



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:13 AM EDT

PDB ID : 1WQS / pdb_00001wqs
Title : Crystal structure of Norovirus 3C-like protease
Authors : Nakamura, K.; Someya, Y.; Kumasaka, T.; Tanaka, N.
Deposited on : 2004-10-01
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

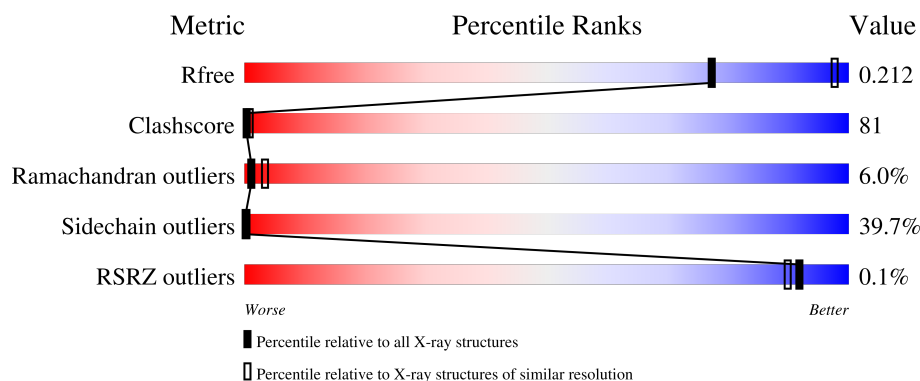
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	173	18% 29% 34% 18%
1	B	173	9% 27% 40% 24%
1	C	173	20% 27% 30% 23%
1	D	173	13% 29% 36% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TLA	A	301	-	-	X	-
4	TAR	A	300	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5367 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.

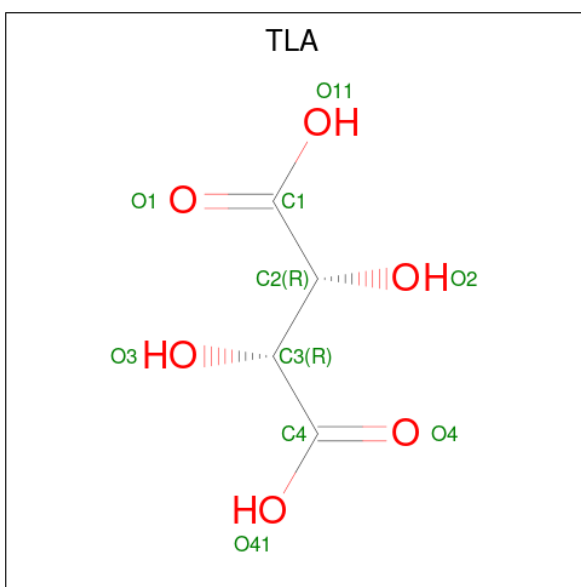
- Molecule 1 is a protein called 3C-like protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1303	829	232	232	10			
1	B	173	Total	C	N	O	S	0	0	0
			1303	829	232	232	10			
1	C	173	Total	C	N	O	S	0	0	0
			1303	829	232	232	10			
1	D	173	Total	C	N	O	S	0	0	0
			1303	829	232	232	10			

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

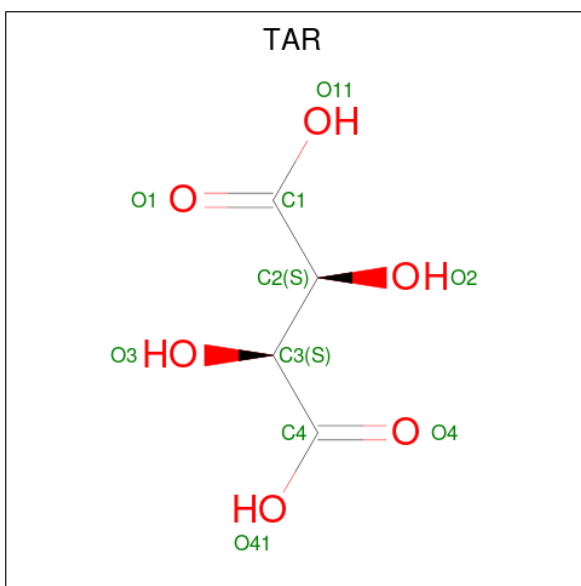
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Hg	0	0
			2	2		
2	B	2	Total	Hg	0	0
			2	2		
2	C	2	Total	Hg	0	0
			2	2		
2	D	2	Total	Hg	0	0
			2	2		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		

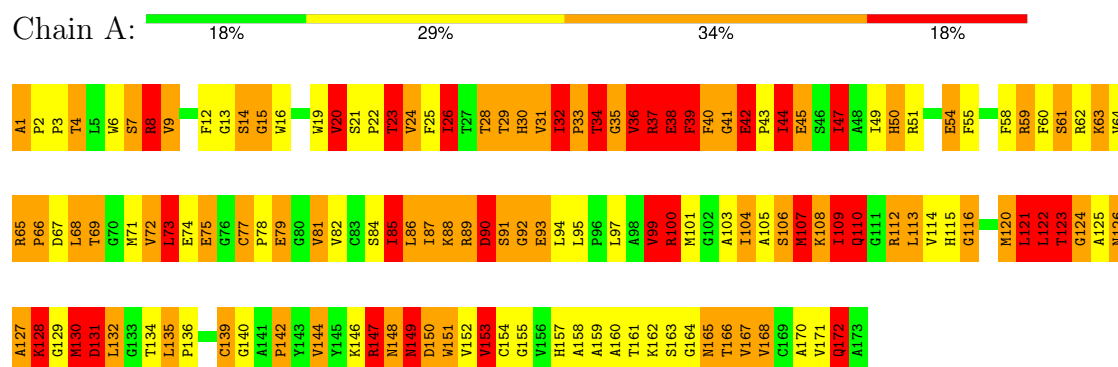
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	B	22	Total 22	O 22	0	0
5	C	41	Total 41	O 41	0	0
5	D	31	Total 31	O 31	0	0

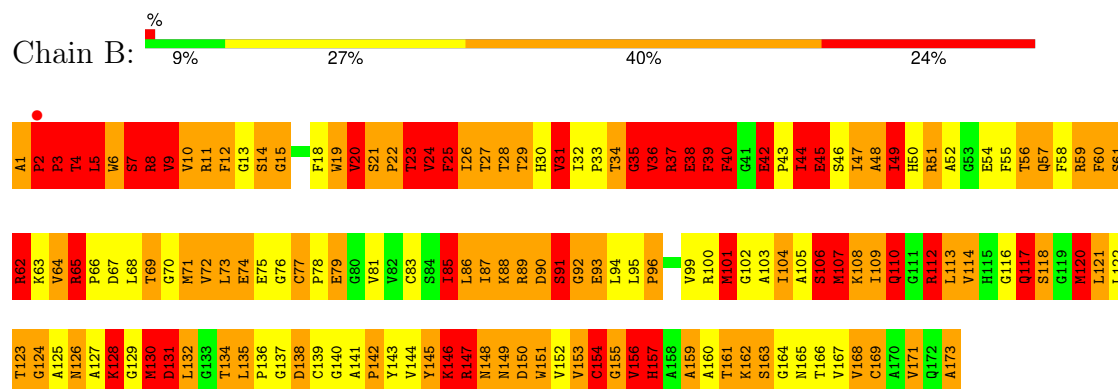
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

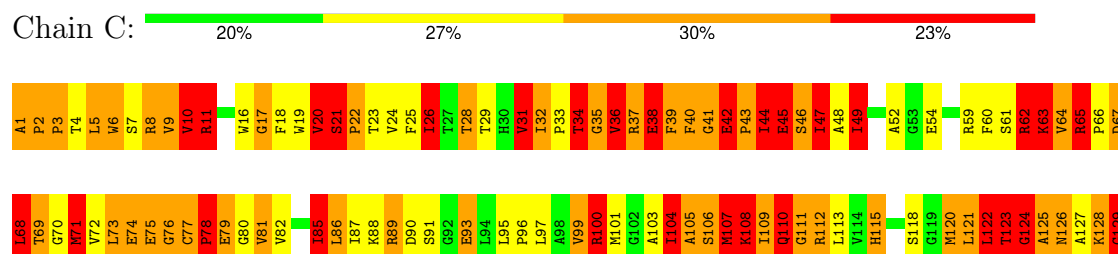
• Molecule 1: 3C-like protease



• Molecule 1: 3C-like protease



• Molecule 1: 3C-like protease





● Molecule 1: 3C-like protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	128.89Å 128.89Å 118.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (8.00-2.80) 95.6 (8.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.240 0.212 , 0.212	Depositor DCC
R_{free} test set	2740 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.54 , 153.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5367	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, TAR, HG

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	2.89	84/1334 (6.3%)	2.95	147/1810 (8.1%)
1	B	3.23	126/1334 (9.4%)	3.39	199/1810 (11.0%)
1	C	2.64	78/1334 (5.8%)	2.76	128/1810 (7.1%)
1	D	3.05	98/1334 (7.3%)	3.12	177/1810 (9.8%)
All	All	2.96	386/5336 (7.2%)	3.06	651/7240 (9.0%)

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	4
1	B	0	4
1	D	0	4
All	All	0	12

