PRO:HA	1.80	0.63
1:B:8:GLN:CB	1:B:31:LYS:NZ	2.62	0.63
1:C:84:ASP:CG	1:C:84:ASP:O	2.40	0.63
1:C:151:TYR:CD1	1:C:151:TYR:N	2.67	0.63
1:A:21:PRO:HD3	1:A:80:PRO:HD3	1.80	0.63
1:B:158:GLY:O	1:B:160:PRO:CD	2.45	0.63
1:C:69:THR:HG22	1:C:71:ARG:H	1.63	0.63
1:B:155:GLY:O	1:B:157:PHE:N	2.31	0.62
1:C:18:LEU:CD2	1:C:22:CYS:HB2	2.27	0.62
1:C:86:GLN:OE1	1:D:88:HIS:NE2	2.32	0.62
1:D:92:LEU:HD13	1:D:112:PHE:CZ	2.34	0.62
1:A:10:ASN:O	1:A:11:PHE:HB2	1.99	0.62
1:C:-1:ASN:O	1:C:-1:ASN:ND2	2.32	0.62
1:D:8:GLN:OE1	1:D:14:HIS:CE1	2.52	0.62
1:D:154:SER:C	1:D:159:ALA:HB3	2.23	0.62
1:A:92:LEU:CD2	1:A:112:PHE:CE2	2.74	0.62
1:D:155:GLY:O	1:D:157:PHE:N	2.32	0.62
1:A:135:GLN:HG2	1:A:136:TYR:CE1	2.34	0.62
1:A:136:TYR:O	1:A:165:GLN:HB2	1.99	0.62
1:B:18:LEU:CD1	1:B:19:ASN:N	2.58	0.62
1:A:92:LEU:HD23	1:A:121:VAL:HG11	1.81	0.62
1:A:63:PRO:O	1:A:64:ARG:HB3	1.99	0.62
1:C:47:GLN:HB3	1:C:51:LYS:C	2.24	0.62
1:C:91:THR:N	1:C:125:ARG:O	2.28	0.62
1:A:58:GLU:O	1:A:59:LYS:C	2.41	0.61
1:C:-1:ASN:N	1:C:-1:ASN:HD22	1.97	0.61
1:B:45:TYR:N	1:B:55:PHE:CE1	2.68	0.61
1:D:41:PRO:CD	1:D:81:ILE:HD12	2.30	0.61
1:B:72:THR:HG22	1:B:73:ASP:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:PHE:CE1	1:D:159:ALA:CB	2.68	0.61
1:A:-6:LYS:CB	1:A:-5:PRO:HD3	2.31	0.61
1:B:69:THR:O	1:B:370:SER:N	2.28	0.61
1:C:90:ILE:O	1:C:90:ILE:HG23	1.98	0.61
1:D:9:GLU:CG	1:D:10:ASN:N	2.61	0.61
1:A:50:CYS:HB2	1:A:51:LYS:HZ1	1.65	0.61
1:A:56:VAL:N	1:B:143:GLN:OE1	2.23	0.61
1:A:169:ARG:NH2	1:A:171:ARG:HE	1.98	0.61
1:D:-2:LEU:HD12	1:D:19:ASN:HD21	1.65	0.61
1:D:65:TRP:CE3	1:D:69:THR:HG21	2.35	0.61
1:B:41:PRO:HG2	1:B:81:ILE:HB	1.83	0.61
1:C:25:LEU:HA	1:C:28:THR:HB	1.82	0.61
1:C:69:THR:CG2	1:C:71:ARG:H	2.13	0.61
1:C:14:HIS:ND1	1:C:29:VAL:HG13	2.15	0.61
1:C:6:PHE:HA	1:C:15:SER:HA	1.82	0.61
1:C:94:GLU:CD	1:C:95:ASN:HD21	2.08	0.61
1:D:-2:LEU:O	1:D:1:PRO:N	2.33	0.61
1:D:28:THR:C	1:D:29:VAL:N	2.58	0.61
1:A:129:GLY:HA2	1:B:84:ASP:O	2.01	0.60
1:A:40:GLY:H	1:B:174:GLN:CG	2.13	0.60
1:D:47:GLN:HG2	1:D:51:LYS:O	2.01	0.60
1:A:64:ARG:HG2	1:A:64:ARG:HH11	0.70	0.60
1:B:9:GLU:HG2	1:B:64:ARG:HG3	1.84	0.60
1:A:25:LEU:O	1:A:29:VAL:O	2.19	0.60
1:C:137:PRO:CD	1:C:165:GLN:NE2	2.58	0.60
1:D:41:PRO:HB2	1:D:81:ILE:HD11	0.67	0.60
1:D:41:PRO:CA	1:D:81:ILE:HD11	2.30	0.60
1:D:159:ALA:O	1:D:160:PRO:C	2.44	0.60
1:C:121:VAL:HB	1:C:164:VAL:CG2	2.27	0.60
1:D:45:TYR:CE2	1:D:50:CYS:HB3	2.37	0.60
1:D:-2:LEU:HA	1:D:19:ASN:ND2	2.16	0.60
1:D:89:LYS:CB	1:D:127:GLN:HG3	2.29	0.60
1:A:130:THR:O	1:A:170:ILE:N	2.31	0.60
1:B:-1:ASN:CB	1:B:1:PRO:CD	2.79	0.60
1:D:9:GLU:HG2	1:D:10:ASN:HB2	1.83	0.60
1:B:92:LEU:HD13	1:B:124:VAL:CG2	2.22	0.59
1:D:88:HIS:N	1:D:88:HIS:ND1	2.50	0.59
1:D:109:VAL:O	1:D:166:SER:HB2	2.02	0.59
1:B:93:TYR:CE1	1:B:102:LYS:HB2	2.37	0.59
1:C:-6:LYS:CG	1:C:-5:PRO:HD3	2.33	0.59
1:C:6:PHE:CD1	1:C:15:SER:HB2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:CD1	1:A:22:CYS:HB3	2.33	0.59
1:B:58:GLU:O	1:B:59:LYS:CB	2.30	0.59
1:C:-6:LYS:HG3	1:C:-5:PRO:HD3	1.83	0.59
1:C:70:SER:HB3	1:D:140:ARG:CG	2.31	0.59
1:D:153:ASP:O	1:D:154:SER:C	2.44	0.59
1:D:306:ASP:O	1:D:171:ARG:NH2	2.35	0.59
1:B:136:TYR:HB3	1:B:137:PRO:HD2	1.83	0.59
1:B:153:ASP:H	1:B:156:ASP:HB3	1.65	0.59
1:C:53:GLU:OE2	1:C:55:PHE:CE1	2.53	0.59
1:B:25:LEU:HD12	1:B:29:VAL:HG21	1.85	0.59
1:D:106:ILE:HG23	1:D:106:ILE:O	2.02	0.59
1:A:2:LYS:O	1:A:3:ILE:HB	2.01	0.59
1:A:69:THR:HG22	1:A:370:SER:HB2	1.83	0.59
1:B:8:GLN:CB	1:B:31:LYS:HZ1	2.15	0.59
1:B:103:MET:SD	1:B:112:PHE:CD1	2.96	0.59
1:A:161:GLN:O	1:A:163:GLN:N	2.35	0.58
1:B:4:ILE:HA	1:B:16:HIS:O	2.03	0.58
1:B:42:TRP:O	1:B:81:ILE:CD1	2.50	0.58
1:C:5:ILE:HD12	1:C:16:HIS:O	2.02	0.58
1:C:161:GLN:HA	1:C:161:GLN:NE2	2.17	0.58
1:B:15:SER:C	1:B:16:HIS:ND1	2.62	0.58
1:C:4:ILE:HG22	1:C:6:PHE:HE1	1.64	0.58
1:C:110:PRO:HG3	1:C:139:TYR:OH	2.02	0.58
1:A:5:ILE:HG12	1:A:35:VAL:HG22	1.85	0.58
1:A:92:LEU:CD2	1:A:112:PHE:CZ	2.87	0.58
1:C:92:LEU:HD12	1:C:92:LEU:N	2.17	0.58
1:B:69:THR:C	1:B:370:SER:N	2.55	0.58
1:C:135:GLN:HB3	1:C:141:GLY:HA3	1.86	0.58
1:A:-1:ASN:CB	1:A:1:PRO:CD	2.75	0.58
1:C:5:ILE:O	1:C:5:ILE:CG1	2.52	0.58
1:A:129:GLY:CA	1:B:84:ASP:HB3	2.33	0.57
1:C:121:VAL:HG11	1:C:164:VAL:HG21	1.86	0.57