All (386) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	PRO	CA-C	40.00	1.73	1.51
1	A	85	ILE	CA-CB	24.66	1.79	1.53
1	B	2	PRO	CA-C	24.49	1.75	1.52
1	B	130	MET	CA-C	21.16	1.83	1.53
1	D	36	VAL	CA-CB	19.60	1.81	1.54
1	C	85	ILE	CA-CB	17.96	1.75	1.54
1	B	24	VAL	CA-CB	16.96	1.77	1.54
1	D	4	THR	CA-CB	16.92	1.80	1.53
1	A	32	ILE	CA-CB	16.22	1.75	1.54
1	A	34	THR	CA-C	16.14	1.74	1.52
1	A	128	LYS	CA-C	15.59	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	ASP	N-CA	15.53	1.66	1.46
1	B	120	MET	SD-CE	-15.12	1.41	1.79
1	B	36	VAL	N-CA	14.57	1.62	1.46
1	D	152	VAL	CA-CB	14.51	1.71	1.54
1	C	131	ASP	CA-C	13.67	1.71	1.52
1	C	48	ALA	CA-CB	-13.59	1.34	1.53
1	A	130	MET	CG-SD	13.34	2.14	1.80
1	B	60	PHE	CA-C	13.33	1.70	1.52
1	B	153	VAL	CA-CB	-13.18	1.37	1.54
1	C	36	VAL	CA-CB	13.15	1.72	1.54
1	D	32	ILE	CA-CB	13.09	1.71	1.54
1	D	23	THR	CA-CB	12.74	1.73	1.53
1	B	24	VAL	CA-C	12.73	1.69	1.52
1	D	154	CYS	CA-CB	12.69	1.72	1.54
1	D	141	ALA	CA-CB	-12.67	1.33	1.53
1	B	127	ALA	CA-C	12.53	1.67	1.52
1	B	127	ALA	CA-CB	12.45	1.72	1.53
1	A	32	ILE	CA-C	-12.43	1.39	1.52
1	B	87	ILE	CA-CB	12.42	1.69	1.54
1	B	36	VAL	CA-C	12.42	1.67	1.52
1	A	110	GLN	N-CA	12.38	1.62	1.46
1	C	123	THR	CA-CB	-12.21	1.33	1.54
1	D	47	ILE	CA-C	-12.22	1.37	1.52
1	A	123	THR	CA-C	12.13	1.69	1.52
1	A	172	GLN	CB-CG	12.07	1.88	1.52
1	A	130	MET	CA-CB	12.06	1.71	1.54
1	A	34	THR	CA-CB	12.06	1.73	1.53
1	D	44	ILE	CA-CB	-11.94	1.38	1.54
1	B	130	MET	N-CA	11.82	1.63	1.46
1	D	131	ASP	CB-CG	11.72	1.81	1.52
1	C	71	MET	SD-CE	-11.68	1.50	1.79
1	B	125	ALA	CA-CB	11.62	1.73	1.53
1	C	70	GLY	CA-C	-11.51	1.44	1.52
1	B	2	PRO	C-O	11.48	1.37	1.24
1	C	130	MET	CA-C	11.45	1.65	1.52
1	D	36	VAL	CA-C	11.43	1.67	1.52
1	A	172	GLN	CG-CD	11.29	1.80	1.52
1	B	62	ARG	CA-C	11.29	1.67	1.52
1	A	36	VAL	C-N	-11.26	1.18	1.33
1	B	44	ILE	CA-C	11.11	1.66	1.52
1	C	28	THR	CA-CB	-11.01	1.35	1.53
1	B	23	THR	CA-C	10.91	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	ARG	C-N	10.89	1.45	1.34
1	D	51	ARG	N-CA	10.83	1.60	1.46
1	C	120	MET	SD-CE	10.80	2.06	1.79
1	D	50	HIS	CA-CB	10.73	1.71	1.53
1	B	34	THR	CA-CB	10.72	1.69	1.53
1	B	62	ARG	CA-CB	10.60	1.71	1.53
1	D	1	ALA	C-N	10.53	1.42	1.33
1	B	61	SER	CA-C	10.52	1.66	1.52
1	C	109	ILE	CA-CB	10.44	1.66	1.54
1	B	71	MET	SD-CE	10.43	2.05	1.79
1	A	128	LYS	N-CA	10.36	1.60	1.46
1	B	36	VAL	CB-CG2	10.36	1.86	1.52
1	B	2	PRO	C-N	10.35	1.58	1.33
1	D	60	PHE	CA-C	10.29	1.65	1.52
1	C	127	ALA	CA-C	10.28	1.65	1.52
1	B	3	PRO	N-CA	10.26	1.60	1.47
1	D	148	ASN	CA-CB	10.26	1.66	1.53
1	C	8	ARG	CA-C	-10.24	1.39	1.52
1	A	130	MET	CB-CG	10.18	1.82	1.52
1	D	37	ARG	N-CA	-10.10	1.33	1.46
1	B	31	VAL	CA-CB	10.02	1.66	1.54
1	A	100	ARG	CG-CD	10.01	1.82	1.52
1	A	72	VAL	CA-CB	-9.97	1.41	1.54
1	A	124	GLY	N-CA	9.96	1.59	1.45
1	A	125	ALA	N-CA	9.96	1.59	1.46
1	B	49	ILE	CA-CB	9.95	1.68	1.54
1	A	35	GLY	C-N	9.92	1.47	1.33
1	B	39	PHE	CA-C	9.73	1.63	1.52
1	A	38	GLU	CA-C	9.60	1.64	1.52
1	D	85	ILE	C-O	-9.58	1.13	1.24
1	A	161	THR	CA-CB	-9.56	1.39	1.53
1	B	173	ALA	CA-CB	9.53	1.83	1.52
1	B	61	SER	N-CA	9.49	1.58	1.46
1	B	1	ALA	C-N	9.37	1.44	1.33
1	D	131	ASP	CA-CB	9.33	1.69	1.53
1	D	130	MET	CA-C	9.32	1.65	1.52
1	A	100	ARG	CB-CG	9.20	1.80	1.52
1	B	83	CYS	CA-CB	9.17	1.66	1.53
1	D	86	LEU	CA-CB	9.12	1.66	1.53
1	B	37	ARG	CA-C	9.09	1.66	1.52
1	B	127	ALA	N-CA	9.07	1.57	1.46
1	A	37	ARG	N-CA	-9.06	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	HIS	CA-C	8.94	1.67	1.52
1	C	20	VAL	CA-C	-8.92	1.40	1.52
1	A	130	MET	CA-C	8.91	1.64	1.52
1	B	62	ARG	CB-CG	8.87	1.79	1.52
1	A	101	MET	SD-CE	-8.83	1.57	1.79
1	A	36	VAL	C-O	-8.83	1.13	1.24
1	B	157	HIS	CA-CB	8.79	1.64	1.53
1	D	24	VAL	CA-CB	8.73	1.64	1.54
1	C	141	ALA	CA-CB	-8.68	1.39	1.53
1	B	47	ILE	CA-CB	8.67	1.66	1.54
1	C	6	TRP	CA-C	8.67	1.64	1.52
1	C	154	CYS	CA-C	8.67	1.63	1.52
1	A	35	GLY	CA-C	-8.65	1.39	1.51
1	D	4	THR	N-CA	8.61	1.57	1.46
1	B	159	ALA	CA-C	-8.57	1.42	1.52
1	B	22	PRO	CA-C	8.50	1.65	1.52
1	C	127	ALA	N-CA	8.50	1.57	1.45
1	C	112	ARG	CA-CB	8.49	1.65	1.53
1	C	173	ALA	CA-C	8.48	1.70	1.52
1	A	49	ILE	CA-CB	-8.46	1.44	1.54
1	C	104	ILE	CA-CB	-8.44	1.42	1.54
1	A	26	ILE	CA-CB	8.41	1.65	1.54
1	B	110	GLN	CB-CG	8.33	1.77	1.52
1	A	109	ILE	CA-C	8.27	1.63	1.52
1	D	90	ASP	CB-CG	8.22	1.72	1.52
1	B	131	ASP	CB-CG	8.18	1.72	1.52
1	D	134	THR	CA-CB	8.09	1.66	1.53
1	A	127	ALA	CA-CB	8.08	1.67	1.53
1	C	29	THR	CA-C	-8.07	1.42	1.52
1	A	160	ALA	CA-CB	-8.05	1.40	1.53
1	A	36	VAL	CA-CB	8.01	1.65	1.54
1	D	59	ARG	CA-C	8.00	1.62	1.52
1	D	104	ILE	CA-CB	8.00	1.65	1.54
1	C	101	MET	SD-CE	8.00	1.99	1.79
1	B	60	PHE	CA-CB	7.99	1.65	1.53
1	B	65	ARG	N-CA	-7.94	1.39	1.46
1	B	123	THR	CA-C	-7.92	1.43	1.53
1	A	43	PRO	CA-C	-7.89	1.43	1.52
1	B	10	VAL	CA-C	-7.84	1.43	1.52
1	B	7	SER	CA-CB	7.82	1.65	1.53
1	D	130	MET	CA-CB	7.82	1.65	1.53
1	B	33	PRO	CA-C	7.81	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	CYS	CA-CB	7.80	1.66	1.53
1	B	24	VAL	N-CA	7.77	1.56	1.46
1	D	71	MET	CA-C	-7.74	1.43	1.52
1	C	148	ASN	CA-C	7.72	1.63	1.52
1	B	146	LYS	CB-CG	7.69	1.75	1.52
1	D	148	ASN	CB-CG	7.68	1.71	1.52
1	C	131	ASP	C-O	7.68	1.33	1.24
1	D	49	ILE	CA-CB	-7.68	1.44	1.54
1	B	63	LYS	CA-C	7.67	1.63	1.52
1	B	110	GLN	CA-CB	7.65	1.67	1.53
1	C	38	GLU	CA-C	-7.64	1.43	1.52
1	C	158	ALA	CA-CB	-7.64	1.42	1.53
1	C	131	ASP	N-CA	7.63	1.56	1.46
1	D	144	VAL	CA-C	-7.63	1.44	1.53
1	C	46	SER	CA-C	-7.62	1.42	1.52
1	B	76	GLY	N-CA	7.61	1.51	1.44
1	D	62	ARG	N-CA	7.59	1.55	1.46
1	C	153	VAL	CA-CB	-7.58	1.44	1.54
1	B	48	ALA	CA-C	7.56	1.61	1.53
1	B	34	THR	N-CA	7.53	1.55	1.46
1	D	130	MET	N-CA	7.53	1.55	1.46
1	A	122	LEU	N-CA	-7.52	1.37	1.46
1	B	28	THR	CA-C	-7.51	1.43	1.52
1	D	148	ASN	CA-C	7.46	1.62	1.53
1	A	47	ILE	CA-CB	7.45	1.64	1.54
1	C	77	CYS	CA-C	-7.44	1.43	1.52
1	B	38	GLU	CA-C	7.37	1.62	1.52
1	C	34	THR	N-CA	-7.36	1.36	1.46
1	C	104	ILE	CA-C	-7.32	1.45	1.53
1	C	126	ASN	CA-C	7.29	1.62	1.52
1	B	154	CYS	CA-CB	7.26	1.64	1.54
1	A	129	GLY	CA-C	7.26	1.62	1.51
1	A	125	ALA	CA-C	7.25	1.62	1.52
1	B	54	GLU	CA-C	7.22	1.62	1.52
1	D	160	ALA	CA-CB	-7.21	1.41	1.53
1	D	139	CYS	CA-C	-7.20	1.43	1.52
1	D	66	PRO	CB-CG	7.19	1.85	1.49
1	C	72	VAL	CA-CB	-7.18	1.45	1.54
1	B	128	LYS	CB-CG	7.17	1.74	1.52
1	A	75	GLU	CA-C	-7.15	1.43	1.52
1	B	109	ILE	CA-CB	7.14	1.64	1.54
1	C	108	LYS	CA-C	-7.13	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	MET	SD-CE	-7.13	1.61	1.79
1	B	64	VAL	CA-CB	-7.12	1.45	1.54
1	B	25	PHE	CA-C	7.12	1.61	1.52
1	D	42	GLU	CA-C	7.11	1.62	1.52
1	A	54	GLU	N-CA	-7.00	1.36	1.46
1	C	62	ARG	CA-C	6.99	1.61	1.52
1	B	167	VAL	N-CA	-6.99	1.38	1.46
1	C	128	LYS	N-CA	6.99	1.56	1.46
1	A	35	GLY	C-O	6.99	1.33	1.23
1	C	85	ILE	CA-C	6.98	1.61	1.52
1	B	12	PHE	CA-CB	6.96	1.60	1.53
1	C	112	ARG	CB-CG	6.96	1.73	1.52
1	B	79	GLU	N-CA	-6.96	1.37	1.46
1	D	51	ARG	CB-CG	6.93	1.73	1.52
1	A	34	THR	N-CA	-6.90	1.37	1.46
1	A	39	PHE	N-CA	6.89	1.54	1.45
1	D	23	THR	CA-C	6.85	1.61	1.52
1	B	12	PHE	CA-C	6.84	1.61	1.53
1	D	61	SER	CA-C	6.83	1.61	1.52
1	B	75	GLU	CB-CG	6.73	1.72	1.52
1	C	131	ASP	CA-CB	6.73	1.64	1.53
1	C	146	LYS	CG-CD	6.73	1.72	1.52
1	D	85	ILE	CA-CB	6.72	1.62	1.54
1	A	31	VAL	C-N	-6.69	1.25	1.33
1	C	123	THR	CB-CG2	-6.68	1.30	1.52
1	C	64	VAL	CA-CB	6.68	1.62	1.54
1	D	131	ASP	C-O	6.66	1.32	1.24
1	A	45	GLU	CG-CD	6.64	1.68	1.52
1	B	117	GLN	CA-CB	6.64	1.61	1.53
1	D	48	ALA	N-CA	-6.64	1.36	1.46
1	B	123	THR	CA-CB	-6.61	1.44	1.52
1	D	88	LYS	CE-NZ	6.61	1.69	1.49
1	D	61	SER	CA-CB	6.59	1.64	1.53
1	C	93	GLU	CA-C	6.58	1.61	1.52
1	A	87	ILE	CA-C	6.57	1.60	1.52
1	C	24	VAL	CA-CB	-6.55	1.46	1.54
1	D	2	PRO	CA-CB	6.54	1.60	1.53
1	A	124	GLY	CA-C	6.54	1.61	1.51
1	A	32	ILE	N-CA	-6.54	1.38	1.46
1	D	101	MET	SD-CE	-6.53	1.63	1.79
1	D	106	SER	CA-C	6.52	1.60	1.52
1	B	110	GLN	CG-CD	6.51	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	ASP	CA-CB	6.50	1.64	1.53
1	C	36	VAL	N-CA	6.48	1.54	1.46
1	A	135	LEU	CG-CD2	6.47	1.74	1.52
1	D	29	THR	CA-C	-6.45	1.44	1.52
1	B	76	GLY	CA-C	6.44	1.60	1.52
1	D	36	VAL	N-CA	6.44	1.54	1.46
1	C	149	ASN	CA-CB	-6.43	1.44	1.53
1	C	17	GLY	N-CA	6.41	1.51	1.45
1	B	129	GLY	C-N	6.40	1.41	1.33
1	A	123	THR	C-N	6.38	1.42	1.33
1	D	3	PRO	CA-CB	6.37	1.62	1.53
1	D	31	VAL	CA-CB	6.35	1.62	1.54
1	B	39	PHE	C-O	6.32	1.31	1.23
1	D	71	MET	SD-CE	6.30	1.95	1.79
1	D	89	ARG	CA-C	6.30	1.60	1.52
1	B	8	ARG	N-CA	6.29	1.53	1.46
1	C	121	LEU	CA-C	-6.28	1.44	1.52
1	C	45	GLU	CG-CD	6.28	1.67	1.52
1	B	62	ARG	CG-CD	6.24	1.71	1.52
1	B	75	GLU	CA-C	6.24	1.61	1.52
1	C	112	ARG	CG-CD	6.22	1.71	1.52
1	D	114	VAL	CA-C	-6.21	1.44	1.52
1	A	121	LEU	CA-C	-6.20	1.45	1.52
1	B	166	THR	CA-C	-6.15	1.45	1.52
1	C	69	THR	CA-CB	-6.15	1.44	1.53
1	B	23	THR	CA-CB	6.14	1.61	1.53
1	B	130	MET	C-O	6.12	1.30	1.23
1	D	90	ASP	CA-CB	6.11	1.63	1.53
1	D	151	TRP	CA-CB	6.10	1.60	1.52
1	B	35	GLY	C-N	6.08	1.42	1.33
1	D	88	LYS	CD-CE	6.07	1.70	1.52
1	C	69	THR	N-CA	-6.04	1.38	1.45
1	D	120	MET	SD-CE	-6.04	1.64	1.79
1	A	45	GLU	CB-CG	6.04	1.70	1.52
1	B	66	PRO	CA-C	6.02	1.61	1.52
1	B	75	GLU	CG-CD	6.00	1.67	1.52
1	B	65	ARG	CA-CB	6.00	1.61	1.53
1	B	161	THR	CA-CB	-5.97	1.43	1.53
1	C	172	GLN	CA-CB	-5.97	1.44	1.53
1	D	111	GLY	CA-C	5.97	1.60	1.51
1	C	105	ALA	CA-C	-5.96	1.44	1.52
1	D	88	LYS	CB-CG	5.95	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	GLU	CA-C	5.94	1.61	1.52
1	B	35	GLY	CA-C	5.93	1.60	1.51
1	D	51	ARG	CG-CD	5.93	1.70	1.52
1	B	72	VAL	N-CA	5.92	1.53	1.46
1	B	33	PRO	CA-CB	5.91	1.61	1.53
1	A	35	GLY	N-CA	5.90	1.53	1.45
1	C	34	THR	CB-CG2	5.89	1.72	1.52
1	A	131	ASP	CA-C	5.88	1.60	1.52
1	D	96	PRO	CA-CB	-5.87	1.46	1.53
1	B	38	GLU	CA-CB	5.86	1.63	1.53
1	D	162	LYS	CD-CE	5.86	1.70	1.52
1	B	149	ASN	CB-CG	5.84	1.66	1.52
1	B	45	GLU	CA-C	5.83	1.60	1.52
1	B	112	ARG	CA-CB	5.83	1.63	1.53
1	B	128	LYS	CA-C	5.82	1.60	1.53
1	D	72	VAL	CA-CB	5.80	1.60	1.54
1	A	33	PRO	N-CA	-5.78	1.39	1.47
1	D	80	GLY	CA-C	-5.77	1.43	1.51
1	C	155	GLY	CA-C	5.76	1.58	1.52
1	B	142	PRO	CA-C	-5.75	1.46	1.52
1	A	120	MET	CA-C	-5.75	1.45	1.52
1	A	108	LYS	CB-CG	5.74	1.69	1.52
1	A	44	ILE	N-CA	-5.73	1.39	1.46
1	D	154	CYS	CB-SG	5.73	2.00	1.81
1	B	57	GLN	CA-C	-5.73	1.45	1.53
1	D	149	ASN	CA-CB	5.72	1.61	1.53
1	B	2	PRO	CA-CB	5.72	1.61	1.54
1	B	139	CYS	CA-C	-5.72	1.45	1.52
1	D	37	ARG	CA-C	-5.72	1.45	1.52
1	D	69	THR	CB-CG2	5.72	1.71	1.52
1	A	113	LEU	CA-CB	5.71	1.61	1.53
1	B	27	THR	CB-CG2	-5.70	1.33	1.52
1	C	49	ILE	CA-CB	5.69	1.61	1.54
1	D	3	PRO	CA-C	5.69	1.60	1.52
1	D	88	LYS	CG-CD	5.68	1.69	1.52
1	B	106	SER	CA-CB	-5.66	1.43	1.53
1	A	25	PHE	CA-C	-5.64	1.45	1.52
1	A	29	THR	CA-CB	5.62	1.62	1.53
1	B	21	SER	C-N	5.62	1.41	1.34
1	D	72	VAL	CA-C	5.60	1.61	1.52
1	B	77	CYS	CA-CB	5.59	1.62	1.54
1	B	2	PRO	N-CD	5.59	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	VAL	CA-CB	5.58	1.64	1.55
1	B	70	GLY	CA-C	-5.57	1.47	1.52
1	C	81	VAL	CA-CB	-5.56	1.48	1.54
1	C	162	LYS	CA-C	5.56	1.60	1.52
1	A	106	SER	CA-C	-5.56	1.46	1.52
1	B	128	LYS	CA-CB	5.54	1.61	1.52
1	C	135	LEU	CA-CB	-5.53	1.46	1.54
1	D	151	TRP	CB-CG	5.53	1.67	1.50
1	D	162	LYS	CG-CD	5.52	1.69	1.52
1	C	173	ALA	CA-CB	5.52	1.70	1.52
1	C	34	THR	CA-C	5.52	1.60	1.52
1	B	14	SER	CA-C	5.50	1.60	1.52
1	B	131	ASP	CA-C	5.49	1.60	1.52
1	A	90	ASP	CA-CB	5.49	1.60	1.52
1	A	85	ILE	CA-C	5.48	1.58	1.53
1	B	112	ARG	CB-CG	5.48	1.68	1.52
1	C	81	VAL	N-CA	-5.47	1.39	1.46
1	A	33	PRO	CB-CG	5.46	1.76	1.49
1	B	173	ALA	CA-C	5.44	1.64	1.52
1	A	90	ASP	CA-C	-5.43	1.46	1.53
1	C	130	MET	N-CA	5.43	1.52	1.46
1	A	150	ASP	CA-C	-5.37	1.46	1.52
1	C	5	LEU	N-CA	5.36	1.52	1.46
1	C	123	THR	C-O	-5.36	1.17	1.23
1	B	15	GLY	N-CA	5.36	1.50	1.45
1	A	23	THR	CA-CB	5.34	1.61	1.54
1	B	42	GLU	CA-C	5.34	1.59	1.52
1	D	2	PRO	C-N	5.34	1.46	1.33
1	A	172	GLN	CA-CB	5.34	1.62	1.53
1	B	108	LYS	CB-CG	5.34	1.68	1.52
1	B	149	ASN	CA-C	5.33	1.59	1.52
1	D	131	ASP	CA-C	5.33	1.59	1.52
1	D	146	LYS	CB-CG	5.32	1.68	1.52
1	C	90	ASP	CA-C	-5.31	1.45	1.52
1	B	60	PHE	CB-CG	5.30	1.62	1.50
1	B	163	SER	CA-C	5.30	1.60	1.52
1	D	56	THR	CA-C	5.29	1.58	1.52
1	D	96	PRO	CA-C	-5.29	1.47	1.52
1	B	167	VAL	CA-CB	5.28	1.64	1.55
1	A	151	TRP	CB-CG	-5.27	1.33	1.50
1	C	68	LEU	CA-C	-5.27	1.45	1.53
1	A	77	CYS	CA-C	-5.26	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	GLY	CA-C	5.25	1.59	1.51
1	C	68	LEU	CB-CG	-5.25	1.43	1.53
1	B	33	PRO	C-N	5.24	1.40	1.33
1	D	36	VAL	C-N	-5.24	1.26	1.33
1	D	51	ARG	CA-CB	5.24	1.62	1.53
1	D	146	LYS	CA-CB	5.24	1.60	1.53
1	A	126	ASN	CA-CB	5.24	1.61	1.53
1	C	110	GLN	CG-CD	5.23	1.65	1.52
1	A	65	ARG	N-CA	5.22	1.52	1.46
1	D	123	THR	CA-C	-5.21	1.45	1.52
1	D	29	THR	CA-CB	5.21	1.61	1.53
1	D	166	THR	CA-CB	5.20	1.61	1.53
1	D	149	ASN	CB-CG	5.20	1.65	1.52
1	A	77	CYS	CB-SG	5.19	1.98	1.81
1	A	121	LEU	N-CA	-5.18	1.39	1.45
1	C	26	ILE	CA-CB	5.17	1.62	1.54
1	A	100	ARG	CD-NE	5.17	1.53	1.46
1	B	129	GLY	CA-C	5.17	1.59	1.51
1	A	105	ALA	CA-C	-5.17	1.46	1.52
1	C	45	GLU	CB-CG	5.16	1.68	1.52
1	B	146	LYS	CG-CD	5.15	1.68	1.52
1	D	20	VAL	CB-CG2	5.15	1.69	1.52
1	B	15	GLY	CA-C	5.15	1.58	1.52
1	B	74	GLU	CA-CB	5.14	1.61	1.53
1	A	49	ILE	CA-C	-5.14	1.46	1.52
1	C	103	ALA	CA-C	-5.14	1.46	1.53
1	B	85	ILE	N-CA	5.10	1.52	1.46
1	D	36	VAL	CB-CG2	5.09	1.69	1.52
1	B	60	PHE	CD2-CE2	5.08	1.53	1.38
1	A	20	VAL	CB-CG1	-5.08	1.35	1.52
1	B	147	ARG	CA-CB	5.07	1.62	1.53
1	B	19	TRP	CA-CB	5.06	1.59	1.52
1	A	86	LEU	CA-C	5.05	1.59	1.52
1	C	10	VAL	N-CA	-5.05	1.40	1.46
1	D	27	THR	CB-CG2	-5.05	1.35	1.52
1	A	91	SER	C-O	-5.05	1.17	1.24
1	C	9	VAL	CA-C	-5.03	1.47	1.52
1	D	86	LEU	CB-CG	5.02	1.63	1.53
1	B	65	ARG	CD-NE	5.01	1.53	1.46