1:C:133:GLY:C	1:C:134:TYR:CD1	2.82	0.57
1:B:113:HIS:CD2	1:B:318:GLN:HA	2.39	0.57
1:C:46:GLU:OE2	1:C:73:ASP:HB3	2.04	0.57
1:C:370:SER:OG	1:C:71:ARG:N	2.35	0.57
1:D:6:PHE:CD2	1:D:11:PHE:O	2.57	0.57
1:D:41:PRO:C	1:D:81:ILE:CD1	2.77	0.57
1:B:14:HIS:NE2	1:B:31:LYS:O	2.33	0.57
1:B:95:ASN:HB3	1:B:99:THR:HB	1.87	0.57
1:B:153:ASP:N	1:B:156:ASP:HB2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLN:OE1	1:D:88:HIS:CE1	2.58	0.57
1:B:144:TYR:CE2	1:B:157:PHE:CE1	2.91	0.57
1:C:79:ARG:HH11	1:C:79:ARG:CG	1.98	0.57
1:C:30:GLU:CD	1:C:31:LYS:HE3	2.28	0.57
1:A:47:GLN:O	1:A:48:ALA:O	2.23	0.57
1:C:89:LYS:HD2	1:C:127:GLN:NE2	2.19	0.57
1:D:145:LEU:CA	1:D:146:LEU:HD12	2.34	0.57
1:A:29:VAL:HG13	1:A:30:GLU:N	2.16	0.57
1:B:102:LYS:HG2	1:B:103:MET:N	2.04	0.57
1:A:43:VAL:HG11	1:B:145:LEU:HD12	1.87	0.56
1:A:44:GLY:C	1:A:45:TYR:CG	2.82	0.56
1:C:-1:ASN:ND2	1:C:-1:ASN:N	2.51	0.56
1:C:46:GLU:O	1:C:76:SER:HB3	2.05	0.56
1:C:94:GLU:HG3	1:C:95:ASN:HD22	1.48	0.56
1:A:111:SER:OG	1:A:114:ALA:N	2.39	0.56
1:A:134:TYR:CD1	1:A:139:TYR:HB3	2.40	0.56
1:C:11:PHE:C	1:C:12:GLN:NE2	2.64	0.56
1:C:91:THR:CG2	1:C:104:GLU:CB	2.82	0.56
1:A:7:GLU:OE2	1:A:13:GLY:C	2.49	0.56
1:B:4:ILE:HG23	1:B:16:HIS:O	2.05	0.56
1:B:8:GLN:HB3	1:B:31:LYS:HZ1	1.70	0.56
1:D:93:TYR:O	1:D:121:VAL:HA	2.06	0.56
1:D:152:LYS:HA	1:D:156:ASP:HB2	1.87	0.56
1:A:138:GLY:O	1:A:139:TYR:C	2.48	0.56
1:B:134:TYR:CE2	1:B:139:TYR:HB3	2.41	0.56
1:C:86:GLN:NE2	1:C:86:GLN:CA	2.69	0.56
1:D:53:GLU:HB3	1:D:55:PHE:CE1	2.38	0.56
1:A:131:TRP:CZ3	1:A:169:ARG:HB2	2.41	0.56
1:A:133:GLY:HA2	1:A:167:VAL:HG23	1.87	0.56
1:A:57:PHE:HZ	1:A:75:LEU:HD21	1.71	0.56
1:A:125:ARG:HG2	1:A:150:ASP:CG	2.32	0.55
1:C:25:LEU:CA	1:C:28:THR:HB	2.36	0.55
1:B:175:TRP:CD1	1:B:175:TRP:N	2.74	0.55
1:D:78:LEU:O	1:D:79:ARG:HB2	2.06	0.55
1:A:3:ILE:HG13	1:A:37:VAL:HG22	1.88	0.55
1:A:45:TYR:HB2	1:A:77:SER:HB2	1.89	0.55
1:A:59:LYS:HB2	1:B:174:GLN:HE22	1.71	0.55
1:A:80:PRO:HG2	1:A:82:LYS:HE3	1.88	0.55
1:B:121:VAL:O	1:B:162:PRO:CB	2.55	0.55
1:C:-6:LYS:CB	1:C:-5:PRO:HD3	2.36	0.55
1:A:157:PHE:CG	1:A:157:PHE:O	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-1:ASN:ND2	1:C:-1:ASN:C	2.65	0.55
1:D:71:ARG:O	1:D:371:ARG:HB2	2.06	0.55
1:D:-2:LEU:CD1	1:D:19:ASN:HD21	2.19	0.55
1:D:159:ALA:O	1:D:162:PRO:CD	2.54	0.55
1:A:44:GLY:O	1:A:45:TYR:CE1	2.59	0.55
1:C:175:TRP:HB2	1:D:1:PRO:N	2.22	0.55
1:D:112:PHE:CE2	1:D:164:VAL:HG12	2.42	0.55
1:A:16:HIS:CE1	1:A:17:GLU:O	2.60	0.55
1:A:61:GLU:O	1:A:63:PRO:HD3	2.06	0.55
1:B:26:LYS:O	1:B:30:GLU:HG3	2.07	0.55
1:B:96:PRO:O	1:B:97:ASN:C	2.50	0.55
1:C:-1:ASN:HD22	1:C:-1:ASN:C	2.06	0.55
1:D:-1:ASN:HB2	1:D:1:PRO:HD3	1.89	0.55
1:D:112:PHE:HB2	1:D:165:GLN:HA	1.89	0.55
1:A:94:GLU:HG3	1:A:119:GLU:HG3	1.87	0.55
1:B:14:HIS:HB2	1:B:16:HIS:HE1	1.72	0.55
1:B:103:MET:HB2	1:B:118:TYR:CE2	2.42	0.54
1:B:134:TYR:CD2	1:B:139:TYR:HB3	2.42	0.54
1:C:22:CYS:SG	1:C:25:LEU:CD2	2.94	0.54
1:C:132:VAL:O	1:C:134:TYR:CD1	2.60	0.54
1:A:90:ILE:CD1	1:A:126:VAL:HG22	2.37	0.54
1:C:1:PRO:HD3	1:D:175:TRP:CZ3	2.42	0.54
1:D:132:VAL:HG22	1:D:170:ILE:HD11	1.86	0.54
1:A:-1:ASN:HB2	1:A:1:PRO:HD3	1.90	0.54
1:A:3:ILE:HG22	1:A:18:LEU:O	2.08	0.54
1:B:8:GLN:O	1:B:9:GLU:C	2.49	0.54
1:C:92:LEU:N	1:C:92:LEU:CD1	2.70	0.54
1:D:69:THR:HG21	1:D:371:ARG:HA	1.75	0.54
1:D:146:LEU:N	1:D:146:LEU:CD1	2.70	0.54
1:C:47:GLN:HB2	1:C:52:GLY:HA3	1.89	0.54
1:C:118:TYR:HE2	1:C:120:LYS:O	1.90	0.54
1:C:152:LYS:N	1:C:156:ASP:OD2	2.41	0.54
1:D:154:SER:OG	1:D:159:ALA:HB3	2.06	0.54
1:A:48:ALA:C	1:A:50:CYS:N	2.65	0.54
1:D:132:VAL:CG2	1:D:170:ILE:CD1	2.86	0.54
1:A:48:ALA:C	1:A:50:CYS:H	2.15	0.54
1:B:103:MET:HE3	1:B:116:HIS:CB	2.38	0.54
1:C:11:PHE:CE2	1:C:63:PRO:HB3	2.42	0.54
1:A:84:ASP:OD1	1:B:129:GLY:N	2.38	0.54
1:C:157:PHE:O	1:C:157:PHE:CD1	2.61	0.54
1:B:112:PHE:HB3	1:B:118:TYR:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLY:O	1:D:70:SER:HB3	2.07	0.54
1:C:143:GLN:NE2	1:D:55:PHE:HA	2.22	0.54
1:D:26:LYS:HD2	1:D:30:GLU:HA	1.89	0.54
1:B:98:PHE:HD1	1:B:98:PHE:H	1.55	0.54
1:C:9:GLU:OE1	1:C:64:ARG:CZ	2.53	0.54
1:B:91:THR:HA	1:B:103:MET:O	2.08	0.53
1:C:69:THR:O	1:C:71:ARG:HG3	2.08	0.53
1:D:111:SER:HB2	1:D:114:ALA:H	1.72	0.53
1:A:18:LEU:HD22	1:A:20:GLY:O	2.09	0.53
1:A:99:THR:HG22	1:A:100:GLY:N	2.22	0.53
1:C:153:ASP:O	1:C:156:ASP:N	2.41	0.53
1:A:11:PHE:CE2	1:A:61:GLU:HB3	2.44	0.53
1:D:95:ASN:C	1:D:95:ASN:ND2	2.60	0.53
1:D:153:ASP:OD2	1:D:155:GLY:CA	2.55	0.53
1:A:153:ASP:O	1:A:156:ASP:OD1	2.27	0.53
1:B:25:LEU:HG	1:B:29:VAL:CG2	2.35	0.53
1:C:3:ILE:HG23	1:C:3:ILE:O	2.09	0.53
1:A:21:PRO:HD3	1:A:80:PRO:CD	2.39	0.53
1:C:69:THR:C	1:C:370:SER:H	2.15	0.53
1:D:87:GLU:CD	1:D:106:ILE:HD11	2.33	0.53
1:B:18:LEU:HG	1:B:42:TRP:CH2	2.44	0.53
1:B:7:GLU:HG2	1:B:8:GLN:HG3	1.91	0.53
1:C:121:VAL:CB	1:C:164:VAL:CG2	2.86	0.53
1:D:137:PRO:HD3	1:D:165:GLN:CD	2.34	0.53
1:A:3:ILE:O	1:A:3:ILE:CG2	2.56	0.53
1:A:22:CYS:SG	1:A:22:CYS:O	2.67	0.53
1:A:4:ILE:HB	1:A:6:PHE:HE1	1.74	0.52
1:B:88:HIS:HD2	1:B:169:ARG:CZ	2.19	0.52
1:B:144:TYR:HD2	1:B:157:PHE:CE1	2.27	0.52
1:C:136:TYR:C	1:C:165:GLN:HB2	2.34	0.52
1:D:8:GLN:HB2	1:D:14:HIS:CE1	2.43	0.52
1:D:95:ASN:ND2	1:D:96:PRO:O	2.42	0.52
1:D:144:TYR:O	1:D:146:LEU:HD11	2.09	0.52
1:A:2:LYS:NZ	1:A:17:GLU:OE1	2.42	0.52
1:A:94:GLU:O	1:A:122:SER:OG	2.27	0.52
1:B:143:GLN:C	1:B:144:TYR:CD1	2.86	0.52
1:B:155:GLY:C	1:B:157:PHE:N	2.62	0.52
1:A:98:PHE:HD1	1:A:123:SER:HB3	1.72	0.52
1:D:24:ASN:OD1	1:D:24:ASN:C	2.51	0.52
1:C:91:THR:C	1:C:92:LEU:HD12	2.34	0.52
1:C:94:GLU:CG	1:C:95:ASN:HD21	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LEU:C	1:C:146:LEU:HD13	2.35	0.52
1:D:88:HIS:O	1:D:131:TRP:CZ2	2.59	0.52
1:A:91:THR:HG23	1:A:104:GLU:HA	1.92	0.52
1:B:58:GLU:N	1:B:62:TYR:OH	2.42	0.52
1:B:142:LEU:HB3	1:B:144:TYR:CE1	2.43	0.52
1:D:41:PRO:CG	1:D:81:ILE:HD12	2.39	0.52
1:B:26:LYS:HA	1:B:29:VAL:O	2.09	0.52
1:B:88:HIS:CD2	1:B:169:ARG:NH1	2.78	0.52
1:C:84:ASP:O	1:D:129:GLY:HA2	2.10	0.52
1:D:65:TRP:CZ3	1:D:69:THR:HG21	2.44	0.52
1:B:46:GLU:HB2	1:B:72:THR:HG23	1.91	0.52
1:C:130:THR:O	1:C:169:ARG:HG3	2.10	0.52
1:A:50:CYS:HB2	1:A:51:LYS:NZ	2.24	0.52
1:A:94:GLU:HG3	1:A:101:LYS:HB3	1.91	0.52
1:B:-1:ASN:HB2	1:B:1:PRO:CD	2.39	0.52
1:B:147:GLU:O	1:B:148:LYS:C	2.52	0.52
1:D:88:HIS:CD2	1:D:169:ARG:NH1	2.78	0.52
1:A:137:PRO:HD3	1:A:165:GLN:CD	2.35	0.52
1:D:55:PHE:HE2	1:D:75:LEU:HD13	1.75	0.52
1:A:99:THR:CG2	1:A:100:GLY:N	2.72	0.52
1:C:25:LEU:CD2	1:C:28:THR:OG1	2.58	0.52
1:C:46:GLU:CD	1:C:73:ASP:HB3	2.35	0.52
1:D:-2:LEU:HD12	1:D:2:LYS:HB2	1.91	0.52
1:D:34:SER:HB3	1:D:63:PRO:O	2.10	0.52
1:D:131:TRP:CZ3	1:D:169:ARG:HB2	2.45	0.52
1:B:135:GLN:HB2	1:B:142:LEU:H	1.74	0.51
1:C:48:ALA:HA	1:C:76:SER:OG	2.09	0.51
1:A:129:GLY:HA2	1:B:84:ASP:HB3	1.92	0.51
1:B:16:HIS:ND1	1:B:16:HIS:N	2.58	0.51
1:D:145:LEU:C	1:D:146:LEU:CD1	2.73	0.51
1:A:89:LYS:HE2	1:A:127:GLN:NE2	2.25	0.51
1:A:135:GLN:HG2	1:A:136:TYR:CD1	2.45	0.51
1:B:2:LYS:HD3	1:B:38:GLN:OE1	2.10	0.51
1:B:3:ILE:HD12	1:B:37:VAL:HG13	1.93	0.51
1:C:36:LEU:C	1:C:36:LEU:CD2	2.83	0.51
1:A:95:ASN:O	1:A:96:PRO:O	2.28	0.51
1:A:20:GLY:O	1:A:21:PRO:C	2.50	0.51
1:C:92:LEU:O	1:C:102:LYS:HA	2.10	0.51
1:C:94:GLU:HG2	1:C:101:LYS:H	1.75	0.51
1:C:133:GLY:H	1:C:146:LEU:HD22	1.76	0.51
1:C:27:GLU:HG2	1:C:27:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:SER:O	1:D:16:HIS:CD2	2.64	0.51
1:D:175:TRP:H	1:D:175:TRP:CD1	2.29	0.51
1:D:94:GLU:HG2	1:D:95:ASN:N	2.12	0.51
1:A:56:VAL:HG13	1:A:81:ILE:HD11	1.92	0.51
1:A:59:LYS:HB2	1:B:174:GLN:NE2	2.25	0.51
1:B:6:PHE:HA	1:B:14:HIS:O	2.10	0.51
1:B:46:GLU:HG3	1:B:73:ASP:HB2	1.92	0.51
1:B:154:SER:OG	1:B:162:PRO:HB3	2.09	0.51
1:C:25:LEU:HD11	1:C:78:LEU:CD1	2.41	0.51
1:C:36:LEU:HD23	1:C:37:VAL:N	2.26	0.51
1:C:124:VAL:HG13	1:C:151:TYR:HB2	1.93	0.51
1:C:175:TRP:CA	1:D:-1:ASN:HB3	2.24	0.51
1:A:370:SER:OG	1:B:142:LEU:CD2	2.59	0.50
1:D:132:VAL:HG21	1:D:170:ILE:HD11	1.92	0.50
1:D:48:ALA:N	1:D:76:SER:OG	2.43	0.50
1:D:65:TRP:CD1	1:D:66:ASP:N	2.79	0.50
1:A:-1:ASN:N	1:A:-1:ASN:OD1	2.43	0.50
1:A:93:TYR:OH	1:A:125:ARG:NH1	2.44	0.50
1:D:9:GLU:O	1:D:10:ASN:HB3	2.10	0.50
1:D:135:GLN:CG	1:D:142:LEU:H	2.08	0.50
1:D:169:ARG:O	1:D:170:ILE:C	2.52	0.50
1:A:92:LEU:HA	1:A:124:VAL:CG1	2.41	0.50
1:A:175:TRP:CD1	1:B:40:GLY:O	2.60	0.50
1:B:27:GLU:C	1:B:328:GLY:H	2.19	0.50
1:B:95:ASN:CB	1:B:99:THR:HB	2.41	0.50
1:B:93:TYR:HE1	1:B:102:LYS:HB2	1.76	0.50
1:C:-1:ASN:HD22	1:C:-1:ASN:H	1.59	0.50
1:A:65:TRP:HA	1:A:68:TRP:CH2	2.47	0.50