All (651) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	VAL	N-CA-C	24.20	148.02	108.81
1	D	24	VAL	N-CA-C	17.59	133.51	108.36
1	D	2	PRO	N-CA-C	-17.57	93.61	110.47
1	D	4	THR	N-CA-C	-17.21	91.60	113.12
1	A	34	THR	N-CA-CB	-16.49	82.62	110.49
1	B	3	PRO	N-CA-C	15.97	145.38	112.47
1	A	32	ILE	CA-C-N	-15.89	103.35	119.56
1	A	32	ILE	C-N-CA	-15.89	103.35	119.56
1	D	109	ILE	N-CA-CB	-15.83	85.11	111.23
1	B	72	VAL	CB-CA-C	-14.82	89.29	111.08
1	D	4	THR	N-CA-CB	14.52	132.63	110.42
1	A	37	ARG	N-CA-CB	-14.43	86.10	110.49
1	D	35	GLY	N-CA-C	14.38	147.27	113.18
1	A	36	VAL	N-CA-C	14.28	139.04	109.34
1	A	128	LYS	N-CA-C	14.12	127.08	110.41
1	A	14	SER	N-CA-C	-14.03	96.45	113.15
1	B	21	SER	N-CA-C	13.95	120.77	108.22
1	C	122	LEU	N-CA-C	13.89	129.30	109.71
1	C	42	GLU	CB-CA-C	13.77	129.97	108.91
1	B	8	ARG	N-CA-C	-13.56	96.24	112.92
1	B	2	PRO	N-CA-C	-13.56	94.15	110.70
1	B	34	THR	N-CA-CB	13.37	131.55	110.57
1	B	39	PHE	CA-C-N	13.33	147.00	121.54
1	B	39	PHE	C-N-CA	13.33	147.00	121.54
1	C	124	GLY	CA-C-N	-12.94	104.23	122.87
1	C	124	GLY	C-N-CA	-12.94	104.23	122.87
1	A	33	PRO	N-CA-C	12.85	130.55	113.84
1	B	168	VAL	CB-CA-C	-12.83	91.59	110.33
1	C	35	GLY	CA-C-O	-12.78	109.61	121.11
1	B	130	MET	N-CA-C	12.71	134.94	107.49
1	C	104	ILE	N-CA-C	-12.43	96.50	110.05
1	A	34	THR	N-CA-C	12.25	136.90	110.80
1	B	126	ASN	N-CA-C	12.19	136.77	110.80
1	B	148	ASN	CA-C-N	12.00	141.09	120.58
1	B	148	ASN	C-N-CA	12.00	141.09	120.58
1	D	37	ARG	N-CA-C	11.99	136.34	110.80
1	B	64	VAL	CA-C-N	11.96	132.81	122.28
1	B	64	VAL	C-N-CA	11.96	132.81	122.28
1	B	160	ALA	N-CA-C	11.94	129.16	108.75
1	B	8	ARG	CA-C-N	-11.93	107.61	123.12
1	B	8	ARG	C-N-CA	-11.93	107.61	123.12
1	A	123	THR	N-CA-C	11.91	132.75	114.64
1	B	93	GLU	N-CA-C	-11.86	92.92	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ASP	CA-C-N	-11.84	98.92	121.54
1	B	90	ASP	C-N-CA	-11.84	98.92	121.54
1	C	131	ASP	CA-C-N	11.80	142.67	122.26
1	C	131	ASP	C-N-CA	11.80	142.67	122.26
1	D	40	PHE	N-CA-C	-11.67	94.88	111.56
1	C	76	GLY	CA-C-O	-11.61	109.99	121.83
1	D	47	ILE	CB-CA-C	-11.41	94.30	110.96
1	A	126	ASN	N-CA-C	11.29	123.28	110.97
1	D	44	ILE	N-CA-C	11.23	132.69	109.34
1	D	36	VAL	N-CA-C	11.14	132.52	109.34
1	B	149	ASN	N-CA-C	10.98	125.19	111.69
1	A	37	ARG	CA-CB-CG	10.95	136.00	114.10
1	B	30	HIS	CA-C-N	-10.80	109.00	121.85
1	B	30	HIS	C-N-CA	-10.80	109.00	121.85
1	A	172	GLN	CB-CG-CD	10.79	130.95	112.60
1	C	42	GLU	N-CA-C	-10.68	94.27	110.50
1	B	64	VAL	CA-C-O	10.66	128.25	119.29
1	A	130	MET	CG-SD-CE	10.60	124.22	100.90
1	C	47	ILE	CB-CA-C	-10.47	96.21	110.98
1	B	110	GLN	N-CA-C	-10.33	95.39	109.54
1	D	47	ILE	N-CA-C	10.31	122.75	107.80
1	D	39	PHE	CA-C-N	10.29	137.49	122.36
1	D	39	PHE	C-N-CA	10.29	137.49	122.36
1	B	90	ASP	CA-C-O	-10.23	109.60	120.55
1	D	37	ARG	N-CA-CB	-10.18	93.29	110.49
1	B	65	ARG	NE-CZ-NH2	10.11	128.30	119.20
1	B	26	ILE	N-CA-CB	-10.04	97.56	111.41
1	D	24	VAL	CB-CA-C	-10.02	97.22	110.84
1	B	138	ASP	CA-C-N	-10.00	104.79	121.39
1	B	138	ASP	C-N-CA	-10.00	104.79	121.39
1	B	25	PHE	N-CA-C	9.98	123.54	108.46
1	D	149	ASN	N-CA-C	-9.96	101.76	113.21
1	B	56	THR	CB-CA-C	-9.93	98.23	110.94
1	C	4	THR	N-CA-C	-9.91	99.92	112.90
1	A	31	VAL	CA-C-N	-9.89	103.83	122.13
1	A	31	VAL	C-N-CA	-9.89	103.83	122.13
1	B	107	MET	N-CA-C	9.89	123.92	108.79
1	D	153	VAL	N-CA-CB	9.77	121.37	110.72
1	D	100	ARG	N-CA-C	-9.72	95.30	109.59
1	B	155	GLY	N-CA-C	9.72	125.27	110.88
1	A	40	PHE	N-CA-C	-9.70	98.01	111.39
1	D	25	PHE	N-CA-C	9.69	124.79	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	ASN	N-CA-C	-9.66	95.66	109.29
1	C	112	ARG	CA-C-N	9.63	135.30	122.30
1	C	112	ARG	C-N-CA	9.63	135.30	122.30
1	B	15	GLY	N-CA-C	9.63	126.08	110.77
1	B	34	THR	O-C-N	9.61	134.63	123.29
1	A	33	PRO	CA-C-N	-9.53	103.33	121.54
1	A	33	PRO	C-N-CA	-9.53	103.33	121.54
1	B	47	ILE	CB-CA-C	-9.48	95.69	110.95
1	B	8	ARG	N-CA-CB	9.47	124.39	110.56
1	B	112	ARG	CA-CB-CG	9.43	132.97	114.10
1	C	154	CYS	N-CA-CB	-9.42	96.80	110.65
1	D	18	PHE	N-CA-C	9.36	124.23	108.13
1	B	69	THR	N-CA-C	-9.36	97.44	110.35
1	D	109	ILE	N-CA-C	9.35	128.78	109.34
1	D	168	VAL	CB-CA-C	-9.34	96.91	110.83
1	D	106	SER	N-CA-C	-9.33	93.21	108.41
1	A	100	ARG	N-CA-C	-9.29	94.11	109.07
1	C	131	ASP	N-CA-C	9.27	130.55	110.80
1	D	130	MET	CA-C-O	9.24	130.78	120.80
1	C	65	ARG	NE-CZ-NH2	9.23	127.50	119.20
1	D	157	HIS	N-CA-C	9.23	123.39	108.63
1	A	36	VAL	CA-C-O	-9.20	109.28	120.78
1	A	147	ARG	N-CA-C	-9.19	91.22	110.80
1	A	171	VAL	N-CA-C	9.17	122.13	108.46
1	A	1	ALA	CA-C-N	9.17	129.83	120.38
1	A	1	ALA	C-N-CA	9.17	129.83	120.38
1	B	46	SER	N-CA-C	9.14	122.22	111.71
1	C	34	THR	N-CA-C	9.12	130.22	110.80
1	D	72	VAL	CB-CA-C	-9.12	96.47	111.51
1	C	89	ARG	CG-CD-NE	-9.11	91.96	112.00
1	B	9	VAL	N-CA-C	-9.11	94.60	107.80
1	C	41	GLY	CA-C-N	-9.06	102.94	123.15
1	C	41	GLY	C-N-CA	-9.06	102.94	123.15
1	B	3	PRO	CA-N-CD	-9.03	99.36	112.00
1	C	40	PHE	N-CA-C	-9.00	99.30	111.54
1	B	24	VAL	CB-CA-C	-8.93	96.64	111.29
1	A	36	VAL	CB-CA-C	-8.92	96.67	111.29
1	B	77	CYS	N-CA-C	-8.90	95.07	109.58
1	D	83	CYS	CA-CB-SG	8.88	134.82	114.40
1	D	50	HIS	CB-CA-C	8.86	131.98	111.77
1	D	153	VAL	CB-CA-C	-8.86	99.92	110.91
1	B	77	CYS	N-CA-CB	8.82	126.25	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	SER	O-C-N	8.75	132.46	122.22
1	D	124	GLY	N-CA-C	8.75	133.93	113.18
1	B	139	CYS	CA-C-N	-8.72	111.30	123.08
1	B	139	CYS	C-N-CA	-8.72	111.30	123.08
1	D	36	VAL	CB-CA-C	-8.72	96.99	111.29
1	B	146	LYS	N-CA-CB	-8.69	97.12	110.77
1	B	91	SER	N-CA-CB	8.67	125.14	110.49
1	A	7	SER	CA-C-N	-8.66	106.70	122.38
1	A	7	SER	C-N-CA	-8.66	106.70	122.38
1	B	146	LYS	CB-CG-CD	8.62	131.12	111.30
1	B	66	PRO	N-CA-C	-8.55	102.73	114.27
1	B	39	PHE	N-CA-C	8.44	122.64	108.13
1	B	46	SER	CA-C-N	8.43	135.32	122.68
1	B	46	SER	C-N-CA	8.43	135.32	122.68
1	D	155	GLY	N-CA-C	8.39	122.63	110.63
1	D	154	CYS	CA-CB-SG	8.38	133.68	114.40
1	C	95	LEU	CB-CA-C	-8.37	98.22	111.02
1	A	135	LEU	CA-CB-CG	8.36	145.56	116.30
1	D	131	ASP	N-CA-C	-8.34	93.03	110.80
1	B	62	ARG	CA-CB-CG	8.34	130.78	114.10
1	D	77	CYS	CA-C-N	-8.32	110.79	120.11
1	D	77	CYS	C-N-CA	-8.32	110.79	120.11
1	B	88	LYS	N-CA-C	-8.31	96.74	109.95
1	B	63	LYS	CB-CA-C	-8.30	93.89	110.42
1	B	101	MET	N-CA-C	8.30	122.41	109.96
1	C	42	GLU	CA-C-N	8.23	128.54	119.90
1	C	42	GLU	C-N-CA	8.23	128.54	119.90
1	D	67	ASP	N-CA-C	-8.20	102.35	111.28
1	A	69	THR	N-CA-C	-8.19	99.05	110.35
1	D	107	MET	CA-C-N	-8.19	109.66	122.67
1	D	107	MET	C-N-CA	-8.19	109.66	122.67
1	B	168	VAL	N-CA-CB	8.18	123.45	111.52
1	C	29	THR	N-CA-C	8.17	120.26	111.36
1	A	42	GLU	CB-CA-C	8.16	122.36	109.55
1	D	65	ARG	NE-CZ-NH2	8.13	126.52	119.20
1	D	85	ILE	CG1-CB-CG2	-8.13	86.31	110.70
1	A	166	THR	N-CA-C	8.11	122.28	110.28
1	D	94	LEU	N-CA-C	-8.08	96.39	109.96
1	A	85	ILE	CA-CB-CG2	8.07	124.22	110.50
1	D	131	ASP	CA-C-N	8.06	137.85	123.34
1	D	131	ASP	C-N-CA	8.06	137.85	123.34
1	D	25	PHE	CA-C-N	8.03	132.07	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	PHE	C-N-CA	8.03	132.07	120.91
1	B	137	GLY	CA-C-N	-8.02	110.59	122.86
1	B	137	GLY	C-N-CA	-8.02	110.59	122.86
1	B	132	LEU	N-CA-C	8.01	123.35	113.50
1	C	21	SER	CA-C-N	8.00	127.57	118.85
1	C	21	SER	C-N-CA	8.00	127.57	118.85
1	D	1	ALA	CA-C-N	-7.98	113.83	119.66
1	D	1	ALA	C-N-CA	-7.98	113.83	119.66
1	A	123	THR	CA-C-O	-7.95	108.49	118.43
1	C	77	CYS	CA-C-N	-7.92	111.75	120.14
1	C	77	CYS	C-N-CA	-7.92	111.75	120.14
1	A	32	ILE	CB-CA-C	-7.91	96.97	111.36
1	B	74	GLU	CB-CA-C	7.90	125.43	110.51
1	D	2	PRO	CA-C-N	-7.89	109.98	119.84
1	D	2	PRO	C-N-CA	-7.89	109.98	119.84
1	B	63	LYS	CA-CB-CG	7.88	129.85	114.10
1	B	70	GLY	CA-C-N	-7.88	110.91	122.65
1	B	70	GLY	C-N-CA	-7.88	110.91	122.65
1	C	149	ASN	N-CA-C	-7.82	101.88	113.61
1	A	37	ARG	CB-CA-C	-7.81	94.88	110.42
1	C	76	GLY	N-CA-C	-7.81	99.32	110.88
1	B	34	THR	CA-C-O	7.79	128.88	120.38
1	B	45	GLU	CA-C-N	7.74	131.43	120.28
1	B	45	GLU	C-N-CA	7.74	131.43	120.28
1	B	24	VAL	N-CA-C	7.74	125.43	109.34
1	A	127	ALA	CA-C-O	-7.72	112.69	121.19
1	C	135	LEU	CB-CA-C	-7.72	96.90	108.87
1	C	81	VAL	CB-CA-C	-7.71	100.63	111.28
1	A	14	SER	CA-C-N	-7.70	116.23	122.16
1	A	14	SER	C-N-CA	-7.70	116.23	122.16
1	D	50	HIS	CA-C-N	7.69	132.76	121.31
1	D	50	HIS	C-N-CA	7.69	132.76	121.31
1	D	148	ASN	N-CA-CB	7.68	118.41	108.96
1	C	127	ALA	N-CA-CB	7.68	122.57	111.05
1	A	134	THR	CA-C-N	-7.67	106.04	123.15
1	A	134	THR	C-N-CA	-7.67	106.04	123.15
1	D	37	ARG	CA-C-O	7.66	131.46	120.51
1	A	72	VAL	CB-CA-C	-7.63	100.31	111.68
1	C	32	ILE	CA-C-N	-7.63	111.89	119.90
1	C	32	ILE	C-N-CA	-7.63	111.89	119.90
1	C	1	ALA	CA-C-N	-7.62	112.53	120.38
1	C	1	ALA	C-N-CA	-7.62	112.53	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	GLU	N-CA-C	7.61	122.43	110.32
1	B	96	PRO	N-CA-C	-7.61	98.31	111.32
1	C	155	GLY	N-CA-C	7.61	121.51	110.63
1	A	90	ASP	N-CA-CB	7.58	120.81	110.57
1	C	43	PRO	N-CA-C	7.58	122.25	110.80
1	D	86	LEU	CA-C-O	7.58	130.38	120.98
1	B	35	GLY	CA-C-O	-7.58	107.38	120.57
1	D	101	MET	N-CA-C	7.57	121.69	110.48
1	D	42	GLU	CA-C-N	7.57	129.30	119.84
1	D	42	GLU	C-N-CA	7.57	129.30	119.84
1	B	144	VAL	CA-C-O	-7.56	115.71	121.68
1	D	46	SER	N-CA-C	-7.54	103.04	111.71
1	D	36	VAL	O-C-N	-7.51	113.18	122.57
1	B	6	TRP	N-CA-C	-7.49	103.05	111.14
1	A	151	TRP	CA-CB-CG	-7.49	99.38	113.60
1	D	69	THR	CB-CA-C	-7.48	98.47	110.81
1	D	51	ARG	NE-CZ-NH2	7.44	125.89	119.20
1	C	172	GLN	O-C-N	7.41	129.80	122.09
1	B	38	GLU	N-CA-C	7.40	126.57	110.80
1	B	114	VAL	N-CA-C	7.40	118.53	107.80
1	B	149	ASN	CA-CB-CG	7.37	119.97	112.60
1	A	40	PHE	CB-CA-C	7.35	122.33	111.89
1	B	19	TRP	CA-C-O	7.35	128.56	120.92
1	B	8	ARG	CB-CA-C	-7.35	98.14	110.56
1	D	108	LYS	CD-CE-NZ	7.34	135.39	111.90
1	D	141	ALA	CA-C-N	7.34	127.26	119.85
1	D	141	ALA	C-N-CA	7.34	127.26	119.85
1	D	88	LYS	N-CA-C	-7.33	97.74	109.76
1	B	114	VAL	CB-CA-C	-7.31	100.29	110.96
1	B	38	GLU	CA-C-N	7.31	133.41	121.86
1	B	38	GLU	C-N-CA	7.31	133.41	121.86
1	D	61	SER	N-CA-C	-7.30	102.49	111.40
1	D	104	ILE	CB-CA-C	-7.27	99.36	111.29
1	B	65	ARG	CD-NE-CZ	7.26	134.56	124.40
1	C	139	CYS	CA-C-N	-7.26	112.26	122.86
1	C	139	CYS	C-N-CA	-7.26	112.26	122.86
1	B	27	THR	OG1-CB-CG2	-7.25	94.79	109.30
1	A	122	LEU	N-CA-C	7.25	119.78	110.65
1	B	127	ALA	CA-C-N	7.24	134.57	122.76
1	B	127	ALA	C-N-CA	7.24	134.57	122.76
1	B	144	VAL	O-C-N	7.24	128.85	122.12
1	C	128	LYS	N-CA-C	7.24	117.79	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	ILE	CA-C-O	-7.22	113.03	121.05
1	D	131	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	108	LYS	N-CA-CB	-7.22	99.54	110.73
1	C	146	LYS	CB-CG-CD	7.21	127.87	111.30
1	B	63	LYS	N-CA-C	-7.19	95.48	110.80
1	D	142	PRO	N-CA-C	7.15	122.74	111.38
1	B	65	ARG	CA-C-N	7.14	127.75	120.04
1	B	65	ARG	C-N-CA	7.14	127.75	120.04
1	C	125	ALA	N-CA-C	7.13	119.31	109.54
1	D	99	VAL	N-CA-C	7.10	119.25	106.61
1	B	64	VAL	O-C-N	7.10	129.64	122.04
1	C	36	VAL	CB-CA-C	-7.08	99.68	111.29
1	D	130	MET	N-CA-C	-7.07	99.70	110.30
1	A	34	THR	CA-C-N	7.06	135.25	121.41
1	A	34	THR	C-N-CA	7.06	135.25	121.41
1	B	48	ALA	N-CA-C	7.06	119.55	110.65
1	B	22	PRO	N-CA-C	-7.06	104.32	113.57
1	A	107	MET	CA-C-N	7.04	133.58	122.60
1	A	107	MET	C-N-CA	7.04	133.58	122.60
1	A	37	ARG	NE-CZ-NH1	-7.04	114.46	121.50
1	B	7	SER	CB-CA-C	7.03	123.17	110.72
1	D	165	ASN	CB-CA-C	-7.03	99.56	110.81
1	B	116	GLY	CA-C-O	-7.01	114.02	121.38
1	A	125	ALA	N-CA-CB	7.00	122.09	110.47
1	A	153	VAL	CB-CA-C	-7.00	99.73	110.50
1	C	70	GLY	O-C-N	6.99	130.23	123.80
1	A	74	GLU	N-CA-C	-6.99	101.52	110.53
1	A	168	VAL	CG1-CB-CG2	-6.99	95.43	110.80
1	A	73	LEU	CB-CA-C	-6.98	100.42	111.17
1	B	76	GLY	CA-C-O	-6.98	115.02	121.72
1	A	25	PHE	CA-C-N	6.95	132.07	123.10
1	A	25	PHE	C-N-CA	6.95	132.07	123.10
1	A	130	MET	CA-CB-CG	6.95	127.99	114.10
1	D	68	LEU	N-CA-C	6.95	120.56	109.24
1	D	107	MET	CB-CA-C	-6.94	98.22	111.48
1	D	130	MET	CA-CB-CG	6.94	127.98	114.10
1	B	171	VAL	CA-C-N	6.93	130.06	120.63
1	B	171	VAL	C-N-CA	6.93	130.06	120.63
1	D	36	VAL	CA-C-O	-6.91	112.15	120.78
1	A	164	GLY	N-CA-C	6.88	129.49	113.18
1	B	110	GLN	CB-CG-CD	6.87	124.28	112.60
1	C	77	CYS	CA-CB-SG	-6.87	98.60	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	THR	CB-CA-C	-6.86	96.78	110.42
1	A	61	SER	N-CA-CB	-6.85	100.47	110.47
1	D	2	PRO	CA-C-O	-6.84	115.97	120.90
1	B	74	GLU	CA-CB-CG	6.84	127.79	114.10
1	B	75	GLU	CB-CG-CD	6.84	124.23	112.60
1	C	147	ARG	NE-CZ-NH1	-6.83	114.67	121.50
1	D	13	GLY	CA-C-N	6.83	129.43	120.28
1	D	13	GLY	C-N-CA	6.83	129.43	120.28
1	C	9	VAL	CB-CA-C	-6.82	102.59	111.25
1	A	112	ARG	CG-CD-NE	6.81	126.99	112.00
1	D	58	PHE	N-CA-C	-6.81	96.22	108.48
1	A	63	LYS	CB-CG-CD	6.80	126.95	111.30
1	D	14	SER	CB-CA-C	-6.76	99.56	110.79
1	B	39	PHE	CA-C-O	6.76	129.37	120.11
1	A	35	GLY	O-C-N	6.75	131.48	122.70
1	D	37	ARG	CB-CA-C	-6.75	96.99	110.42
1	D	33	PRO	N-CA-C	6.75	122.11	111.38
1	B	13	GLY	CA-C-N	6.74	132.94	121.14
1	B	13	GLY	C-N-CA	6.74	132.94	121.14
1	A	39	PHE	N-CA-CB	6.73	124.05	111.53
1	B	154	CYS	CA-CB-SG	6.73	129.88	114.40
1	B	27	THR	N-CA-CB	6.71	122.84	111.57
1	A	124	GLY	CA-C-N	-6.68	113.62	123.11
1	A	124	GLY	C-N-CA	-6.68	113.62	123.11
1	A	91	SER	N-CA-C	-6.66	96.61	110.80
1	C	108	LYS	CB-CG-CD	6.64	126.58	111.30
1	C	131	ASP	CA-C-O	6.63	130.00	120.51
1	B	128	LYS	CB-CG-CD	6.62	126.52	111.30
1	B	148	ASN	O-C-N	6.62	129.93	122.32
1	C	148	ASN	CB-CA-C	6.61	123.57	110.42
1	A	85	ILE	CG1-CB-CG2	-6.61	90.88	110.70
1	B	71	MET	N-CA-C	6.60	120.59	109.76
1	B	150	ASP	N-CA-C	6.60	119.11	109.07
1	B	134	THR	N-CA-C	6.58	120.22	110.48
1	C	115	HIS	N-CA-C	-6.57	99.11	109.50
1	B	135	LEU	CA-C-N	6.57	128.05	119.84
1	B	135	LEU	C-N-CA	6.57	128.05	119.84
1	B	156	VAL	CA-C-N	-6.56	112.22	121.99
1	B	156	VAL	C-N-CA	-6.56	112.22	121.99
1	B	83	CYS	N-CA-C	-6.55	100.21	110.36
1	C	31	VAL	N-CA-C	-6.54	103.77	113.39
1	B	138	ASP	N-CA-C	-6.54	103.63	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	D	1	ALA	N-CA-C	6.52	129.27	111.00
1	D	158	ALA	N-CA-C	6.52	119.35	111.40
1	C	147	ARG	CA-C-N	-6.50	109.12	121.54
1	C	147	ARG	C-N-CA	-6.50	109.12	121.54
1	B	146	LYS	CB-CA-C	6.48	120.51	110.14
1	A	123	THR	CA-C-N	6.48	134.11	121.41
1	A	123	THR	C-N-CA	6.48	134.11	121.41
1	B	8	ARG	CA-CB-CG	6.48	127.06	114.10
1	D	138	ASP	CA-C-N	-6.48	110.77	120.94
1	D	138	ASP	C-N-CA	-6.48	110.77	120.94
1	A	85	ILE	N-CA-CB	6.47	118.89	111.90
1	C	112	ARG	CA-CB-CG	6.46	127.02	114.10
1	B	21	SER	CB-CA-C	-6.45	101.70	110.22
1	D	89	ARG	N-CA-CB	-6.44	101.19	111.43
1	C	63	LYS	N-CA-C	-6.43	100.65	110.30
1	A	42	GLU	CA-C-N	6.42	126.80	119.93
1	A	42	GLU	C-N-CA	6.42	126.80	119.93
1	D	89	ARG	N-CA-C	6.42	119.17	109.41
1	B	36	VAL	CB-CA-C	-6.42	99.23	110.71
1	C	36	VAL	N-CA-CB	6.41	121.81	111.23
1	C	149	ASN	N-CA-CB	-6.39	101.27	110.80
1	A	39	PHE	N-CA-C	6.39	119.13	109.23
1	B	40	PHE	CB-CA-C	6.38	123.11	110.42
1	C	123	THR	CA-C-O	-6.37	114.19	121.58
1	D	151	TRP	N-CA-C	6.37	119.20	107.99
1	B	32	ILE	CA-C-N	-6.36	113.12	119.99
1	B	32	ILE	C-N-CA	-6.36	113.12	119.99
1	D	57	GLN	CB-CA-C	-6.36	98.88	111.60
1	A	30	HIS	CA-C-N	-6.35	110.53	121.97
1	A	30	HIS	C-N-CA	-6.35	110.53	121.97
1	B	108	LYS	CB-CA-C	6.35	122.28	111.68
1	D	150	ASP	N-CA-C	6.34	119.80	109.59
1	C	148	ASN	N-CA-CB	-6.31	99.82	110.49
1	D	65	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	D	28	THR	CA-C-N	6.31	129.02	120.38
1	D	28	THR	C-N-CA	6.31	129.02	120.38
1	A	120	MET	N-CA-CB	6.30	120.83	110.69
1	B	92	GLY	CA-C-O	6.29	131.52	120.57
1	D	108	LYS	CA-CB-CG	6.28	126.66	114.10
1	B	130	MET	O-C-N	-6.26	113.60	122.87
1	B	74	GLU	N-CA-CB	-6.25	100.93	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	CYS	CB-CA-C	6.23	120.02	109.55
1	A	43	PRO	N-CA-C	6.23	121.41	111.26
1	C	71	MET	N-CA-C	6.22	119.29	110.14
1	B	92	GLY	CA-C-N	6.22	131.72	121.39
1	B	92	GLY	C-N-CA	6.22	131.72	121.39
1	A	38	GLU	N-CA-C	6.22	118.58	108.76
1	A	128	LYS	O-C-N	-6.21	116.03	122.18
1	D	146	LYS	CA-C-O	6.21	127.00	120.36
1	A	129	GLY	N-CA-C	-6.20	98.48	113.18
1	C	109	ILE	CB-CA-C	6.20	119.91	111.97
1	B	43	PRO	CA-N-CD	-6.18	103.35	112.00
1	D	131	ASP	CB-CA-C	6.17	122.70	110.42
1	C	35	GLY	N-CA-C	-6.16	100.41	111.19
1	A	85	ILE	CB-CA-C	6.16	118.33	111.80
1	D	2	PRO	O-C-N	-6.16	118.48	121.31
1	A	107	MET	N-CA-CB	6.14	119.75	110.42
1	A	32	ILE	O-C-N	6.11	128.07	121.10
1	A	88	LYS	N-CA-C	-6.11	98.55	108.52
1	D	64	VAL	CB-CA-C	-6.10	102.22	112.16
1	B	92	GLY	O-C-N	6.07	130.59	122.70
1	C	2	PRO	CB-CA-C	6.06	118.32	110.92
1	B	57	GLN	CA-C-O	-6.05	114.81	121.89
1	D	71	MET	O-C-N	6.05	130.91	123.10
1	A	14	SER	N-CA-CB	-6.04	101.15	110.46
1	B	43	PRO	CB-CA-C	-6.04	101.60	111.56
1	A	35	GLY	CA-C-O	-6.03	110.07	120.57
1	D	85	ILE	N-CA-CB	6.03	118.29	110.57
1	B	75	GLU	CB-CA-C	6.03	122.41	110.42
1	C	107	MET	CA-C-N	-6.03	113.77	123.23
1	C	107	MET	C-N-CA	-6.03	113.77	123.23
1	B	61	SER	N-CA-CB	6.01	120.45	110.47
1	C	133	GLY	N-CA-C	6.01	119.56	111.20
1	A	108	LYS	CG-CD-CE	6.00	125.11	111.30
1	C	167	VAL	N-CA-C	6.00	118.65	108.86
1	D	107	MET	N-CA-C	-6.00	101.31	109.95
1	C	64	VAL	N-CA-C	-5.98	106.49	112.17
1	A	165	ASN	CB-CA-C	5.97	122.31	110.42
1	C	20	VAL	N-CA-C	-5.97	104.49	111.00
1	A	95	LEU	N-CA-CB	-5.96	102.79	111.20
1	B	166	THR	CA-C-N	-5.96	114.22	122.69
1	B	166	THR	C-N-CA	-5.96	114.22	122.69
1	C	77	CYS	CB-CA-C	-5.96	98.43	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	ILE	CG1-CB-CG2	-5.96	92.83	110.70
1	A	68	LEU	N-CA-C	5.95	119.28	110.48
1	C	72	VAL	CB-CA-C	-5.94	103.43	111.15
1	D	47	ILE	CA-C-N	-5.93	113.92	123.23
1	D	47	ILE	C-N-CA	-5.93	113.92	123.23
1	B	37	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	44	ILE	CG1-CB-CG2	-5.92	92.93	110.70
1	D	85	ILE	O-C-N	-5.92	115.74	121.90
1	A	155	GLY	N-CA-C	5.92	119.15	110.80
1	B	155	GLY	CA-C-N	-5.91	112.75	122.67
1	B	155	GLY	C-N-CA	-5.91	112.75	122.67
1	C	36	VAL	CA-C-N	-5.91	111.69	122.38
1	C	36	VAL	C-N-CA	-5.91	111.69	122.38
1	C	69	THR	CA-C-N	-5.90	117.24	122.73
1	C	69	THR	C-N-CA	-5.90	117.24	122.73
1	A	24	VAL	N-CA-C	5.90	116.79	108.36
1	A	107	MET	CA-CB-CG	5.90	125.90	114.10
1	C	20	VAL	N-CA-CB	5.90	120.41	110.56
1	B	130	MET	CA-CB-CG	5.89	125.89	114.10
1	A	112	ARG	CD-NE-CZ	5.89	132.65	124.40
1	D	42	GLU	N-CA-CB	5.89	118.24	109.88
1	C	24	VAL	N-CA-C	5.88	117.17	109.58
1	C	169	CYS	CA-C-N	-5.88	112.02	122.07
1	C	169	CYS	C-N-CA	-5.88	112.02	122.07
1	B	36	VAL	CG1-CB-CG2	5.88	123.73	110.80
1	C	39	PHE	N-CA-C	5.87	118.79	108.75
1	D	43	PRO	CA-N-CD	-5.87	103.79	112.00
1	C	67	ASP	CA-C-N	-5.84	112.34	123.32
1	C	67	ASP	C-N-CA	-5.84	112.34	123.32
1	C	65	ARG	CD-NE-CZ	5.83	132.56	124.40
1	D	96	PRO	CB-CA-C	-5.82	106.10	111.40
1	A	37	ARG	CA-C-N	5.82	132.81	121.63
1	A	37	ARG	C-N-CA	5.82	132.81	121.63
1	D	50	HIS	CA-CB-CG	5.81	119.61	113.80
1	D	168	VAL	N-CA-C	5.80	116.30	108.17
1	A	149	ASN	N-CA-C	-5.80	105.86	113.17
1	B	67	ASP	N-CA-CB	5.78	119.54	110.46
1	D	146	LYS	CD-CE-NZ	5.78	130.40	111.90
1	A	172	GLN	N-CA-CB	5.77	118.55	109.83
1	B	5	LEU	CB-CG-CD2	-5.76	93.41	110.70
1	B	128	LYS	CA-CB-CG	5.76	125.62	114.10
1	B	144	VAL	CA-C-N	5.76	132.80	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	VAL	C-N-CA	5.76	132.80	122.09
1	B	90	ASP	N-CA-C	5.75	118.42	111.40
1	C	111	GLY	N-CA-C	-5.75	99.56	113.18
1	D	61	SER	CA-C-N	5.74	132.51	121.54
1	D	61	SER	C-N-CA	5.74	132.51	121.54
1	D	90	ASP	CA-C-O	-5.74	114.30	121.02
1	B	127	ALA	N-CA-CB	5.74	119.58	110.57
1	B	75	GLU	N-CA-CB	-5.73	100.80	110.49
1	C	129	GLY	CA-C-N	5.72	130.85	122.39
1	C	129	GLY	C-N-CA	5.72	130.85	122.39
1	D	3	PRO	CA-C-N	-5.70	111.58	122.53
1	D	3	PRO	C-N-CA	-5.70	111.58	122.53
1	A	130	MET	CA-C-O	-5.70	112.63	118.90
1	C	36	VAL	N-CA-C	5.70	121.19	109.34
1	D	37	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	C	11	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	B	171	VAL	N-CA-C	5.67	121.14	109.34
1	D	101	MET	CA-C-N	-5.67	112.32	123.04
1	D	101	MET	C-N-CA	-5.67	112.32	123.04
1	A	47	ILE	CB-CA-C	-5.67	102.17	110.62
1	A	8	ARG	N-CA-C	5.66	120.18	113.16
1	D	66	PRO	O-C-N	5.65	130.27	122.64
1	B	87	ILE	CA-C-N	-5.62	113.82	122.87
1	B	87	ILE	C-N-CA	-5.62	113.82	122.87
1	D	49	ILE	CA-C-N	-5.62	113.22	123.34
1	D	49	ILE	C-N-CA	-5.62	113.22	123.34
1	B	38	GLU	CA-CB-CG	5.62	125.34	114.10
1	D	4	THR	CA-C-N	-5.62	111.77	120.31
1	D	4	THR	C-N-CA	-5.62	111.77	120.31
1	C	93	GLU	N-CA-CB	-5.62	101.00	110.49
1	B	46	SER	O-C-N	5.62	128.79	122.22
1	C	132	LEU	N-CA-CB	-5.62	102.16	110.53
1	D	135	LEU	N-CA-C	5.61	114.76	108.25
1	B	52	ALA	N-CA-C	5.61	120.14	108.53
1	B	20	VAL	N-CA-C	-5.60	104.71	112.50
1	D	51	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	61	SER	CA-CB-OG	-5.58	99.93	111.10
1	C	105	ALA	CA-C-N	-5.58	112.17	121.89
1	C	105	ALA	C-N-CA	-5.58	112.17	121.89
1	D	14	SER	N-CA-C	-5.58	105.19	111.28
1	C	78	PRO	CB-CA-C	5.58	118.61	110.63
1	A	116	GLY	N-CA-C	-5.56	102.68	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	VAL	CB-CA-C	-5.55	102.60	110.82
1	B	108	LYS	CB-CG-CD	5.55	124.06	111.30
1	A	36	VAL	O-C-N	-5.54	115.64	122.57
1	D	127	ALA	CB-CA-C	-5.54	103.62	111.76
1	A	121	LEU	O-C-N	5.54	129.47	123.10
1	C	147	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	A	123	THR	CA-CB-CG2	-5.53	101.10	110.50
1	A	160	ALA	O-C-N	-5.52	117.18	123.48
1	D	44	ILE	CG1-CB-CG2	5.52	127.25	110.70
1	B	57	GLN	CB-CG-CD	-5.51	103.23	112.60
1	A	41	GLY	CA-C-N	-5.51	111.26	122.45
1	A	41	GLY	C-N-CA	-5.51	111.26	122.45
1	C	37	ARG	CA-CB-CG	5.50	125.11	114.10
1	C	87	ILE	CB-CA-C	-5.50	104.30	110.96
1	B	71	MET	CA-C-O	-5.50	114.70	120.80
1	B	90	ASP	N-CA-CB	5.49	118.26	110.13
1	B	50	HIS	N-CA-CB	5.49	119.56	111.43
1	D	65	ARG	CA-C-N	5.49	126.70	119.84
1	D	65	ARG	C-N-CA	5.49	126.70	119.84
1	D	13	GLY	O-C-N	5.48	129.82	122.70
1	B	4	THR	CA-C-N	-5.48	111.08	121.54
1	B	4	THR	C-N-CA	-5.48	111.08	121.54
1	C	87	ILE	N-CA-C	5.48	116.61	108.23
1	D	90	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	172	GLN	CB-CG-CD	-5.47	103.30	112.60
1	D	50	HIS	O-C-N	5.46	129.09	121.83
1	B	159	ALA	O-C-N	5.46	128.75	123.29
1	D	108	LYS	N-CA-CB	5.46	119.65	110.92
1	B	117	GLN	CA-CB-CG	5.45	125.00	114.10
1	B	37	ARG	CA-C-O	5.45	126.26	119.78
1	C	10	VAL	CB-CA-C	-5.44	103.73	111.19
1	D	13	GLY	N-CA-C	-5.42	100.33	113.18
1	A	109	ILE	N-CA-CB	-5.42	102.29	111.23
1	D	62	ARG	CB-CG-CD	5.42	123.76	111.30
1	B	44	ILE	N-CA-CB	-5.40	102.31	111.23
1	A	77	CYS	N-CA-CB	5.40	117.33	110.04
1	A	33	PRO	CB-CA-C	5.39	119.51	111.85
1	B	29	THR	N-CA-C	5.39	120.27	111.37
1	B	23	THR	CB-CA-C	5.39	119.96	111.39
1	C	100	ARG	N-CA-C	-5.38	100.63	109.40
1	D	39	PHE	O-C-N	5.37	129.91	123.36
1	A	125	ALA	N-CA-C	-5.37	98.49	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	PHE	N-CA-C	5.36	122.23	110.80
1	A	131	ASP	OD1-CG-OD2	-5.35	110.05	122.90
1	C	7	SER	N-CA-C	-5.35	105.98	113.37
1	A	58	PHE	CB-CA-C	-5.35	100.47	109.72
1	D	130	MET	N-CA-CB	5.34	118.04	109.28
1	A	100	ARG	NH1-CZ-NH2	-5.33	112.37	119.30
1	B	6	TRP	CA-C-N	-5.33	111.73	122.55
1	B	6	TRP	C-N-CA	-5.33	111.73	122.55
1	D	64	VAL	N-CA-CB	5.32	121.01	110.95
1	C	127	ALA	N-CA-C	-5.32	101.67	109.81
1	D	26	ILE	N-CA-CB	-5.32	101.83	110.13
1	C	42	GLU	CG-CD-OE2	-5.32	106.17	118.40
1	A	3	PRO	CB-CG-CD	-5.30	89.12	106.10
1	B	123	THR	N-CA-C	-5.29	99.35	108.56
1	C	109	ILE	CA-C-N	-5.29	111.44	121.54
1	C	109	ILE	C-N-CA	-5.29	111.44	121.54
1	A	152	VAL	N-CA-C	5.28	116.51	108.80
1	B	14	SER	N-CA-C	-5.27	106.35	112.89
1	D	162	LYS	CD-CE-NZ	5.27	128.76	111.90
1	D	51	ARG	CB-CA-C	-5.27	101.29	109.61
1	B	129	GLY	CA-C-O	-5.25	111.42	120.57
1	D	95	LEU	CD1-CG-CD2	-5.25	99.24	110.80
1	D	4	THR	CB-CA-C	-5.25	100.90	109.56
1	D	104	ILE	CA-CB-CG2	5.25	119.42	110.50
1	C	11	ARG	CG-CD-NE	5.25	123.54	112.00
1	C	166	THR	N-CA-C	5.25	118.49	110.20
1	B	149	ASN	N-CA-CB	-5.24	102.40	110.20
1	D	96	PRO	CA-C-O	-5.24	114.36	120.85
1	B	144	VAL	N-CA-C	-5.23	102.24	109.46
1	C	118	SER	CA-C-N	5.23	128.68	121.26
1	C	118	SER	C-N-CA	5.23	128.68	121.26
1	A	36	VAL	N-CA-CB	5.22	119.85	111.23
1	D	27	THR	N-CA-C	5.22	116.47	108.42
1	B	110	GLN	CA-CB-CG	5.22	124.54	114.10
1	A	107	MET	O-C-N	5.21	128.78	122.68
1	B	131	ASP	OD1-CG-OD2	-5.21	110.38	122.90
1	A	110	GLN	N-CA-C	5.21	121.90	110.80
1	A	147	ARG	CD-NE-CZ	5.21	131.69	124.40
1	D	116	GLY	CA-C-N	-5.21	115.81	123.00
1	D	116	GLY	C-N-CA	-5.21	115.81	123.00
1	A	15	GLY	O-C-N	5.20	127.09	123.14
1	A	61	SER	CA-C-O	5.19	125.28	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PRO	CB-CA-C	5.19	118.88	111.04
1	D	40	PHE	N-CA-CB	5.19	120.55	112.25
1	B	118	SER	CA-C-O	5.18	127.57	121.87
1	B	155	GLY	O-C-N	-5.18	118.76	123.78
1	D	148	ASN	CA-CB-CG	5.17	117.78	112.60
1	C	63	LYS	CB-CG-CD	5.17	123.20	111.30
1	C	91	SER	N-CA-C	5.17	119.22	113.02
1	D	40	PHE	CB-CA-C	5.16	118.43	111.82
1	A	115	HIS	CA-C-N	-5.16	114.31	121.23
1	A	115	HIS	C-N-CA	-5.16	114.31	121.23
1	C	121	LEU	O-C-N	5.15	129.14	123.16
1	D	113	LEU	CA-C-N	-5.15	116.25	123.10
1	D	113	LEU	C-N-CA	-5.15	116.25	123.10
1	A	36	VAL	CA-C-N	-5.14	111.71	121.54
1	A	36	VAL	C-N-CA	-5.14	111.71	121.54
1	C	67	ASP	N-CA-C	-5.14	106.27	112.54
1	D	72	VAL	N-CA-C	-5.14	102.16	109.51
1	A	132	LEU	CA-CB-CG	5.14	134.30	116.30
1	B	36	VAL	N-CA-CB	-5.13	102.32	111.92
1	C	77	CYS	N-CA-CB	5.13	119.50	110.37
1	A	110	GLN	CA-CB-CG	5.12	124.34	114.10
1	D	35	GLY	CA-C-O	-5.12	111.67	120.57
1	D	5	LEU	N-CA-C	5.11	117.75	111.82
1	B	57	GLN	CA-C-N	5.11	129.95	122.39
1	B	57	GLN	C-N-CA	5.11	129.95	122.39
1	B	112	ARG	CD-NE-CZ	5.11	131.55	124.40
1	C	168	VAL	CB-CA-C	-5.11	103.52	110.77
1	D	134	THR	N-CA-C	-5.11	103.94	110.53
1	C	136	PRO	CA-CB-CG	-5.10	94.80	104.50
1	A	7	SER	N-CA-C	-5.09	105.85	111.71
1	A	90	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	65	ARG	CD-NE-CZ	5.08	131.51	124.40
1	D	86	LEU	N-CA-C	5.08	118.73	111.92
1	B	3	PRO	CA-C-O	-5.08	111.35	120.60
1	B	40	PHE	N-CA-C	-5.08	99.98	110.80
1	D	162	LYS	CG-CD-CE	5.07	122.96	111.30
1	A	130	MET	N-CA-C	5.07	121.16	114.12
1	C	85	ILE	CA-CB-CG1	5.06	119.01	110.40
1	A	9	VAL	CB-CA-C	-5.06	104.83	111.25
1	A	112	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	B	54	GLU	CB-CA-C	5.05	118.71	110.17
1	D	46	SER	CB-CA-C	-5.05	101.30	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	134	THR	N-CA-CB	5.04	117.65	110.44
1	C	22	PRO	CA-C-N	5.04	128.45	120.89
1	C	22	PRO	C-N-CA	5.04	128.45	120.89
1	D	114	VAL	CA-C-O	-5.04	115.15	120.39
1	D	118	SER	O-C-N	5.04	128.53	122.79
1	D	66	PRO	CB-CA-C	5.04	119.87	111.56
1	B	106	SER	CA-CB-OG	-5.04	101.03	111.10
1	A	144	VAL	CB-CA-C	-5.03	103.12	110.62
1	B	47	ILE	CA-C-N	5.03	129.59	122.24
1	B	47	ILE	C-N-CA	5.03	129.59	122.24
1	B	54	GLU	N-CA-CB	-5.03	103.01	110.61
1	A	41	GLY	CA-C-O	5.03	125.88	119.80
1	A	50	HIS	N-CA-C	5.03	118.20	107.70
1	B	157	HIS	CB-CA-C	5.03	119.16	110.77
1	A	99	VAL	CB-CA-C	-5.01	102.16	111.18
1	B	61	SER	N-CA-C	-5.01	99.12	107.99
1	D	15	GLY	CA-C-N	5.01	130.59	122.53
1	D	15	GLY	C-N-CA	5.01	130.59	122.53
1	C	34	THR	N-CA-CB	-5.00	102.03	110.49
1	C	68	LEU	N-CA-C	5.00	116.89	109.69