1:B:43:VAL:HG22	1:B:81:ILE:HD11	1.94	0.50
1:C:143:GLN:HE22	1:D:55:PHE:HB3	1.76	0.50
1:A:126:VAL:HG12	1:A:126:VAL:O	2.12	0.50
1:A:145:LEU:C	1:A:146:LEU:HD12	2.35	0.50
1:B:7:GLU:HA	1:B:14:HIS:CE1	2.46	0.50
1:C:47:GLN:CB	1:C:52:GLY:HA3	2.42	0.50
1:C:51:LYS:HG2	1:C:52:GLY:H	1.69	0.50
1:C:91:THR:HG23	1:C:104:GLU:CA	2.40	0.50
1:B:119:GLU:OE2	1:B:119:GLU:N	2.44	0.50
1:B:53:GLU:OE2	1:B:72:THR:OG1	2.28	0.50
1:B:93:TYR:HE2	1:B:125:ARG:HH21	1.59	0.50
1:C:22:CYS:O	1:C:23:PRO:C	2.53	0.50
1:C:65:TRP:HE3	1:C:72:THR:HG21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LEU:HD22	1:D:43:VAL:HG21	1.94	0.50
1:C:-4:GLN:O	1:C:-3:PRO:C	2.55	0.49
1:D:67:SER:O	1:D:68:TRP:HB3	2.11	0.49
1:D:69:THR:HG21	1:D:371:ARG:H	1.77	0.49
1:B:-1:ASN:CB	1:B:1:PRO:HD2	2.41	0.49
1:B:157:PHE:HE1	1:B:159:ALA:HB2	1.74	0.49
1:C:174:GLN:N	1:C:174:GLN:CD	2.71	0.49
1:D:144:TYR:O	1:D:146:LEU:HD12	2.12	0.49
1:D:98:PHE:CE1	1:D:123:SER:HB3	2.47	0.49
1:A:32:ALA:HB2	1:A:75:LEU:CB	2.24	0.49
1:B:88:HIS:HD2	1:B:169:ARG:NE	2.11	0.49
1:B:92:LEU:HD22	1:B:92:LEU:N	2.28	0.49
1:C:95:ASN:HB3	1:C:96:PRO:CD	2.42	0.49
1:C:157:PHE:O	1:C:157:PHE:HD1	1.95	0.49
1:A:9:GLU:O	1:A:10:ASN:CB	2.61	0.49
1:A:110:PRO:O	1:A:166:SER:CB	2.55	0.49
1:B:43:VAL:CG2	1:B:81:ILE:HG12	2.43	0.49
1:C:18:LEU:CD2	1:C:22:CYS:CB	2.86	0.49
1:C:174:GLN:NE2	1:D:59:LYS:HB2	2.26	0.49
1:A:6:PHE:CG	1:A:15:SER:HB3	2.47	0.49
1:A:86:GLN:CB	1:B:88:HIS:HE1	2.18	0.49
1:A:105:VAL:C	1:A:106:ILE:HG13	2.37	0.49
1:B:43:VAL:HG23	1:B:81:ILE:HG12	1.95	0.49
1:A:3:ILE:HG13	1:A:37:VAL:CG2	2.42	0.49
1:A:94:GLU:HB2	1:A:101:LYS:O	2.12	0.49
1:A:98:PHE:H	1:A:123:SER:CB	2.24	0.49
1:A:130:THR:O	1:A:169:ARG:HG3	2.12	0.49
1:D:41:PRO:HG2	1:D:81:ILE:CD1	2.40	0.49
1:A:11:PHE:HE2	1:A:61:GLU:HB3	1.78	0.49
1:B:46:GLU:HG3	1:B:73:ASP:CB	2.42	0.49
1:B:144:TYR:HE2	1:B:157:PHE:HE1	1.56	0.49
1:B:45:TYR:O	1:B:55:PHE:CZ	2.66	0.49
1:B:103:MET:SD	1:B:112:PHE:CE1	3.06	0.49
1:B:135:GLN:HG2	1:B:136:TYR:CD1	2.48	0.49
1:C:38:GLN:O	1:C:39:ALA:HB2	2.13	0.49
1:B:126:VAL:HG12	1:B:148:LYS:HA	1.95	0.48
1:C:2:LYS:HB2	1:C:39:ALA:HB3	1.95	0.48
1:C:43:VAL:CG1	1:C:81:ILE:HD11	2.18	0.48
1:B:7:GLU:HB2	1:B:14:HIS:CD2	2.48	0.48
1:B:53:GLU:CD	1:B:72:THR:HG1	2.21	0.48
1:B:144:TYR:HE2	1:B:159:ALA:HB2	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:TYR:N	1:B:55:PHE:HE1	2.08	0.48
1:B:55:PHE:CZ	1:B:72:THR:HG21	2.45	0.48
1:C:172:ASP:O	1:C:173:MET:HG2	2.14	0.48
1:D:-1:ASN:HB2	1:D:1:PRO:CD	2.43	0.48
1:D:13:GLY:HA3	1:D:14:HIS:ND1	2.27	0.48
1:A:120:LYS:NZ	1:A:162:PRO:CB	2.77	0.48
1:B:18:LEU:CD1	1:B:20:GLY:H	2.27	0.48
1:C:5:ILE:O	1:C:5:ILE:HG12	2.13	0.48
1:C:103:MET:HE1	1:C:116:HIS:HB2	1.95	0.48
1:C:137:PRO:O	1:C:139:TYR:N	2.47	0.48
1:B:1:PRO:CG	1:B:80:PRO:HB3	2.44	0.48
1:B:8:GLN:C	1:B:9:GLU:O	2.54	0.48
1:C:25:LEU:HD11	1:C:78:LEU:HD12	1.94	0.48
1:C:94:GLU:HB3	1:C:118:TYR:OH	2.14	0.48
1:B:46:GLU:HG3	1:B:73:ASP:N	2.29	0.48
1:B:153:ASP:CG	1:B:154:SER:N	2.71	0.48
1:A:64:ARG:NH1	1:A:64:ARG:CG	2.36	0.48
1:B:6:PHE:C	1:B:14:HIS:CD2	2.92	0.48
1:A:370:SER:C	1:A:371:ARG:N	2.69	0.48
1:A:83:VAL:CG1	1:B:173:MET:SD	3.00	0.48
1:B:1:PRO:O	1:B:19:ASN:HA	2.14	0.48
1:A:98:PHE:HE1	1:A:151:TYR:O	1.96	0.48
1:C:5:ILE:H	1:C:5:ILE:HD12	1.77	0.48
1:C:9:GLU:HB3	1:C:64:ARG:HH11	1.79	0.48
1:D:26:LYS:NZ	1:D:30:GLU:O	2.36	0.47
1:D:26:LYS:HA	1:D:29:VAL:O	2.14	0.47
1:A:23:PRO:O	1:A:24:ASN:HB2	2.13	0.47
1:A:55:PHE:CD1	1:A:55:PHE:N	2.82	0.47
1:C:6:PHE:HA	1:C:14:HIS:O	2.14	0.47
1:C:159:ALA:HB1	1:C:161:GLN:O	2.14	0.47
1:D:-3:PRO:C	1:D:-1:ASN:N	2.72	0.47
1:D:102:LYS:O	1:D:102:LYS:CG	2.62	0.47
1:B:55:PHE:HE2	1:B:72:THR:CG2	2.18	0.47
1:B:65:TRP:HA	1:B:68:TRP:CZ2	2.50	0.47
1:C:-1:ASN:HA	1:D:175:TRP:CE3	2.49	0.47
1:D:95:ASN:HD21	1:D:99:THR:CB	2.26	0.47
1:B:121:VAL:HG21	1:B:164:VAL:HB	1.95	0.47
1:D:72:THR:HB	1:D:73:ASP:H	1.33	0.47
1:A:131:TRP:CZ2	1:A:169:ARG:HD3	2.49	0.47
1:D:159:ALA:HB1	1:D:162:PRO:CA	2.43	0.47
1:A:36:LEU:HD23	1:A:37:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-6:LYS:N	1:C:-5:PRO:CD	2.77	0.47
1:D:125:ARG:O	1:D:125:ARG:HG3	2.10	0.47
1:C:106:ILE:O	1:C:306:ASP:HB2	2.14	0.47
1:C:136:TYR:O	1:C:165:GLN:HB2	2.14	0.47
1:D:23:PRO:O	1:D:48:ALA:HB1	2.15	0.47
1:A:59:LYS:CD	1:B:174:GLN:HE22	2.23	0.47