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ILE	Peptide
1	A	128	LYS	Mainchain
1	A	130	MET	Peptide
1	A	32	ILE	Mainchain
1	B	145	TYR	Sidechain
1	B	157	HIS	Sidechain
1	B	2	PRO	Mainchain
1	B	35	GLY	Mainchain
1	D	145	TYR	Sidechain
1	D	25	PHE	Sidechain
1	D	36	VAL	Peptide
1	D	37	ARG	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1303	0	1312	201	4
1	B	1303	0	1310	254	0
1	C	1303	0	1312	170	1
1	D	1303	0	1310	250	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	10	0	4	6	1
4	A	10	0	3	4	0
5	A	33	0	0	40	2
5	B	22	0	0	25	0
5	C	41	0	0	27	6
5	D	31	0	0	40	0
All	All	5367	0	5251	842	7

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 81.

All (842) 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:32:ILE:CA	1:A:32:ILE:CB	1.75	1.62
1:C:85:ILE:CA	1:C:85:ILE:CB	1.75	1.59
1:B:62:ARG:CG	1:B:62:ARG:CB	1.79	1.59
1:D:4:THR:CB	1:D:4:THR:CA	1.80	1.59
1:A:128:LYS:C	1:A:128:LYS:CA	1.75	1.58
1:A:100:ARG:CG	1:A:100:ARG:CB	1.80	1.57
3:A:301:TLA:C2	3:A:301:TLA:C3	1.82	1.57
1:B:24:VAL:CB	1:B:24:VAL:CA	1.77	1.57
1:B:110:GLN:CG	1:B:110:GLN:CB	1.77	1.57
1:B:146:LYS:CG	1:B:146:LYS:CB	1.75	1.55
1:D:36:VAL:CB	1:D:36:VAL:CA	1.81	1.54
1:B:2:PRO:C	1:B:2:PRO:CA	1.74	1.54
1:A:85:ILE:CB	1:A:85:ILE:CA	1.79	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ASP:CB	1:D:131:ASP:CG	1.81	1.53
1:A:100:ARG:CG	1:A:100:ARG:CD	1.82	1.53
1:A:130:MET:CG	1:A:130:MET:CB	1.83	1.53
1:D:88:LYS:CE	1:D:88:LYS:NZ	1.69	1.52
1:A:33:PRO:CB	1:A:33:PRO:CG	1.77	1.51
1:A:172:GLN:CD	1:A:172:GLN:CG	1.80	1.51
1:B:130:MET:CA	1:B:130:MET:C	1.83	1.50
1:A:172:GLN:CG	1:A:172:GLN:CB	1.88	1.50
1:B:173:ALA:CA	1:B:173:ALA:CB	1.84	1.50
1:B:36:VAL:CB	1:B:36:VAL:CG2	1.86	1.49
1:D:108:LYS:HE3	1:D:108:LYS:CA	1.42	1.44
1:C:120:MET:SD	1:C:120:MET:CE	2.06	1.43
1:B:71:MET:SD	1:B:71:MET:CE	2.05	1.42
1:D:108:LYS:HE3	1:D:108:LYS:N	1.31	1.42
1:D:66:PRO:CB	1:D:66:PRO:CG	1.85	1.39
1:A:130:MET:CG	1:A:130:MET:SD	2.14	1.36
1:A:88:LYS:HD2	5:A:1030:HOH:O	1.28	1.32
1:D:22:PRO:HB3	1:D:65:ARG:O	1.16	1.29
1:A:9:VAL:HB	5:A:1030:HOH:O	1.14	1.28
1:B:44:ILE:HG13	5:B:1019:HOH:O	1.16	1.28
1:C:77:CYS:HB2	1:C:78:PRO:CD	1.58	1.27
1:D:108:LYS:CE	1:D:108:LYS:H	1.45	1.26
1:C:164:GLY:HA2	5:C:1043:HOH:O	1.37	1.21
1:D:43:PRO:HD2	1:D:46:SER:OG	1.39	1.20
1:D:108:LYS:N	1:D:108:LYS:CE	2.03	1.20
1:B:20:VAL:HG11	1:B:26:ILE:HD13	1.20	1.19
1:D:37:ARG:O	5:D:1026:HOH:O	1.56	1.18
1:A:31:VAL:HG13	5:A:1004:HOH:O	1.46	1.15
1:C:77:CYS:HB2	1:C:78:PRO:HD2	1.23	1.11
1:B:7:SER:HA	1:B:88:LYS:HZ1	1.13	1.11
1:A:28:THR:HB	5:A:1006:HOH:O	1.52	1.09
1:B:22:PRO:HB3	1:B:65:ARG:O	1.50	1.08
1:C:2:PRO:HB2	5:C:1032:HOH:O	1.54	1.07
1:A:32:ILE:H	1:A:33:PRO:HD3	1.08	1.07
1:D:100:ARG:O	5:D:1030:HOH:O	1.72	1.07
1:B:73:LEU:C	1:B:73:LEU:HD12	1.76	1.06
1:C:38:GLU:CD	1:C:41:GLY:HA2	1.80	1.06
1:D:157:HIS:HE1	5:D:1019:HOH:O	1.35	1.05
1:D:168:VAL:HG13	5:D:1038:HOH:O	1.57	1.05
1:B:72:VAL:HG12	1:B:73:LEU:N	1.64	1.05
1:B:2:PRO:HB2	1:C:130:MET:HG2	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:CYS:SG	1:A:78:PRO:HD2	1.96	1.04
1:B:113:LEU:HG	5:B:1014:HOH:O	1.59	1.03
1:B:5:LEU:HD23	1:B:5:LEU:C	1.79	1.03
1:D:119:GLY:HA2	5:D:1030:HOH:O	1.59	1.02
1:D:86:LEU:HD11	1:D:144:VAL:HG21	1.42	1.01
1:A:31:VAL:O	1:A:31:VAL:HG22	1.60	1.00
1:D:119:GLY:CA	5:D:1030:HOH:O	2.09	1.00
1:C:35:GLY:O	1:C:36:VAL:HG13	1.62	1.00
1:D:22:PRO:HB3	1:D:65:ARG:C	1.88	0.99
1:A:30:HIS:NE2	4:A:300:TAR:O4	1.95	0.99
1:C:139:CYS:SG	5:C:1030:HOH:O	2.20	0.98
1:A:139:CYS:SG	4:A:300:TAR:O4	2.22	0.97
1:C:149:ASN:ND2	1:C:149:ASN:H	1.53	0.97
1:D:22:PRO:CB	1:D:65:ARG:O	2.11	0.97
1:B:85:ILE:HD11	1:B:87:ILE:HD11	1.44	0.97
1:C:115:HIS:HB2	5:C:1042:HOH:O	1.64	0.97
1:A:32:ILE:CB	1:A:32:ILE:C	2.36	0.96
1:C:78:PRO:HG2	1:C:81:VAL:CG2	1.94	0.96
1:A:128:LYS:HB2	1:A:131:ASP:OD1	1.67	0.94
1:B:19:TRP:CZ2	1:B:40:PHE:CD2	2.55	0.94
1:D:90:ASP:HA	5:D:1029:HOH:O	1.68	0.94
1:C:38:GLU:OE2	1:C:41:GLY:HA2	1.67	0.93
1:D:73:LEU:HD12	1:D:73:LEU:O	1.67	0.93
1:A:32:ILE:H	1:A:33:PRO:CD	1.81	0.93
1:D:144:VAL:O	1:D:145:TYR:HB3	1.65	0.93
1:A:154:CYS:N	5:A:1026:HOH:O	2.01	0.93
1:B:23:THR:O	1:B:60:PHE:HB2	1.67	0.93
1:C:100:ARG:HD2	5:C:1039:HOH:O	1.66	0.93
1:A:139:CYS:SG	4:A:300:TAR:C4	2.57	0.92
1:B:130:MET:C	1:B:130:MET:HA	1.93	0.92
1:D:108:LYS:CA	1:D:108:LYS:CE	2.37	0.92
1:C:146:LYS:H	1:C:146:LYS:HD2	1.33	0.91
1:B:72:VAL:CG1	1:B:73:LEU:N	2.33	0.91
1:B:105:ALA:HB3	1:B:107:MET:CE	2.01	0.91
1:C:77:CYS:CB	1:C:78:PRO:CD	2.43	0.91
1:C:153:VAL:HG12	5:C:1027:HOH:O	1.70	0.91
1:D:85:ILE:HD11	1:D:99:VAL:HG21	1.52	0.91
1:B:38:GLU:HB2	5:B:1009:HOH:O	1.71	0.90
1:B:7:SER:HA	1:B:88:LYS:NZ	1.86	0.90
1:C:38:GLU:OE1	1:C:41:GLY:HA2	1.71	0.90
1:B:37:ARG:O	1:B:44:ILE:HG22	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:H	1:C:149:ASN:HD22	1.02	0.90
1:B:57:GLN:C	1:B:58:PHE:HD2	1.79	0.90
1:D:168:VAL:HA	5:D:1038:HOH:O	1.69	0.90
1:D:73:LEU:HD12	1:D:73:LEU:C	1.95	0.90
1:A:126:ASN:O	1:A:131:ASP:HB3	1.73	0.89
1:D:23:THR:HB	1:D:59:ARG:HD2	1.55	0.89
1:A:32:ILE:N	1:A:33:PRO:HD3	1.86	0.88
1:B:162:LYS:HD2	1:B:162:LYS:H	1.38	0.88
1:A:93:GLU:OE2	1:D:3:PRO:HD3	1.73	0.88
1:B:77:CYS:HB3	1:B:81:VAL:HG11	1.56	0.88
1:B:9:VAL:O	1:B:88:LYS:HE3	1.71	0.88
1:A:77:CYS:SG	1:A:81:VAL:HG22	2.13	0.88
1:A:1:ALA:HB1	1:A:2:PRO:HD2	1.55	0.87
1:A:50:HIS:HB3	1:A:172:GLN:HE22	1.38	0.87
1:B:85:ILE:CG2	1:B:99:VAL:HG21	2.05	0.87
1:B:2:PRO:HB2	1:C:130:MET:CG	2.04	0.87
1:C:75:GLU:HG3	1:C:172:GLN:HE21	1.40	0.87
1:A:123:THR:HG21	1:D:96:PRO:HB2	1.55	0.86
1:B:141:ALA:N	5:B:1025:HOH:O	2.08	0.86
1:A:168:VAL:HB	5:A:1020:HOH:O	1.76	0.86
5:B:1017:HOH:O	1:C:124:GLY:HA3	1.74	0.86
1:A:16:TRP:HB2	5:A:1005:HOH:O	1.74	0.86
1:B:19:TRP:HZ2	1:B:40:PHE:CD2	1.94	0.86
1:D:108:LYS:H	1:D:108:LYS:HE2	1.38	0.86
1:A:36:VAL:HB	1:A:37:ARG:HB2	1.56	0.86
1:C:74:GLU:OE2	1:C:145:TYR:OH	1.92	0.86
1:B:37:ARG:O	1:B:44:ILE:CG2	2.23	0.86
1:B:7:SER:CA	1:B:88:LYS:HZ1	1.88	0.85
1:A:79:GLU:CD	1:B:161:THR:HG21	2.02	0.85
1:B:64:VAL:HG23	1:B:65:ARG:N	1.90	0.85
1:B:106:SER:C	1:B:107:MET:HG2	1.99	0.85
1:C:125:ALA:HB2	1:D:100:ARG:HH22	1.40	0.85
1:A:33:PRO:O	1:A:35:GLY:N	2.09	0.85
1:B:20:VAL:O	1:B:71:MET:N	2.10	0.85
1:B:42:GLU:O	5:B:1009:HOH:O	1.94	0.85
1:B:65:ARG:HG2	5:B:1023:HOH:O	1.77	0.84
1:C:80:GLY:CA	5:C:1039:HOH:O	2.24	0.84
1:D:44:ILE:HB	5:D:1026:HOH:O	1.78	0.84
1:D:20:VAL:O	1:D:70:GLY:HA2	1.78	0.84
1:D:104:ILE:HD13	1:D:104:ILE:H	1.42	0.84
1:D:37:ARG:HG2	1:D:38:GLU:H	1.40	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:PRO:HG2	1:C:81:VAL:HG21	1.60	0.83
1:B:5:LEU:HD23	1:B:6:TRP:N	1.94	0.83
1:B:135:LEU:HB3	1:B:136:PRO:HD2	1.58	0.83
1:C:79:GLU:OE1	1:D:165:ASN:HB3	1.79	0.83
1:B:135:LEU:HB3	1:B:136:PRO:CD	2.09	0.83
1:A:123:THR:O	1:A:123:THR:HG22	1.79	0.82
1:C:85:ILE:CA	1:C:85:ILE:CG2	2.57	0.82
1:B:24:VAL:HG12	1:B:25:PHE:H	1.45	0.82
1:D:19:TRP:CZ2	1:D:40:PHE:CD2	2.67	0.82
1:D:6:TRP:CH2	1:D:94:LEU:HB3	2.13	0.82
1:D:14:SER:HB2	1:D:31:VAL:HG22	1.61	0.82
1:D:37:ARG:CG	1:D:38:GLU:H	1.70	0.82
1:B:6:TRP:CG	1:B:94:LEU:HD23	2.14	0.82
1:A:32:ILE:N	1:A:33:PRO:CD	2.38	0.81
1:A:13:GLY:C	1:A:15:GLY:H	1.83	0.81
1:B:20:VAL:CG1	1:B:26:ILE:HD13	2.09	0.81
1:C:146:LYS:H	1:C:146:LYS:CD	1.89	0.81
1:A:6:TRP:O	1:A:88:LYS:NZ	2.14	0.81
1:D:109:ILE:HG21	1:D:159:ALA:HB1	1.62	0.81
1:A:32:ILE:HG13	1:A:33:PRO:N	1.96	0.81
1:B:6:TRP:CD2	1:B:94:LEU:HD23	2.16	0.81
1:B:38:GLU:CB	5:B:1009:HOH:O	2.26	0.81
1:D:57:GLN:O	1:D:58:PHE:HD1	1.63	0.81
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.45	0.80
1:A:146:LYS:NZ	1:A:149:ASN:O	2.14	0.80
1:D:14:SER:CB	1:D:31:VAL:HG22	2.12	0.80
1:D:85:ILE:CD1	1:D:99:VAL:HG21	2.11	0.80
1:C:16:TRP:CH2	1:C:88:LYS:HB3	2.16	0.80
1:A:32:ILE:C	1:A:32:ILE:HG13	2.07	0.80
1:B:109:ILE:O	1:B:162:LYS:CE	2.30	0.80
1:D:52:ALA:N	5:D:1027:HOH:O	2.14	0.80
1:A:31:VAL:HG12	5:A:1006:HOH:O	1.80	0.79
1:A:64:VAL:O	5:A:1013:HOH:O	1.99	0.79
1:C:2:PRO:HD3	1:C:151:TRP:CH2	2.16	0.79
1:C:125:ALA:O	1:C:126:ASN:OD1	1.99	0.79
1:A:77:CYS:SG	1:A:78:PRO:CD	2.70	0.79
1:C:78:PRO:HG2	1:C:81:VAL:HG23	1.64	0.79
1:A:139:CYS:O	5:A:1005:HOH:O	1.99	0.79
1:A:42:GLU:HB2	5:A:1009:HOH:O	1.82	0.79
1:A:32:ILE:CG1	1:A:33:PRO:N	2.46	0.79
1:D:55:PHE:CE2	1:D:172:GLN:HB2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:O	1:A:31:VAL:CG2	2.29	0.78
1:A:159:ALA:N	5:A:1035:HOH:O	2.16	0.78
1:C:149:ASN:HD22	1:C:149:ASN:N	1.79	0.78
1:B:3:PRO:O	1:B:5:LEU:N	2.16	0.78
1:D:94:LEU:N	1:D:94:LEU:HD12	1.99	0.78
1:A:85:ILE:CB	1:A:85:ILE:HA	2.08	0.78
1:B:2:PRO:C	1:B:2:PRO:N	2.43	0.78
1:B:40:PHE:CD1	5:B:1008:HOH:O	2.37	0.78
1:B:102:GLY:O	1:B:117:GLN:NE2	2.17	0.77
1:A:1:ALA:HB1	1:A:2:PRO:CD	2.15	0.77
1:C:125:ALA:N	5:C:1031:HOH:O	2.18	0.77
1:D:66:PRO:HD2	1:D:67:ASP:OD1	1.84	0.77
1:A:148:ASN:HB3	1:A:149:ASN:OD1	1.84	0.77
1:B:24:VAL:CB	1:B:24:VAL:C	2.58	0.77
1:B:64:VAL:CG2	1:B:65:ARG:N	2.48	0.77
1:A:158:ALA:C	5:A:1035:HOH:O	2.28	0.76
1:D:73:LEU:C	1:D:73:LEU:CD1	2.57	0.76
1:D:4:THR:CB	1:D:4:THR:C	2.57	0.76
1:A:128:LYS:HD2	1:D:146:LYS:HE2	1.67	0.76
1:C:128:LYS:CG	1:C:129:GLY:N	2.48	0.76
1:C:18:PHE:CD2	1:C:142:PRO:HG3	2.21	0.76
1:A:32:ILE:C	1:A:32:ILE:CG1	2.59	0.76
1:B:140:GLY:O	1:B:156:VAL:HG12	1.84	0.76
1:C:38:GLU:OE2	1:C:41:GLY:CA	2.33	0.76
1:B:140:GLY:C	1:B:156:VAL:HG12	2.11	0.76
1:C:131:ASP:HB2	5:C:1044:HOH:O	1.87	0.75
1:B:38:GLU:CA	5:B:1009:HOH:O	2.33	0.75
1:C:38:GLU:OE2	1:C:41:GLY:C	2.29	0.75
1:A:30:HIS:CD2	4:A:300:TAR:O4	2.39	0.75
1:B:105:ALA:HB3	1:B:107:MET:HE3	1.67	0.75
1:D:47:ILE:HG13	1:D:60:PHE:CD2	2.21	0.75
1:D:4:THR:CB	1:D:4:THR:HA	2.14	0.74
1:C:81:VAL:HG12	1:C:82:VAL:N	2.02	0.74
1:C:100:ARG:HG2	1:C:100:ARG:HH21	1.52	0.74
1:D:36:VAL:CB	1:D:36:VAL:C	2.60	0.74
1:D:148:ASN:C	1:D:150:ASP:H	1.94	0.74
1:C:19:TRP:HZ2	1:C:40:PHE:CD2	2.06	0.74
1:D:101:MET:HA	5:D:1030:HOH:O	1.86	0.74
1:A:128:LYS:CB	1:A:131:ASP:OD1	2.35	0.73
1:C:148:ASN:HB2	1:C:149:ASN:HD22	1.53	0.73
1:B:146:LYS:HG2	1:B:146:LYS:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	1:A:81:VAL:HG13	1.89	0.73
1:C:19:TRP:CZ2	1:C:40:PHE:CD2	2.76	0.73
1:C:154:CYS:N	5:C:1027:HOH:O	2.20	0.73
1:B:64:VAL:CG2	1:B:65:ARG:H	2.02	0.73
1:C:3:PRO:HD2	5:C:1032:HOH:O	1.89	0.73
1:B:153:VAL:HG12	1:B:154:CYS:N	2.04	0.72
1:C:75:GLU:HG3	1:C:172:GLN:NE2	2.03	0.72
1:C:147:ARG:O	1:C:148:ASN:O	2.07	0.72
1:B:15:GLY:HA3	1:B:31:VAL:HG21	1.69	0.72
1:B:85:ILE:CG2	1:B:99:VAL:CG2	2.67	0.72
1:C:80:GLY:HA2	5:C:1039:HOH:O	1.88	0.72
1:C:148:ASN:HA	5:C:1046:HOH:O	1.89	0.72
1:A:60:PHE:HA	5:A:1031:HOH:O	1.87	0.72
1:A:85:ILE:CA	1:A:85:ILE:HB	2.12	0.72
1:B:78:PRO:O	1:B:81:VAL:HG12	1.89	0.72
1:D:132:LEU:HA	5:D:1036:HOH:O	1.90	0.72
1:C:147:ARG:O	1:C:148:ASN:C	2.31	0.72
1:B:55:PHE:CD1	1:B:56:THR:N	2.58	0.72
1:A:127:ALA:O	1:A:128:LYS:HG2	1.89	0.72
1:C:66:PRO:CD	5:C:1038:HOH:O	2.37	0.72
1:C:66:PRO:HD2	5:C:1038:HOH:O	1.88	0.71
1:D:107:MET:HG3	1:D:109:ILE:HD11	1.72	0.71
1:B:141:ALA:HB2	5:B:1025:HOH:O	1.89	0.71
1:C:125:ALA:CB	1:D:100:ARG:HH22	2.02	0.71
1:A:146:LYS:NZ	1:A:149:ASN:C	2.48	0.71
1:C:80:GLY:O	1:C:100:ARG:HD3	1.90	0.71
1:B:72:VAL:HG11	1:B:147:ARG:NH2	2.06	0.71
1:B:90:ASP:C	1:B:92:GLY:N	2.49	0.70
1:D:168:VAL:CA	5:D:1038:HOH:O	2.33	0.70
1:A:66:PRO:HD2	1:A:67:ASP:H	1.56	0.70
1:D:43:PRO:HD2	1:D:46:SER:HG	1.54	0.70
1:A:85:ILE:CA	1:A:85:ILE:CG1	2.67	0.70
5:C:1043:HOH:O	1:D:79:GLU:HB2	1.91	0.70
1:D:1:ALA:HB3	1:D:6:TRP:HE1	1.55	0.70
1:D:51:ARG:C	5:D:1027:HOH:O	2.33	0.70
1:D:6:TRP:CD2	1:D:94:LEU:HD23	2.27	0.69
1:A:28:THR:CB	5:A:1006:HOH:O	2.24	0.69
1:D:21:SER:CB	1:D:24:VAL:HG23	2.22	0.69
1:D:102:GLY:O	1:D:117:GLN:OE1	2.11	0.69
1:A:47:ILE:HD12	1:A:60:PHE:CD2	2.28	0.69
1:D:59:ARG:HH21	1:D:59:ARG:HB2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301:TLA:C2	3:A:301:TLA:C4	2.71	0.69
1:B:24:VAL:HG12	1:B:25:PHE:N	2.07	0.68
1:C:23:THR:O	1:C:60:PHE:HD1	1.76	0.68
1:B:146:LYS:CG	1:B:146:LYS:N	2.55	0.68
1:A:123:THR:HA	1:D:98:ALA:HB2	1.74	0.68
1:B:24:VAL:CA	1:B:24:VAL:CG1	2.70	0.68
1:B:90:ASP:C	1:B:92:GLY:H	2.02	0.68
1:A:153:VAL:HG12	5:A:1026:HOH:O	1.93	0.68
1:B:109:ILE:O	1:B:162:LYS:HE2	1.93	0.68
1:B:140:GLY:O	1:B:156:VAL:CG1	2.41	0.68
1:C:8:ARG:HD3	1:C:19:TRP:O	1.93	0.68
1:C:77:CYS:HB2	1:C:78:PRO:HD3	1.69	0.68
1:C:125:ALA:O	1:C:126:ASN:CG	2.36	0.68
1:C:100:ARG:HH21	1:C:100:ARG:CG	2.07	0.68
1:B:22:PRO:O	1:B:64:VAL:CG2	2.41	0.67
1:C:123:THR:O	1:C:124:GLY:O	2.12	0.67
1:D:97:LEU:HD22	1:D:123:THR:HG21	1.77	0.67
1:D:117:GLN:C	5:D:1038:HOH:O	2.37	0.67
1:B:58:PHE:HD2	1:B:58:PHE:N	1.90	0.67
1:A:50:HIS:CB	1:A:172:GLN:HE22	2.06	0.67
3:A:301:TLA:C2	3:A:301:TLA:H3	2.18	0.67
1:C:71:MET:HE2	1:C:153:VAL:CG2	2.25	0.67
1:D:26:ILE:HD11	1:D:73:LEU:CD2	2.25	0.67
1:D:57:GLN:O	1:D:58:PHE:CD1	2.46	0.67
1:C:46:SER:O	1:C:61:SER:OG	2.11	0.67
1:A:73:LEU:HA	1:A:153:VAL:HG23	1.77	0.67
1:B:1:ALA:HB1	5:C:1045:HOH:O	1.94	0.67
1:B:25:PHE:CE2	1:B:40:PHE:HE2	2.13	0.67
1:A:33:PRO:O	1:A:34:THR:C	2.36	0.66
5:C:1043:HOH:O	1:D:79:GLU:CB	2.43	0.66
1:B:35:GLY:C	1:B:36:VAL:CG1	2.68	0.66
1:C:17:GLY:HA3	1:C:25:PHE:CZ	2.30	0.66
1:D:21:SER:HB2	1:D:24:VAL:HG23	1.76	0.66
1:A:42:GLU:OE1	5:A:1031:HOH:O	2.13	0.66
1:C:2:PRO:O	1:C:6:TRP:HD1	1.78	0.66
1:C:38:GLU:HB2	1:C:42:GLU:O	1.96	0.66
1:C:78:PRO:CG	1:C:81:VAL:HG21	2.24	0.66
1:D:37:ARG:CG	1:D:38:GLU:N	2.47	0.66
1:B:123:THR:O	1:B:124:GLY:C	2.39	0.66
1:A:13:GLY:C	1:A:15:GLY:N	2.48	0.66
1:A:128:LYS:C	1:A:128:LYS:CB	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:HG22	1:C:122:LEU:HD23	1.78	0.66
1:B:87:ILE:HD12	1:B:138:ASP:HB3	1.76	0.66
1:D:168:VAL:CG1	5:D:1038:HOH:O	2.25	0.66
1:B:143:TYR:HE2	1:B:157:HIS:HB2	1.61	0.65
1:D:6:TRP:CE2	1:D:94:LEU:HD23	2.31	0.65
1:D:162:LYS:CD	5:D:1023:HOH:O	2.44	0.65
1:B:85:ILE:CD1	1:B:87:ILE:HD11	2.22	0.65
1:C:128:LYS:HG2	1:C:129:GLY:N	2.11	0.65
1:D:47:ILE:HG13	1:D:60:PHE:HD2	1.61	0.65
1:A:88:LYS:CD	5:A:1030:HOH:O	2.07	0.65
1:C:128:LYS:CG	1:C:129:GLY:H	2.09	0.65
1:B:22:PRO:CB	1:B:65:ARG:O	2.38	0.65
1:A:79:GLU:OE1	1:B:161:THR:HG21	1.97	0.65
1:A:32:ILE:CA	1:A:32:ILE:HB	2.15	0.65
1:A:165:ASN:HD21	1:B:100:ARG:NH1	1.95	0.64
1:B:6:TRP:C	1:B:88:LYS:HZ1	2.05	0.64
1:A:38:GLU:HB2	1:A:42:GLU:O	1.98	0.64
1:A:148:ASN:HA	5:A:1027:HOH:O	1.97	0.64
1:B:95:LEU:HD11	1:B:131:ASP:O	1.97	0.64
1:D:108:LYS:HE3	1:D:108:LYS:C	2.20	0.64
1:B:112:ARG:NH2	1:B:159:ALA:HB2	2.13	0.64
1:D:127:ALA:HB2	5:D:1033:HOH:O	1.97	0.64
5:B:1017:HOH:O	1:C:124:GLY:CA	2.38	0.63
1:B:65:ARG:HB3	1:B:68:LEU:CD1	2.27	0.63
1:C:109:ILE:HD12	1:C:110:GLN:N	2.13	0.63
1:C:123:THR:O	1:C:124:GLY:C	2.41	0.63
3:A:301:TLA:C3	3:A:301:TLA:O2	2.46	0.63
1:B:25:PHE:C	1:B:26:ILE:HD12	2.23	0.63
1:B:162:LYS:H	1:B:162:LYS:CD	2.11	0.63
1:A:128:LYS:HG3	1:A:131:ASP:OD1	1.98	0.63
1:C:85:ILE:CB	1:C:85:ILE:C	2.69	0.63
1:A:36:VAL:HG12	1:A:37:ARG:CZ	2.29	0.63
1:D:71:MET:HE3	1:D:151:TRP:HB3	1.81	0.63
1:A:126:ASN:O	1:A:131:ASP:CB	2.46	0.63
1:A:42:GLU:CB	5:A:1009:HOH:O	2.43	0.62
1:A:54:GLU:O	1:A:54:GLU:HG3	1.99	0.62
1:B:22:PRO:O	1:B:64:VAL:HG22	1.98	0.62
1:C:128:LYS:HG3	1:C:129:GLY:H	1.64	0.62
1:A:50:HIS:CB	1:A:172:GLN:NE2	2.62	0.62
1:B:55:PHE:HD1	1:B:56:THR:H	1.48	0.62
1:D:57:GLN:C	1:D:58:PHE:HD1	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HB2	1:A:131:ASP:CG	2.23	0.62
1:A:28:THR:CG2	5:A:1006:HOH:O	2.46	0.62
1:D:108:LYS:H	1:D:108:LYS:NZ	1.96	0.62
1:B:94:LEU:N	1:B:94:LEU:HD12	2.15	0.62
1:B:57:GLN:O	1:B:58:PHE:HD2	1.82	0.62
1:C:6:TRP:C	1:C:8:ARG:H	2.06	0.62
1:A:128:LYS:N	1:A:131:ASP:HB2	2.14	0.62
1:B:42:GLU:CD	1:B:62:ARG:HD2	2.24	0.61
1:A:50:HIS:HB3	1:A:172:GLN:NE2	2.12	0.61
1:B:44:ILE:HD13	1:B:44:ILE:C	2.25	0.61
1:B:105:ALA:HB3	1:B:107:MET:HE2	1.83	0.61
1:D:52:ALA:CA	5:D:1027:HOH:O	2.47	0.61
1:D:21:SER:CB	1:D:22:PRO:CD	2.78	0.61
1:D:66:PRO:HD2	1:D:67:ASP:H	1.66	0.61
1:D:104:ILE:HA	1:D:117:GLN:HA	1.82	0.61
1:A:131:ASP:O	1:D:1:ALA:HB2	2.01	0.61
1:C:66:PRO:N	5:C:1038:HOH:O	2.30	0.61
1:C:77:CYS:CB	1:C:78:PRO:HD2	2.15	0.61
1:C:100:ARG:CD	5:C:1039:HOH:O	2.34	0.61
1:D:1:ALA:HB3	1:D:6:TRP:NE1	2.14	0.61
1:B:90:ASP:O	1:B:92:GLY:N	2.34	0.61
1:D:47:ILE:HG22	1:D:49:ILE:HG12	1.81	0.61
1:A:114:VAL:HG11	1:A:168:VAL:HG21	1.83	0.61
1:B:35:GLY:C	1:B:36:VAL:HG13	2.24	0.61
1:B:48:ALA:HB3	1:B:59:ARG:HB3	1.81	0.61
1:A:8:ARG:HB2	1:A:19:TRP:HB2	1.83	0.60
1:B:19:TRP:NE1	1:B:65:ARG:HD3	2.15	0.60
1:B:145:TYR:O	1:B:151:TRP:HD1	1.84	0.60
1:D:39:PHE:N	1:D:42:GLU:O	2.34	0.60
1:C:16:TRP:CZ2	1:C:88:LYS:HB3	2.36	0.60
1:D:12:PHE:CD2	1:D:25:PHE:HZ	2.19	0.60
1:B:89:ARG:NH2	1:B:138:ASP:OD2	2.35	0.60
1:D:66:PRO:CD	1:D:67:ASP:OD1	2.49	0.60
1:D:135:LEU:HD22	1:D:136:PRO:HD2	1.82	0.60
1:B:72:VAL:HG11	1:B:147:ARG:HH21	1.67	0.60
1:B:113:LEU:C	1:B:113:LEU:HD23	2.27	0.60
1:D:51:ARG:HA	1:D:56:THR:HA	1.83	0.60
1:D:19:TRP:CH2	1:D:40:PHE:CD2	2.90	0.60
1:D:94:LEU:N	1:D:94:LEU:CD1	2.64	0.60
1:A:23:THR:OG1	1:A:59:ARG:HD2	2.02	0.59
1:A:85:ILE:HG13	1:A:87:ILE:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:HG23	1:B:45:GLU:OE2	2.01	0.59