1:A:136:TYR:HB3	1:A:137:PRO:HD2	1.97	0.47
1:B:26:LYS:HE2	1:B:74:SER:C	2.39	0.47
1:C:25:LEU:HA	1:C:28:THR:CB	2.45	0.47
1:A:59:LYS:HB2	1:B:174:GLN:OE1	2.14	0.47
1:A:65:TRP:CG	1:A:66:ASP:N	2.83	0.47
1:C:2:LYS:CB	1:C:39:ALA:HB3	2.45	0.47
1:C:14:HIS:ND1	1:C:29:VAL:CG1	2.77	0.47
1:C:72:THR:HG23	1:C:72:THR:O	2.15	0.47
1:D:95:ASN:ND2	1:D:99:THR:OG1	2.25	0.47
1:A:101:LYS:HG3	1:A:118:TYR:CE1	2.50	0.47
1:B:7:GLU:O	1:B:31:LYS:HD2	2.15	0.47
1:B:25:LEU:O	1:B:29:VAL:HG23	2.15	0.47
1:C:9:GLU:HA	1:C:34:SER:OG	2.15	0.47
1:C:90:ILE:HG22	1:C:105:VAL:HB	1.97	0.47
1:C:98:PHE:CE1	1:C:123:SER:HB3	2.50	0.47
1:A:46:GLU:C	1:A:76:SER:OG	2.58	0.46
1:A:135:GLN:CG	1:A:136:TYR:CE1	2.98	0.46
1:B:18:LEU:HD11	1:B:20:GLY:H	1.80	0.46
1:C:88:HIS:O	1:C:131:TRP:HZ2	1.97	0.46
1:C:153:ASP:O	1:C:154:SER:C	2.58	0.46
1:D:144:TYR:CZ	1:D:158:GLY:O	2.68	0.46
1:C:43:VAL:HG11	1:D:145:LEU:HD22	1.97	0.46
1:C:75:LEU:HD12	1:C:76:SER:H	1.80	0.46
1:C:88:HIS:CD2	1:C:169:ARG:NH1	2.83	0.46
1:A:48:ALA:CA	1:A:76:SER:HB2	2.45	0.46
1:A:120:LYS:NZ	1:A:162:PRO:HB2	2.29	0.46
1:B:25:LEU:CD1	1:B:29:VAL:HG21	2.45	0.46
1:B:27:GLU:C	1:B:328:GLY:N	2.72	0.46
1:B:370:SER:O	1:B:71:ARG:HB2	2.16	0.46
1:D:147:GLU:O	1:D:148:LYS:C	2.57	0.46
1:B:46:GLU:HA	1:B:72:THR:HG22	1.97	0.46
1:C:-6:LYS:H	1:C:-5:PRO:CD	2.28	0.46
1:D:15:SER:O	1:D:16:HIS:HD2	1.98	0.46
1:D:154:SER:O	1:D:157:PHE:CD1	2.69	0.46
1:B:27:GLU:O	1:B:328:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLU:CG	1:B:73:ASP:OD2	2.63	0.46
1:D:46:GLU:HB2	1:D:53:GLU:HB2	1.96	0.46
1:A:54:GLN:C	1:A:55:PHE:CG	2.94	0.46
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.53	0.46
1:B:26:LYS:CG	1:B:76:SER:HA	2.44	0.46
1:B:103:MET:HE3	1:B:116:HIS:HB3	1.97	0.46
1:B:24:ASN:OD1	1:B:26:LYS:HB2	2.16	0.46
1:C:53:GLU:CD	1:C:55:PHE:CE1	2.85	0.46
1:A:133:GLY:CA	1:A:167:VAL:HG23	2.46	0.46
1:A:131:TRP:CE3	1:A:169:ARG:HB2	2.51	0.46
1:A:144:TYR:CZ	1:A:159:ALA:HB2	2.50	0.46
1:B:95:ASN:O	1:B:122:SER:HB2	2.15	0.46
1:C:-1:ASN:O	1:C:1:PRO:C	2.58	0.46
1:C:42:TRP:CH2	1:C:80:PRO:HG3	2.51	0.46
1:D:9:GLU:O	1:D:10:ASN:CB	2.63	0.46
1:A:10:ASN:HB2	1:A:12:GLN:NE2	2.27	0.46
1:A:28:THR:HG21	1:A:29:VAL:CG1	2.40	0.46
1:B:9:GLU:HG2	1:B:64:ARG:CG	2.46	0.46
1:B:19:ASN:N	1:B:19:ASN:OD1	2.49	0.46
1:B:119:GLU:N	1:B:119:GLU:CD	2.74	0.46
1:C:121:VAL:CG2	1:C:164:VAL:HG23	2.45	0.46
1:D:102:LYS:O	1:D:102:LYS:HG3	2.15	0.46
1:C:26:LYS:HD3	1:C:26:LYS:N	2.31	0.45
1:C:134:TYR:OH	1:C:168:ARG:NE	2.30	0.45
1:C:-1:ASN:HB2	1:C:1:PRO:HD2	1.98	0.45
1:C:3:ILE:HD12	1:C:37:VAL:HG22	1.97	0.45
1:A:48:ALA:N	1:A:76:SER:HB2	2.31	0.45
1:B:132:VAL:O	1:B:132:VAL:HG22	2.16	0.45
1:C:174:GLN:O	1:D:39:ALA:HB1	2.15	0.45
1:D:3:ILE:HB	1:D:42:TRP:CE2	2.51	0.45
1:A:47:GLN:C	1:A:48:ALA:O	2.57	0.45
1:C:41:PRO:HB2	1:C:81:ILE:HG13	1.97	0.45
1:C:59:LYS:HB2	1:D:174:GLN:OE1	2.16	0.45
1:A:86:GLN:H	1:B:88:HIS:CE1	2.34	0.45
1:C:46:GLU:HB2	1:C:55:PHE:CZ	2.52	0.45
1:D:-1:ASN:N	1:D:-1:ASN:OD1	2.48	0.45
1:D:114:ALA:C	1:D:117:GLY:H	2.24	0.45
1:D:142:LEU:HA	1:D:142:LEU:HD12	1.56	0.45
1:A:136:TYR:HB3	1:A:137:PRO:CD	2.47	0.45
1:B:4:ILE:CG2	1:B:16:HIS:O	2.64	0.45
1:B:106:ILE:O	1:B:106:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-1:ASN:O	1:D:39:ALA:CB	2.55	0.45
1:D:152:LYS:HA	1:D:156:ASP:CB	2.46	0.45
1:A:94:GLU:HG2	1:A:119:GLU:HB2	1.98	0.45
1:B:18:LEU:HG	1:B:42:TRP:HH2	1.80	0.45
1:C:-4:GLN:HA	1:C:-3:PRO:HD3	1.59	0.45
1:C:-4:GLN:C	1:C:-3:PRO:O	2.55	0.45
1:C:135:GLN:CB	1:C:142:LEU:H	2.19	0.45
1:C:173:MET:C	1:C:174:GLN:OE1	2.59	0.45
1:D:6:PHE:CD1	1:D:6:PHE:N	2.84	0.45
1:D:45:TYR:CD2	1:D:50:CYS:HA	2.52	0.45
1:D:131:TRP:CZ3	1:D:169:ARG:HD3	2.51	0.45
1:A:1:PRO:HB2	1:A:42:TRP:CZ2	2.52	0.45
1:A:48:ALA:O	1:A:50:CYS:N	2.51	0.45
1:B:7:GLU:N	1:B:14:HIS:CD2	2.85	0.45
1:B:53:GLU:O	1:B:53:GLU:HG2	2.16	0.45
1:C:120:LYS:HB2	1:C:162:PRO:O	2.17	0.45
1:D:49:ASN:O	1:D:51:LYS:HG3	2.17	0.45
1:D:132:VAL:HG23	1:D:170:ILE:CG1	2.47	0.45
1:C:144:TYR:O	1:C:146:LEU:HD13	2.17	0.44
1:D:69:THR:HB	1:D:71:ARG:CA	2.47	0.44
1:A:18:LEU:CD2	1:A:22:CYS:CB	2.88	0.44
1:A:125:ARG:HA	1:A:150:ASP:HA	2.00	0.44
1:B:144:TYR:CD2	1:B:157:PHE:CD1	3.05	0.44
1:C:157:PHE:CE1	1:C:159:ALA:HB2	2.52	0.44
1:B:6:PHE:HB2	1:B:34:SER:HB2	1.99	0.44