1:D:51:ARG:HG2	5:D:1027:HOH:O	2.02	0.59
1:C:2:PRO:O	1:C:6:TRP:CD1	2.54	0.59
1:C:10:VAL:HG23	1:C:11:ARG:O	2.02	0.59
1:C:44:ILE:HG22	1:C:45:GLU:N	2.16	0.59
1:A:42:GLU:OE2	5:A:1009:HOH:O	2.17	0.59
1:B:42:GLU:HG2	1:B:62:ARG:HD3	1.84	0.59
1:A:128:LYS:C	1:A:128:LYS:HA	2.11	0.59
1:D:6:TRP:CZ2	1:D:94:LEU:HB3	2.38	0.59
1:D:65:ARG:HB3	1:D:68:LEU:CD1	2.33	0.59
1:B:107:MET:C	1:B:109:ILE:HD12	2.28	0.59
1:B:36:VAL:HG23	1:B:36:VAL:O	2.03	0.59
1:B:146:LYS:CG	1:B:146:LYS:CA	2.77	0.59
1:A:24:VAL:HG22	1:A:59:ARG:HD3	1.85	0.59
1:B:121:LEU:HD22	1:B:164:GLY:O	2.02	0.59
1:D:14:SER:HB3	1:D:31:VAL:CG2	2.33	0.59
1:A:32:ILE:HG13	1:A:33:PRO:CA	2.33	0.58
1:B:3:PRO:C	1:B:5:LEU:N	2.57	0.58
1:C:97:LEU:HA	5:C:1041:HOH:O	2.02	0.58
1:D:165:ASN:ND2	5:D:1012:HOH:O	2.31	0.58
1:A:31:VAL:CG1	5:A:1006:HOH:O	2.46	0.58
1:B:29:THR:C	1:B:31:VAL:H	2.10	0.58
1:D:131:ASP:HA	5:D:1035:HOH:O	2.03	0.58
1:B:3:PRO:C	1:B:5:LEU:H	2.10	0.58
1:C:21:SER:CB	1:C:22:PRO:CD	2.82	0.58
1:D:95:LEU:HD11	5:D:1036:HOH:O	2.03	0.58
1:D:148:ASN:C	1:D:150:ASP:N	2.60	0.58
1:A:86:LEU:HB2	1:A:142:PRO:HG2	1.85	0.58
1:B:36:VAL:CG2	1:B:36:VAL:CA	2.76	0.58
1:D:14:SER:CB	1:D:31:VAL:CG2	2.81	0.58
1:B:20:VAL:HG11	1:B:26:ILE:CD1	2.13	0.58
1:B:93:GLU:C	1:B:94:LEU:HD12	2.28	0.58
1:C:104:ILE:CG2	1:C:105:ALA:N	2.65	0.58
1:D:91:SER:HB3	1:D:93:GLU:HG3	1.85	0.58
1:B:141:ALA:CA	5:B:1025:HOH:O	2.48	0.58
1:D:36:VAL:CA	1:D:36:VAL:CG1	2.78	0.58
1:D:46:SER:CB	1:D:47:ILE:HD12	2.34	0.58
1:A:36:VAL:HG12	1:A:37:ARG:NH2	2.20	0.57
1:D:36:VAL:CB	1:D:36:VAL:N	2.65	0.57
1:A:150:ASP:HB2	5:A:1028:HOH:O	2.04	0.57
1:B:58:PHE:N	1:B:58:PHE:CD2	2.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:CB	1:A:32:ILE:N	2.61	0.57
1:B:6:TRP:CZ2	1:B:86:LEU:HD12	2.38	0.57
1:B:73:LEU:HD12	1:B:74:GLU:N	2.17	0.57
1:D:44:ILE:HG23	1:D:45:GLU:N	2.17	0.57
1:A:36:VAL:HG23	1:A:37:ARG:H	1.70	0.57
1:B:148:ASN:HB3	1:B:149:ASN:HD22	1.69	0.57
1:C:1:ALA:HB1	1:C:5:LEU:HD23	1.85	0.57
1:D:21:SER:HB2	1:D:24:VAL:CG2	2.35	0.57
1:D:55:PHE:CD2	1:D:172:GLN:HB2	2.39	0.57
1:B:96:PRO:HB2	1:C:123:THR:CG2	2.34	0.57
1:D:9:VAL:O	1:D:88:LYS:HD3	2.03	0.57
1:D:86:LEU:HD11	1:D:144:VAL:CG2	2.28	0.57
1:A:32:ILE:CA	1:A:32:ILE:CG1	2.75	0.57
1:B:12:PHE:CD2	1:B:25:PHE:HZ	2.23	0.57
1:A:104:ILE:N	5:A:1034:HOH:O	2.37	0.57
1:B:19:TRP:CD1	1:B:65:ARG:HD3	2.40	0.57
1:B:24:VAL:O	1:B:25:PHE:HB2	2.05	0.56
1:B:64:VAL:HG23	1:B:65:ARG:HB2	1.86	0.56
1:A:66:PRO:CD	1:A:67:ASP:H	2.14	0.56
1:B:68:LEU:HD21	5:B:1023:HOH:O	2.05	0.56
1:B:146:LYS:HG2	1:B:146:LYS:H	1.69	0.56
1:B:153:VAL:HG12	1:B:155:GLY:H	1.69	0.56
1:C:89:ARG:NH2	1:C:138:ASP:OD2	2.38	0.56
1:C:148:ASN:HB2	1:C:149:ASN:ND2	2.20	0.56
1:D:127:ALA:CB	5:D:1034:HOH:O	2.54	0.56
1:D:153:VAL:HG12	1:D:154:CYS:N	2.20	0.56
1:A:72:VAL:HG12	1:A:73:LEU:N	2.20	0.56
1:B:85:ILE:HG23	1:B:99:VAL:CG2	2.35	0.56
1:D:6:TRP:CG	1:D:94:LEU:HD23	2.40	0.56
1:A:77:CYS:SG	1:A:81:VAL:CG2	2.92	0.56
1:B:44:ILE:HD13	1:B:44:ILE:O	2.05	0.56
1:C:81:VAL:CG1	1:C:82:VAL:N	2.66	0.56
1:C:85:ILE:HD11	1:C:99:VAL:CG1	2.36	0.56
1:D:108:LYS:NZ	1:D:109:ILE:N	2.54	0.56
1:B:85:ILE:HG22	1:B:99:VAL:HG21	1.86	0.56
1:B:141:ALA:CB	5:B:1025:HOH:O	2.51	0.56
1:D:14:SER:HB3	1:D:31:VAL:HG22	1.88	0.56
1:A:82:VAL:HG23	1:A:99:VAL:O	2.06	0.56
1:A:12:PHE:HD1	5:A:1004:HOH:O	1.89	0.55
1:D:127:ALA:HA	1:D:131:ASP:HB3	1.88	0.55
1:B:112:ARG:HH22	1:B:159:ALA:HB2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:THR:C	1:B:31:VAL:N	2.64	0.55
1:B:57:GLN:O	1:B:58:PHE:CD2	2.60	0.55
1:C:18:PHE:HD2	1:C:142:PRO:HG3	1.72	0.55
1:A:60:PHE:CA	5:A:1031:HOH:O	2.49	0.55
1:A:146:LYS:C	1:A:147:ARG:O	2.44	0.55
1:B:2:PRO:C	1:B:2:PRO:CB	2.77	0.55
1:B:107:MET:O	1:B:109:ILE:HD12	2.07	0.55
1:A:120:MET:HE1	1:B:100:ARG:HG2	1.89	0.55
1:B:36:VAL:CG2	1:B:36:VAL:HB	2.22	0.55
1:C:109:ILE:HG12	1:C:159:ALA:HB1	1.89	0.55
1:D:26:ILE:HD11	1:D:73:LEU:HD22	1.89	0.55
1:B:73:LEU:C	1:B:73:LEU:CD1	2.61	0.55
1:A:99:VAL:HG13	1:A:121:LEU:HD12	1.87	0.55
1:A:128:LYS:CG	1:A:131:ASP:OD1	2.54	0.55
1:B:90:ASP:O	1:B:91:SER:C	2.39	0.55
1:B:25:PHE:C	1:B:25:PHE:CD1	2.85	0.54
1:B:96:PRO:HB2	1:C:123:THR:HG21	1.88	0.54
1:A:103:ALA:HB1	5:A:1034:HOH:O	2.06	0.54
1:D:104:ILE:HG22	1:D:117:GLN:HB2	1.90	0.54
1:B:9:VAL:HB	1:B:88:LYS:HE3	1.90	0.54
1:B:87:ILE:HD13	1:B:141:ALA:CB	2.38	0.54
1:D:51:ARG:HG3	1:D:56:THR:OG1	2.07	0.54
1:A:6:TRP:CE3	1:A:94:LEU:HD23	2.43	0.54
1:C:6:TRP:C	1:C:8:ARG:N	2.66	0.54
1:C:148:ASN:CB	1:C:149:ASN:HD22	2.20	0.54
1:B:148:ASN:N	5:B:1026:HOH:O	2.41	0.54
1:D:21:SER:HB3	1:D:22:PRO:CD	2.38	0.54
1:A:78:PRO:HG2	1:A:81:VAL:HG11	1.90	0.54
1:A:85:ILE:HG13	1:A:87:ILE:HD12	1.90	0.54
1:C:52:ALA:HA	5:C:1017:HOH:O	2.08	0.54
1:B:18:PHE:CE1	1:B:153:VAL:HG21	2.43	0.53
1:C:158:ALA:O	1:C:159:ALA:HB2	2.08	0.53
1:B:5:LEU:C	1:B:5:LEU:CD2	2.61	0.53
1:D:86:LEU:CD1	1:D:144:VAL:HG21	2.28	0.53
1:A:28:THR:HG22	1:A:30:HIS:H	1.73	0.53
1:C:80:GLY:C	1:C:100:ARG:HD3	2.34	0.53
1:C:99:VAL:HG12	1:C:121:LEU:HA	1.91	0.53
1:B:104:ILE:HD11	5:B:1012:HOH:O	2.09	0.53
1:A:79:GLU:CG	1:B:161:THR:HG21	2.37	0.53
1:A:107:MET:CG	1:A:109:ILE:HD11	2.39	0.53
1:B:130:MET:HE1	1:C:1:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ARG:HH21	1:D:59:ARG:CB	2.21	0.53
1:D:144:VAL:O	1:D:145:TYR:CB	2.43	0.53
1:A:77:CYS:SG	1:A:78:PRO:N	2.80	0.53
1:C:85:ILE:HD11	1:C:99:VAL:HG11	1.91	0.53
1:D:37:ARG:HG2	1:D:38:GLU:HG3	1.91	0.53
1:A:140:GLY:HA3	5:A:1005:HOH:O	2.09	0.53
1:B:36:VAL:CG2	1:B:36:VAL:C	2.82	0.53
1:D:33:PRO:O	1:D:34:THR:C	2.51	0.53
1:C:33:PRO:HA	5:C:1013:HOH:O	2.09	0.52
1:C:76:GLY:HA2	1:C:154:CYS:O	2.09	0.52
1:D:162:LYS:CD	1:D:162:LYS:H	2.21	0.52
1:B:9:VAL:HB	1:B:88:LYS:CE	2.40	0.52
1:B:37:ARG:HD3	1:B:38:GLU:HB3	1.91	0.52
1:B:109:ILE:HG22	1:B:110:GLN:HG2	1.91	0.52
1:C:65:ARG:HG2	1:C:65:ARG:HH21	1.74	0.52
1:B:19:TRP:CE2	1:B:65:ARG:HD3	2.45	0.52
1:B:96:PRO:HG2	1:C:123:THR:HG21	1.91	0.52
1:A:66:PRO:CD	1:A:67:ASP:N	2.71	0.52
1:B:77:CYS:CB	1:B:81:VAL:HG11	2.34	0.52
1:C:78:PRO:HD2	1:C:81:VAL:HG21	1.90	0.52
1:D:19:TRP:HZ2	1:D:40:PHE:CD2	2.26	0.52
1:B:57:GLN:C	1:B:58:PHE:CD2	2.71	0.52
1:D:46:SER:HB2	1:D:47:ILE:HD12	1.90	0.52
1:A:4:THR:O	1:A:7:SER:HB3	2.09	0.52
1:B:149:ASN:N	5:B:1026:HOH:O	2.42	0.52
1:B:55:PHE:HD2	1:B:171:VAL:O	1.93	0.52
1:D:26:ILE:HG22	1:D:156:VAL:HG11	1.92	0.52
1:A:90:ASP:OD1	3:A:301:TLA:C2	2.58	0.52
1:D:146:LYS:NZ	1:D:149:ASN:HA	2.25	0.52
1:D:37:ARG:C	5:D:1026:HOH:O	2.29	0.51
1:D:1:ALA:CB	1:D:6:TRP:HE1	2.21	0.51
1:D:108:LYS:HZ1	1:D:109:ILE:N	2.08	0.51
1:A:107:MET:HE3	1:A:168:VAL:CG1	2.40	0.51
1:B:37:ARG:C	1:B:44:ILE:HG21	2.35	0.51
1:B:77:CYS:HB3	1:B:78:PRO:HD2	1.91	0.51
1:D:52:ALA:HA	5:D:1027:HOH:O	2.10	0.51
1:B:22:PRO:O	1:B:64:VAL:HG21	2.10	0.51
1:C:62:ARG:O	1:C:64:VAL:HG23	2.09	0.51
1:C:31:VAL:HG21	1:C:139:CYS:HB2	1.91	0.51
1:C:64:VAL:HG12	1:C:64:VAL:O	2.10	0.51
1:D:54:GLU:O	1:D:54:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LYS:H	1:D:162:LYS:HD2	1.74	0.51
1:B:8:ARG:HG3	1:B:18:PHE:CE2	2.45	0.51
1:D:42:GLU:CA	1:D:42:GLU:OE1	2.59	0.51
1:D:28:THR:HG21	1:D:139:CYS:HB3	1.93	0.51
1:A:90:ASP:OD1	3:A:301:TLA:C1	2.58	0.51
1:B:6:TRP:O	1:B:88:LYS:NZ	2.42	0.51
1:B:21:SER:HB2	1:B:24:VAL:HG23	1.92	0.51
1:B:26:ILE:HG23	1:B:156:VAL:HG22	1.91	0.51
1:D:28:THR:HG22	1:D:140:GLY:HA2	1.92	0.51
1:B:173:ALA:CB	1:B:173:ALA:C	2.82	0.50
1:C:1:ALA:CB	1:C:5:LEU:HD23	2.40	0.50
1:C:35:GLY:O	1:C:36:VAL:CG1	2.48	0.50
1:A:35:GLY:N	5:A:1008:HOH:O	2.43	0.50
1:C:129:GLY:C	1:C:130:MET:HE3	2.36	0.50
1:A:66:PRO:HD2	1:A:67:ASP:N	2.23	0.50
1:D:12:PHE:CD2	1:D:25:PHE:CZ	2.99	0.50
1:D:44:ILE:CG2	1:D:45:GLU:N	2.74	0.50
1:B:39:PHE:N	5:B:1009:HOH:O	2.44	0.50
1:D:4:THR:CA	1:D:4:THR:CG2	2.86	0.50
1:D:47:ILE:HG22	1:D:49:ILE:H	1.76	0.50
1:A:159:ALA:HB3	1:A:168:VAL:CG2	2.42	0.50
1:A:30:HIS:CD2	1:A:30:HIS:C	2.90	0.50
1:B:37:ARG:C	1:B:44:ILE:CG2	2.85	0.50
1:C:20:VAL:HG11	1:C:26:ILE:HD12	1.94	0.50
1:B:27:THR:OG1	1:B:28:THR:N	2.45	0.50
1:C:78:PRO:CD	1:C:81:VAL:HG21	2.42	0.49
1:C:125:ALA:HB2	1:D:100:ARG:NH2	2.17	0.49
1:D:45:GLU:C	1:D:47:ILE:N	2.64	0.49
1:A:50:HIS:HB2	1:A:172:GLN:NE2	2.26	0.49
1:A:123:THR:HB	1:A:126:ASN:OD1	2.12	0.49
1:B:65:ARG:CG	5:B:1023:HOH:O	2.48	0.49
1:D:12:PHE:HD1	1:D:12:PHE:O	1.96	0.49
1:D:145:TYR:CE2	1:D:152:VAL:HG22	2.47	0.49
1:A:128:LYS:HG3	1:A:131:ASP:CG	2.38	0.49
1:B:29:THR:O	1:B:31:VAL:N	2.46	0.49
1:B:55:PHE:CD2	1:B:171:VAL:O	2.66	0.49
1:D:44:ILE:O	1:D:44:ILE:HG12	2.13	0.49
1:A:147:ARG:HG2	1:A:147:ARG:NH1	2.15	0.49
1:C:107:MET:HB3	1:D:105:ALA:HB2	1.95	0.49