1:B:89:LYS:HG3	1:B:106:ILE:HG12	1.99	0.44
1:B:108:ASP:OD1	1:B:168:ARG:HA	2.17	0.44
1:C:94:GLU:CG	1:C:100:GLY:HA3	2.48	0.44
1:C:135:GLN:HE22	1:C:142:LEU:HD13	1.81	0.44
1:D:169:ARG:NH1	1:D:169:ARG:HG2	2.31	0.44
1:C:86:GLN:N	1:C:86:GLN:OE1	2.36	0.44
1:D:23:PRO:O	1:D:24:ASN:CB	2.52	0.44
1:D:108:ASP:HB3	1:D:139:TYR:OH	2.17	0.44
1:D:154:SER:CB	1:D:162:PRO:HD3	2.47	0.44
1:A:7:GLU:CD	1:A:12:GLN:O	2.60	0.44
1:A:10:ASN:HB2	1:A:12:GLN:HE21	1.70	0.44
1:A:120:LYS:NZ	1:A:162:PRO:CG	2.79	0.44
1:C:5:ILE:HD11	1:C:16:HIS:O	2.15	0.44
1:D:95:ASN:OD1	1:D:99:THR:HB	2.18	0.44
1:A:4:ILE:O	1:A:6:PHE:CE1	2.71	0.44
1:A:16:HIS:CE1	1:A:17:GLU:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG22	1:B:134:TYR:CE2	2.53	0.44
1:D:-2:LEU:HD11	1:D:2:LYS:HD2	1.99	0.44
1:A:130:THR:HB	1:B:83:VAL:HG13	1.99	0.44
1:A:49:ASN:O	1:A:51:LYS:HE2	2.18	0.44
1:B:169:ARG:NH1	1:B:169:ARG:HG2	2.32	0.44
1:C:134:TYR:HD1	1:C:166:SER:O	2.01	0.44
1:B:22:CYS:HA	1:B:23:PRO:HD3	1.11	0.44
1:C:25:LEU:HD23	1:C:28:THR:OG1	2.18	0.44
1:C:41:PRO:C	1:C:81:ILE:HG13	2.43	0.44
1:A:7:GLU:O	1:A:8:GLN:C	2.60	0.43
1:A:45:TYR:CE1	1:A:54:GLN:HB3	2.53	0.43
1:B:121:VAL:O	1:B:162:PRO:HB3	2.18	0.43
1:C:-6:LYS:H	1:C:-5:PRO:HD2	1.83	0.43
1:C:147:GLU:O	1:C:148:LYS:C	2.61	0.43
1:D:50:CYS:O	1:D:51:LYS:HG2	2.18	0.43
1:A:102:LYS:HE2	1:A:102:LYS:HB3	1.12	0.43
1:A:109:VAL:HA	1:A:110:PRO:HD2	1.85	0.43
1:A:8:GLN:CB	1:A:12:GLN:O	2.64	0.43
1:C:22:CYS:O	1:C:24:ASN:N	2.52	0.43
1:C:93:TYR:CE1	1:C:102:LYS:HE3	2.53	0.43
1:A:7:GLU:OE1	1:A:7:GLU:C	2.59	0.43
1:B:7:GLU:C	1:B:31:LYS:HZ3	2.27	0.43
1:B:46:GLU:CD	1:B:72:THR:HA	2.43	0.43
1:D:46:GLU:HB3	1:D:53:GLU:N	2.34	0.43
1:D:49:ASN:O	1:D:50:CYS:C	2.61	0.43
1:A:370:SER:C	1:A:371:ARG:H	2.27	0.43
1:B:1:PRO:HG2	1:B:80:PRO:HB3	2.00	0.43
1:B:26:LYS:HG2	1:B:75:LEU:O	2.18	0.43
1:B:90:ILE:HG22	1:B:105:VAL:HB	1.99	0.43
1:C:121:VAL:HG21	1:C:164:VAL:CG2	2.48	0.43
1:D:41:PRO:HG2	1:D:81:ILE:HD13	2.00	0.43
1:B:7:GLU:HA	1:B:14:HIS:HE2	1.75	0.43
1:A:40:GLY:O	1:B:174:GLN:HG3	2.19	0.43
1:B:174:GLN:HE21	1:B:174:GLN:HB3	1.66	0.43
1:C:158:GLY:O	1:C:160:PRO:HD3	2.19	0.43
1:A:112:PHE:N	1:A:165:GLN:O	2.48	0.43
1:B:69:THR:O	1:B:69:THR:HG23	2.19	0.43
1:C:1:PRO:HB3	1:C:80:PRO:HB3	2.00	0.43
1:D:92:LEU:HD13	1:D:112:PHE:HZ	1.80	0.43
1:A:72:THR:OG1	1:A:73:ASP:N	2.52	0.43
1:A:105:VAL:HG12	1:A:106:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:HD3	1:B:30:GLU:HA	2.01	0.43
1:B:90:ILE:CD1	1:B:167:VAL:HG21	2.49	0.43
1:B:103:MET:CE	1:B:112:PHE:CD1	2.99	0.43
1:C:24:ASN:O	1:C:27:GLU:HB3	2.18	0.43
1:B:49:ASN:N	1:B:49:ASN:ND2	2.65	0.43
1:B:112:PHE:O	1:B:116:HIS:N	2.48	0.43
1:C:1:PRO:HD3	1:D:175:TRP:CE3	2.53	0.43
1:C:110:PRO:O	1:C:138:GLY:N	2.48	0.43
1:A:18:LEU:HD21	1:A:22:CYS:HB3	1.98	0.42
1:A:173:MET:HE2	1:A:173:MET:HB2	1.89	0.42
1:B:95:ASN:HB2	1:B:99:THR:O	2.19	0.42
1:D:6:PHE:HD1	1:D:6:PHE:H	1.65	0.42
1:C:83:VAL:O	1:C:83:VAL:HG12	2.19	0.42
1:D:122:SER:O	1:D:157:PHE:HE2	2.01	0.42
1:B:101:LYS:HE3	1:B:119:GLU:OE1	2.20	0.42
1:C:45:TYR:O	1:C:75:LEU:HD12	2.19	0.42
1:D:132:VAL:HG12	1:D:134:TYR:CE1	2.55	0.42
1:A:3:ILE:CG1	1:A:37:VAL:HG22	2.49	0.42
1:A:44:GLY:O	1:A:45:TYR:CE2	2.71	0.42
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.87	0.42
1:D:41:PRO:O	1:D:81:ILE:CD1	2.68	0.42
1:D:45:TYR:CD2	1:D:50:CYS:HB3	2.54	0.42
1:A:123:SER:O	1:A:124:VAL:HG13	2.18	0.42
1:B:151:TYR:N	1:B:151:TYR:CD1	2.88	0.42
1:C:16:HIS:CE1	1:C:18:LEU:HD12	2.54	0.42
1:C:44:GLY:HA3	1:C:78:LEU:HD23	2.01	0.42
1:C:91:THR:CG2	1:C:104:GLU:HA	2.45	0.42
1:A:92:LEU:HA	1:A:124:VAL:HG13	2.02	0.42
1:B:47:GLN:C	1:B:76:SER:HB2	2.44	0.42
1:C:144:TYR:CE1	1:C:159:ALA:HA	2.54	0.42
1:D:-2:LEU:C	1:D:1:PRO:CD	2.92	0.42
1:A:46:GLU:HG2	1:A:52:GLY:HA3	2.01	0.42
1:A:125:ARG:HG2	1:A:150:ASP:OD1	2.20	0.42
1:C:153:ASP:O	1:C:155:GLY:N	2.52	0.42
1:A:144:TYR:HE1	1:A:158:GLY:O	2.03	0.42
1:B:8:GLN:CB	1:B:31:LYS:HZ3	2.33	0.42
1:D:95:ASN:HD22	1:D:96:PRO:N	2.18	0.42
1:D:97:ASN:HD21	1:D:152:LYS:HE2	1.85	0.42
1:A:26:LYS:C	1:A:28:THR:H	2.26	0.42
1:B:134:TYR:O	1:B:164:VAL:HA	2.20	0.42
1:C:25:LEU:HD22	1:C:28:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:GLY:O	1:C:34:SER:OG	2.37	0.42
1:C:65:TRP:CD1	1:C:65:TRP:N	2.87	0.42
1:D:25:LEU:HD11	1:D:78:LEU:HD22	2.02	0.42
1:D:49:ASN:O	1:D:51:LYS:CG	2.68	0.42
1:D:110:PRO:HA	1:D:166:SER:HB2	2.01	0.42
1:D:93:TYR:CE1	1:D:102:LYS:HB3	2.54	0.42
1:B:112:PHE:O	1:B:113:HIS:C	2.61	0.41
1:A:44:GLY:C	1:A:45:TYR:CD2	2.99	0.41
1:A:92:LEU:HA	1:A:124:VAL:HG12	2.01	0.41
1:A:95:ASN:O	1:A:96:PRO:C	2.61	0.41
1:B:154:SER:O	1:B:159:ALA:HB3	2.19	0.41
1:C:159:ALA:HA	1:C:160:PRO:HD3	1.69	0.41
1:A:16:HIS:HE1	1:A:18:LEU:HG	1.86	0.41
1:A:32:ALA:CB	1:A:75:LEU:H	2.33	0.41
1:A:36:LEU:HD23	1:A:37:VAL:H	1.84	0.41
1:A:95:ASN:C	1:A:96:PRO:O	2.63	0.41
1:C:137:PRO:HD3	1:C:165:GLN:CD	2.39	0.41
1:D:71:ARG:O	1:D:371:ARG:CB	2.66	0.41
1:A:28:THR:HG22	1:A:328:GLY:N	2.36	0.41
1:B:24:ASN:O	1:B:25:LEU:C	2.59	0.41
1:B:109:VAL:HA	1:B:110:PRO:HD2	1.90	0.41
1:C:2:LYS:O	1:C:39:ALA:N	2.54	0.41
1:A:6:PHE:HB3	1:A:7:GLU:H	1.50	0.41
1:A:159:ALA:HA	1:A:160:PRO:HD2	1.88	0.41
1:B:-2:LEU:O	1:B:-1:ASN:C	2.61	0.41
1:C:35:VAL:CG1	1:C:36:LEU:N	2.82	0.41
1:C:122:SER:O	1:C:153:ASP:HA	2.21	0.41
1:D:55:PHE:CE2	1:D:75:LEU:HD13	2.55	0.41
1:D:153:ASP:CG	1:D:155:GLY:HA3	2.45	0.41
1:B:45:TYR:CE2	1:B:50:CYS:O	2.74	0.41
1:B:146:LEU:HD13	1:B:146:LEU:N	2.35	0.41
1:D:7:GLU:HG2	1:D:31:LYS:O	2.20	0.41
1:A:18:LEU:CD2	1:A:22:CYS:HB3	2.50	0.41
1:A:93:TYR:CE1	1:A:102:LYS:CE	3.03	0.41
1:A:135:GLN:O	1:A:165:GLN:HG3	2.21	0.41
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.75	0.41
1:C:44:GLY:N	1:C:55:PHE:O	2.53	0.41
1:D:6:PHE:HD2	1:D:11:PHE:O	2.00	0.41
1:D:26:LYS:HD3	1:D:26:LYS:HA	1.09	0.41
1:D:47:GLN:CG	1:D:51:LYS:O	2.69	0.41
1:D:65:TRP:CD1	1:D:66:ASP:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLN:HA	1:D:162:PRO:HD2	1.82	0.41
1:A:36:LEU:CD2	1:A:37:VAL:N	2.84	0.41
1:A:64:ARG:O	1:A:65:TRP:C	2.64	0.41
1:B:42:TRP:C	1:B:81:ILE:HD11	2.39	0.41
1:C:93:TYR:HE2	1:C:125:ARG:HB2	1.86	0.41
1:C:121:VAL:CG2	1:C:164:VAL:CG2	2.99	0.41
1:C:132:VAL:HG21	1:D:56:VAL:HG21	2.03	0.41
1:D:-2:LEU:O	1:D:-1:ASN:O	2.35	0.41
1:A:69:THR:HG22	1:A:370:SER:CB	2.51	0.41
1:B:87:GLU:OE1	1:B:106:ILE:HD13	2.21	0.41
1:B:161:GLN:OE1	1:B:163:GLN:HB2	2.21	0.41
1:C:37:VAL:CG1	1:C:59:LYS:HA	2.43	0.41
1:C:65:TRP:CE3	1:C:72:THR:HG21	2.54	0.41
1:A:54:GLN:C	1:A:55:PHE:CD1	2.99	0.40
1:A:54:GLN:H	1:A:54:GLN:HG2	1.38	0.40
1:B:121:VAL:O	1:B:162:PRO:HB2	2.20	0.40
1:A:48:ALA:O	1:A:49:ASN:C	2.64	0.40
1:A:64:ARG:NH1	1:A:66:ASP:OD2	2.54	0.40
1:B:90:ILE:HD12	1:B:167:VAL:HG21	2.03	0.40
1:C:151:TYR:HB3	1:C:156:ASP:HB3	2.03	0.40
1:D:9:GLU:HG2	1:D:10:ASN:CB	2.48	0.40
1:D:131:TRP:CH2	1:D:169:ARG:CD	3.04	0.40
1:A:-4:GLN:HA	1:A:-3:PRO:HD3	1.72	0.40
1:A:22:CYS:HA	1:A:23:PRO:HD3	1.77	0.40
1:C:102:LYS:HE3	1:C:102:LYS:HB3	1.86	0.40
1:D:98:PHE:HE1	1:D:123:SER:HB3	1.86	0.40
1:D:108:ASP:O	1:D:109:VAL:HG13	2.21	0.40
1:D:132:VAL:CG2	1:D:170:ILE:CG1	2.99	0.40
1:A:24:ASN:ND2	1:A:48:ALA:HB1	2.36	0.40
1:A:50:CYS:N	1:A:77:SER:OG	2.52	0.40
1:B:45:TYR:O	1:B:55:PHE:HZ	2.04	0.40
1:C:89:LYS:HB3	1:C:127:GLN:HB3	2.04	0.40
1:D:137:PRO:O	1:D:138:GLY:C	2.63	0.40
1:D:144:TYR:C	1:D:146:LEU:CD1	2.94	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASN:ND2	1:D:-4:GLN:O[1_554]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:OG	1:A:136:TYR:CD2[3_555]	2.02	0.18
1:C:371:ARG:CD	1:C:371:ARG:CD[4_555]	2.03	0.17

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	183/204 (90%)	144 (79%)	21 (12%)	18 (10%)	0	3
1	B	179/204 (88%)	130 (73%)	34 (19%)	15 (8%)	0	4
1	C	185/204 (91%)	137 (74%)	31 (17%)	17 (9%)	0	3
1	D	181/204 (89%)	136 (75%)	29 (16%)	16 (9%)	0	4
All	All	728/816 (89%)	547 (75%)	115 (16%)	66 (9%)	0	3

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	48	ALA
1	A	65	TRP
1	A	73	ASP
1	A	96	PRO
1	A	306	ASP
1	A	160	PRO
1	B	9	GLU
1	B	71	ARG
1	B	156	ASP
1	C	-5	PRO
1	C	-4	GLN
1	C	-3	PRO
1	C	21	PRO
1	C	29	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	14	HIS
1	D	70	SER
1	D	119	GLU
1	D	152	LYS
1	A	14	HIS
1	A	32	ALA
1	B	59	LYS
1	B	75	LEU
1	C	-6	LYS
1	C	64	ARG
1	C	71	ARG
1	C	154	SER
1	C	156	ASP
1	D	-1	ASN
1	D	9	GLU
1	D	328	GLY
1	D	65	TRP
1	D	156	ASP
1	D	162	PRO
1	D	167	VAL
1	A	59	LYS
1	A	110	PRO
1	A	139	TYR
1	A	174	GLN
1	B	14	HIS
1	B	63	PRO
1	B	70	SER
1	B	370	SER
1	B	148	LYS
1	C	74	SER
1	D	67	SER
1	D	71	ARG
1	A	64	ARG
1	A	74	SER
1	B	10	ASN
1	C	138	GLY
1	D	68	TRP
1	A	67	SER
1	B	306	ASP
1	C	306	ASP
1	C	136	TYR
1	C	148	LYS

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Mol	Chain	Res	Type
1	D	50	CYS
1	B	124	VAL
1	D	137	PRO
1	A	162	PRO
1	B	35	VAL
1	C	23	PRO
1	B	95	ASN
1	C	22	CYS
1	A	136	TYR

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/177 (92%)	97 (60%)	65 (40%)	0	0
1	B	159/177 (90%)	101 (64%)	58 (36%)	0	1
1	C	163/177 (92%)	105 (64%)	58 (36%)	0	1
1	D	161/177 (91%)	105 (65%)	56 (35%)	0	1
All	All	645/708 (91%)	408 (63%)	237 (37%)	0	1

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	LEU
1	A	4	ILE
1	A	5	ILE
1	A	7	GLU
1	A	9	GLU
1	A	10	ASN
1	A	18	LEU
1	A	22	CYS
1	A	25	LEU
1	A	26	LYS
1	A	27	GLU
1	A	29	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	31	LYS
1	A	34	SER
1	A	36	LEU
1	A	37	VAL
1	A	47	GLN
1	A	49	ASN
1	A	51	LYS
1	A	55	PHE
1	A	56	VAL
1	A	58	GLU
1	A	64	ARG
1	A	67	SER
1	A	70	SER
1	A	370	SER
1	A	71	ARG
1	A	73	ASP
1	A	74	SER
1	A	78	LEU
1	A	79	ARG
1	A	81	ILE
1	A	83	VAL
1	A	87	GLU
1	A	91	THR
1	A	94	GLU
1	A	95	ASN
1	A	102	LYS
1	A	103	MET
1	A	107	ASP
1	A	108	ASP
1	A	109	VAL
1	A	111	SER
1	A	113	HIS
1	A	318	GLN
1	A	119	GLU
1	A	122	SER
1	A	123	SER
1	A	124	VAL
1	A	125	ARG
1	A	127	GLN
1	A	130	THR
1	A	135	GLN
1	A	139	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	142	LEU
1	A	143	GLN
1	A	150	ASP
1	A	152	LYS
1	A	157	PHE
1	A	163	GLN
1	A	167	VAL
1	A	170	ILE
1	A	172	ASP
1	A	173	MET
1	A	174	GLN
1	B	-2	LEU
1	B	-1	ASN
1	B	2	LYS
1	B	3	ILE
1	B	4	ILE
1	B	8	GLN
1	B	9	GLU
1	B	12	GLN
1	B	14	HIS
1	B	16	HIS
1	B	19	ASN
1	B	25	LEU
1	B	27	GLU
1	B	29	VAL
1	B	30	GLU
1	B	31	LYS
1	B	34	SER
1	B	37	VAL
1	B	47	GLN
1	B	49	ASN
1	B	50	CYS
1	B	51	LYS
1	B	53	GLU
1	B	55	PHE
1	B	64	ARG
1	B	67	SER
1	B	370	SER
1	B	71	ARG
1	B	371	ARG
1	B	74	SER
1	B	75	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	77	SER
1	B	79	ARG
1	B	89	LYS
1	B	90	ILE
1	B	91	THR
1	B	92	LEU
1	B	94	GLU
1	B	95	ASN
1	B	98	PHE
1	B	102	LYS
1	B	318	GLN
1	B	120	LYS
1	B	122	SER
1	B	132	VAL
1	B	139	TYR
1	B	142	LEU
1	B	143	GLN
1	B	146	LEU
1	B	147	GLU
1	B	154	SER
1	B	160	PRO
1	B	167	VAL
1	B	170	ILE
1	B	172	ASP
1	B	173	MET
1	B	174	GLN
1	B	175	TRP
1	C	-6	LYS
1	C	-4	GLN
1	C	-2	LEU
1	C	-1	ASN
1	C	2	LYS
1	C	3	ILE
1	C	4	ILE
1	C	5	ILE
1	C	6	PHE
1	C	8	GLN
1	C	18	LEU
1	C	26	LYS
1	C	27	GLU
1	C	28	THR
1	C	29	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	30	GLU
1	C	31	LYS
1	C	43	VAL
1	C	51	LYS
1	C	58	GLU
1	C	64	ARG
1	C	69	THR
1	C	370	SER
1	C	371	ARG
1	C	72	THR
1	C	74	SER
1	C	75	LEU
1	C	81	ILE
1	C	83	VAL
1	C	85	SER
1	C	86	GLN
1	C	87	GLU
1	C	89	LYS
1	C	91	THR
1	C	95	ASN
1	C	101	LYS
1	C	103	MET
1	C	104	GLU
1	C	108	ASP
1	C	318	GLN
1	C	122	SER
1	C	124	VAL
1	C	125	ARG
1	C	126	VAL
1	C	132	VAL
1	C	142	LEU
1	C	146	LEU
1	C	147	GLU
1	C	150	ASP
1	C	154	SER
1	C	164	VAL
1	C	166	SER
1	C	167	VAL
1	C	170	ILE
1	C	171	ARG
1	C	172	ASP
1	C	173	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	174	GLN
1	D	-2	LEU
1	D	2	LYS
1	D	5	ILE
1	D	6	PHE
1	D	8	GLN
1	D	10	ASN
1	D	12	GLN
1	D	14	HIS
1	D	26	LYS
1	D	28	THR
1	D	29	VAL
1	D	35	VAL
1	D	36	LEU
1	D	37	VAL
1	D	38	GLN
1	D	50	CYS
1	D	51	LYS
1	D	53	GLU
1	D	55	PHE
1	D	67	SER
1	D	69	THR
1	D	71	ARG
1	D	371	ARG
1	D	72	THR
1	D	74	SER
1	D	76	SER
1	D	77	SER
1	D	78	LEU
1	D	79	ARG
1	D	81	ILE
1	D	82	LYS
1	D	86	GLN
1	D	87	GLU
1	D	88	HIS
1	D	89	LYS
1	D	90	ILE
1	D	91	THR
1	D	94	GLU
1	D	95	ASN
1	D	98	PHE
1	D	99	THR

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Mol	Chain	Res	Type
1	D	105	VAL
1	D	318	GLN
1	D	120	LYS
1	D	121	VAL
1	D	122	SER
1	D	124	VAL
1	D	125	ARG
1	D	127	GLN
1	D	140	ARG
1	D	142	LEU
1	D	143	GLN
1	D	161	GLN
1	D	170	ILE
1	D	172	ASP
1	D	174	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	16	HIS
1	A	54	GLN
1	A	86	GLN
1	A	95	ASN
1	A	127	GLN
1	B	8	GLN
1	B	12	GLN
1	B	49	ASN
1	B	88	HIS
1	B	116	HIS
1	B	318	GLN
1	B	135	GLN
1	B	165	GLN
1	B	174	GLN
1	C	-1	ASN
1	C	47	GLN
1	C	95	ASN
1	C	113	HIS
1	C	127	GLN
1	C	135	GLN
1	C	143	GLN
1	C	165	GLN

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Mol	Chain	Res	Type
1	D	19	ASN
1	D	95	ASN
1	D	113	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.