1:C:146:LYS:HD2	1:C:146:LYS:N	2.15	0.49
1:B:11:ARG:HG3	1:B:12:PHE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ARG:CZ	5:D:1027:HOH:O	2.61	0.49
1:D:88:LYS:HE3	5:D:1028:HOH:O	2.13	0.49
1:D:100:ARG:C	5:D:1030:HOH:O	2.36	0.49
1:A:77:CYS:SG	1:A:78:PRO:O	2.57	0.49
1:C:2:PRO:HB2	1:C:3:PRO:HD2	1.95	0.49
1:C:162:LYS:O	1:C:163:SER:O	2.31	0.49
1:A:107:MET:HG3	1:A:109:ILE:HD11	1.94	0.48
1:B:40:PHE:HA	5:B:1008:HOH:O	2.13	0.48
1:A:116:GLY:HA3	5:A:1020:HOH:O	2.12	0.48
1:D:102:GLY:N	1:D:118:SER:O	2.34	0.48
1:D:104:ILE:HD13	1:D:104:ILE:N	2.21	0.48
1:B:25:PHE:O	1:B:26:ILE:HD12	2.12	0.48
1:C:1:ALA:HB1	1:C:5:LEU:CD2	2.43	0.48
1:C:49:ILE:N	1:C:49:ILE:HD12	2.28	0.48
1:D:108:LYS:N	1:D:108:LYS:NZ	2.58	0.48
1:A:121:LEU:C	1:A:122:LEU:HD13	2.39	0.48
1:A:140:GLY:CA	5:A:1005:HOH:O	2.61	0.48
1:B:102:GLY:N	1:B:118:SER:O	2.38	0.48
1:A:16:TRP:CB	5:A:1005:HOH:O	2.47	0.48
1:A:116:GLY:C	5:A:1020:HOH:O	2.57	0.48
1:B:48:ALA:O	1:B:49:ILE:C	2.56	0.48
1:B:51:ARG:HB2	1:B:56:THR:HG23	1.95	0.48
1:A:157:HIS:CD2	5:A:1035:HOH:O	2.67	0.48
1:D:30:HIS:C	1:D:30:HIS:CD2	2.91	0.48
1:C:68:LEU:C	1:C:68:LEU:HD12	2.36	0.48
1:D:47:ILE:HG22	1:D:49:ILE:N	2.29	0.48
1:D:120:MET:N	5:D:1030:HOH:O	2.43	0.48
1:D:126:ASN:OD1	1:D:131:ASP:OD1	2.31	0.48
1:A:79:GLU:HG2	1:B:161:THR:HG21	1.96	0.48
1:A:99:VAL:HG13	1:A:121:LEU:CD1	2.43	0.48
1:B:19:TRP:CZ2	1:B:40:PHE:HD2	2.24	0.48
1:C:31:VAL:O	1:C:32:ILE:C	2.57	0.48
1:D:26:ILE:HG23	1:D:55:PHE:CE1	2.48	0.48
1:D:51:ARG:HB2	1:D:56:THR:HG23	1.96	0.48
1:B:24:VAL:O	1:B:25:PHE:CB	2.62	0.47
1:B:65:ARG:HB3	1:B:68:LEU:HD12	1.95	0.47
1:B:28:THR:O	1:B:29:THR:C	2.56	0.47
1:C:104:ILE:HG23	1:C:105:ALA:N	2.29	0.47
1:D:1:ALA:N	1:D:6:TRP:HE1	2.12	0.47
1:D:108:LYS:CE	1:D:108:LYS:C	2.83	0.47
1:D:164:GLY:HA2	5:D:1024:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HB3	1:A:93:GLU:HG2	1.96	0.47
1:C:109:ILE:HD12	1:C:110:GLN:H	1.79	0.47
1:D:32:ILE:HG22	1:D:33:PRO:HD2	1.96	0.47
1:B:6:TRP:O	1:B:88:LYS:CE	2.62	0.47
1:B:93:GLU:OE2	1:C:1:ALA:N	2.46	0.47
1:C:44:ILE:O	1:C:47:ILE:HG12	2.14	0.47
1:D:12:PHE:O	1:D:12:PHE:CD1	2.66	0.47
1:A:32:ILE:CA	1:A:32:ILE:CG2	2.80	0.47
1:A:87:ILE:HD11	1:A:97:LEU:HD12	1.96	0.47
1:B:7:SER:CA	1:B:88:LYS:NZ	2.63	0.47
1:B:85:ILE:HG23	1:B:99:VAL:HG23	1.96	0.47
1:B:109:ILE:HD13	1:B:114:VAL:HG23	1.97	0.47
1:C:28:THR:HG21	1:C:157:HIS:O	2.15	0.47
1:D:19:TRP:CH2	1:D:40:PHE:HD2	2.33	0.47
1:D:43:PRO:CD	1:D:46:SER:OG	2.34	0.47
1:A:122:LEU:HB3	5:D:1011:HOH:O	2.15	0.47
1:B:135:LEU:CB	1:B:136:PRO:CD	2.75	0.47
1:B:25:PHE:C	1:B:26:ILE:CD1	2.88	0.47
1:B:153:VAL:CG1	1:B:154:CYS:N	2.73	0.47
1:D:85:ILE:CD1	1:D:99:VAL:CG2	2.89	0.47
1:D:162:LYS:HD2	5:D:1023:HOH:O	2.13	0.47
1:A:16:TRP:CH2	1:A:88:LYS:HB3	2.51	0.46
1:A:146:LYS:HZ3	1:A:149:ASN:C	2.19	0.46
1:A:166:THR:HG22	1:A:167:VAL:N	2.28	0.46
1:D:107:MET:H	1:D:107:MET:HG2	1.60	0.46
1:A:79:GLU:HG2	1:B:163:SER:OG	2.15	0.46
1:B:14:SER:OG	1:B:31:VAL:HG22	2.16	0.46
1:C:86:LEU:HB2	1:C:142:PRO:HG2	1.98	0.46
1:D:65:ARG:HB3	1:D:68:LEU:CG	2.45	0.46
1:B:6:TRP:O	1:B:9:VAL:HB	2.15	0.46
1:B:109:ILE:O	1:B:162:LYS:HE3	2.14	0.46
1:C:44:ILE:HA	1:C:47:ILE:HG12	1.97	0.46
1:D:123:THR:HB	1:D:132:LEU:HB3	1.97	0.46
1:B:12:PHE:CE2	1:B:25:PHE:CZ	3.04	0.46
1:B:122:LEU:HA	1:B:122:LEU:HD12	1.77	0.46
1:A:39:PHE:CZ	1:A:44:ILE:HD11	2.51	0.46
1:A:120:MET:HE1	1:B:100:ARG:CG	2.46	0.46
1:C:109:ILE:HG12	1:C:159:ALA:CB	2.45	0.46
1:D:80:GLY:O	1:D:81:VAL:C	2.56	0.46
1:D:132:LEU:HD13	5:D:1036:HOH:O	2.15	0.46
1:B:96:PRO:CG	1:C:123:THR:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:CG1	1:C:88:LYS:HD2	2.46	0.46
1:C:107:MET:CG	1:C:109:ILE:HG23	2.46	0.46
1:C:138:ASP:O	1:C:139:CYS:C	2.59	0.46
1:A:38:GLU:HB2	1:A:42:GLU:C	2.41	0.46
1:A:139:CYS:C	5:A:1005:HOH:O	2.51	0.46
1:B:37:ARG:HD3	1:B:37:ARG:C	2.40	0.46
1:B:145:TYR:O	1:B:151:TRP:CD1	2.67	0.46
1:C:96:PRO:O	1:C:96:PRO:HG2	2.16	0.46
1:D:99:VAL:HG22	1:D:121:LEU:HD12	1.97	0.46
1:A:19:TRP:CD2	1:A:65:ARG:HG3	2.50	0.46
1:D:135:LEU:CD2	1:D:136:PRO:HD2	2.45	0.46
1:D:135:LEU:HD23	1:D:135:LEU:HA	1.53	0.46
1:D:162:LYS:HG3	5:D:1023:HOH:O	2.15	0.45
1:A:88:LYS:CE	5:A:1030:HOH:O	2.49	0.45
1:D:44:ILE:HA	1:D:47:ILE:HD13	1.98	0.45
1:D:65:ARG:HB3	1:D:68:LEU:HG	1.97	0.45
1:A:26:ILE:HG13	1:A:55:PHE:CZ	2.51	0.45
1:A:85:ILE:HG13	1:A:87:ILE:HD11	1.99	0.45
1:B:36:VAL:CG2	1:B:36:VAL:O	2.64	0.45
1:C:108:LYS:NZ	1:D:104:ILE:HD11	2.31	0.45
1:A:29:THR:O	1:A:33:PRO:HD3	2.16	0.45
1:A:144:VAL:HG12	1:A:153:VAL:HG13	1.97	0.45
5:C:1043:HOH:O	1:D:79:GLU:HB3	2.12	0.45
1:D:36:VAL:HB	1:D:37:ARG:HB2	1.99	0.45
1:D:55:PHE:CE2	1:D:172:GLN:HG3	2.51	0.45
1:D:26:ILE:HD11	1:D:73:LEU:HD23	1.97	0.45
1:C:73:LEU:HD23	1:C:153:VAL:O	2.17	0.45
1:C:149:ASN:ND2	1:C:149:ASN:N	2.34	0.45
1:C:157:HIS:HE1	1:C:167:VAL:HG22	1.82	0.45
1:D:62:ARG:O	1:D:64:VAL:N	2.50	0.45
1:D:108:LYS:C	1:D:108:LYS:NZ	2.74	0.45
1:B:38:GLU:HA	5:B:1009:HOH:O	2.08	0.45
1:B:150:ASP:N	5:B:1026:HOH:O	2.32	0.45
1:C:62:ARG:O	1:C:63:LYS:C	2.60	0.45
1:D:85:ILE:N	1:D:85:ILE:HD13	2.31	0.45
1:C:67:ASP:N	5:C:1038:HOH:O	2.08	0.45
1:C:5:LEU:O	1:C:8:ARG:HB2	2.17	0.45
1:D:104:ILE:HG12	1:D:104:ILE:O	2.16	0.45
1:B:57:GLN:CG	1:B:58:PHE:N	2.79	0.45
1:B:85:ILE:HG21	1:B:99:VAL:HG21	1.91	0.45
1:A:85:ILE:N	1:A:97:LEU:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HA	1:B:121:LEU:HD12	1.72	0.44
1:D:138:ASP:O	1:D:139:CYS:C	2.58	0.44
1:B:19:TRP:CH2	1:B:40:PHE:CD2	3.05	0.44
1:D:99:VAL:HA	1:D:120:MET:O	2.16	0.44
1:A:116:GLY:CA	5:A:1020:HOH:O	2.65	0.44
1:B:72:VAL:HG23	1:B:150:ASP:OD1	2.18	0.44
1:B:130:MET:HA	1:B:131:ASP:N	2.32	0.44
1:C:131:ASP:HB3	1:C:132:LEU:H	1.30	0.44
1:A:30:HIS:HE2	1:A:139:CYS:HG	1.66	0.44
1:B:19:TRP:CH2	1:B:40:PHE:HD2	2.36	0.44
1:C:106:SER:O	1:D:105:ALA:HB1	2.18	0.44
1:D:46:SER:HG	1:D:46:SER:H	1.64	0.44
1:D:65:ARG:HA	1:D:66:PRO:HD3	1.33	0.44
1:A:123:THR:O	1:A:123:THR:CG2	2.55	0.44
1:D:18:PHE:CD2	1:D:142:PRO:HG3	2.52	0.44
1:D:26:ILE:HG23	1:D:55:PHE:HE1	1.82	0.44
1:D:139:CYS:HB3	1:D:157:HIS:O	2.18	0.44
1:A:87:ILE:CD1	1:A:97:LEU:HD12	2.47	0.44
1:A:92:GLY:N	5:A:1018:HOH:O	2.50	0.44
1:A:147:ARG:HG3	1:A:148:ASN:N	2.33	0.44
1:B:6:TRP:C	1:B:88:LYS:NZ	2.75	0.44
1:B:35:GLY:C	1:B:36:VAL:HG12	2.43	0.44
1:B:51:ARG:HA	1:B:56:THR:HA	1.99	0.44
1:D:114:VAL:HG11	1:D:168:VAL:HG21	2.00	0.44
1:D:160:ALA:HB2	1:D:167:VAL:HG12	1.99	0.44
1:B:3:PRO:O	1:B:4:THR:C	2.60	0.43
1:B:120:MET:HA	1:B:165:ASN:O	2.18	0.43
1:C:65:ARG:HG3	1:C:67:ASP:OD1	2.18	0.43
1:C:100:ARG:O	1:D:120:MET:HE1	2.18	0.43
1:D:65:ARG:NH2	1:D:68:LEU:HD21	2.33	0.43
1:A:100:ARG:CG	1:A:100:ARG:NE	2.73	0.43
1:A:165:ASN:ND2	1:B:100:ARG:NH1	2.62	0.43
1:C:130:MET:O	1:C:131:ASP:OD1	2.36	0.43
1:D:120:MET:HE2	1:D:165:ASN:OD1	2.18	0.43
1:A:87:ILE:HD13	1:A:97:LEU:HG	2.01	0.43
1:D:21:SER:HB3	1:D:22:PRO:HD2	1.99	0.43
1:A:114:VAL:CG1	1:A:168:VAL:HG21	2.47	0.43
1:B:96:PRO:CB	1:C:123:THR:HG21	2.48	0.43
1:D:15:GLY:HA3	1:D:31:VAL:HG21	2.00	0.43
1:D:59:ARG:HH21	1:D:59:ARG:CG	2.31	0.43
1:B:9:VAL:CB	1:B:88:LYS:HE3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HG12	1:B:154:CYS:H	1.78	0.43
1:C:44:ILE:CG2	1:C:45:GLU:N	2.78	0.43
1:C:162:LYS:O	1:C:163:SER:C	2.61	0.43
1:D:37:ARG:HG2	1:D:38:GLU:CG	2.48	0.43
1:B:109:ILE:HD13	1:B:114:VAL:CG2	2.48	0.43
1:C:47:ILE:HD12	1:C:60:PHE:CD2	2.53	0.43
1:C:80:GLY:HA3	5:C:1039:HOH:O	2.05	0.43
1:D:43:PRO:HD2	1:D:43:PRO:O	2.18	0.43
1:A:55:PHE:CE2	1:A:172:GLN:HG2	2.53	0.43
1:C:19:TRP:CZ2	1:C:40:PHE:HD2	2.33	0.43
1:D:6:TRP:CD1	1:D:94:LEU:HD23	2.54	0.43
1:D:12:PHE:CE2	1:D:25:PHE:CZ	3.06	0.43
1:D:114:VAL:CG1	1:D:168:VAL:HG21	2.48	0.43
1:B:146:LYS:CG	1:B:146:LYS:H	2.26	0.43
1:B:168:VAL:HG12	1:B:169:CYS:N	2.33	0.43
1:D:21:SER:HB3	1:D:24:VAL:H	1.84	0.43
1:D:51:ARG:NE	5:D:1027:HOH:O	2.51	0.43
1:D:153:VAL:HG12	1:D:155:GLY:H	1.83	0.43
1:B:12:PHE:CE2	1:B:25:PHE:HZ	2.37	0.43
1:C:10:VAL:CG1	1:C:19:TRP:HD1	2.32	0.43
1:D:6:TRP:CZ3	1:D:94:LEU:HB3	2.53	0.43
1:D:49:ILE:HG12	1:D:49:ILE:H	1.10	0.43
1:D:107:MET:HG3	1:D:109:ILE:CD1	2.45	0.43
1:A:20:VAL:HG23	1:A:71:MET:HB2	2.01	0.42
1:A:40:PHE:O	1:A:41:GLY:C	2.60	0.42
1:B:56:THR:HG22	1:B:58:PHE:HE2	1.84	0.42
1:B:59:ARG:HD3	1:B:59:ARG:C	2.43	0.42
1:D:127:ALA:HB3	5:D:1034:HOH:O	2.19	0.42
1:D:128:LYS:H	1:D:131:ASP:CG	2.26	0.42
1:A:61:SER:N	5:A:1031:HOH:O	2.41	0.42
1:C:107:MET:HB3	1:C:107:MET:HE2	1.86	0.42
1:D:12:PHE:HE2	1:D:40:PHE:CE2	2.37	0.42
1:A:26:ILE:CG1	1:A:55:PHE:CZ	3.02	0.42
1:C:32:ILE:CG2	1:C:33:PRO:CD	2.98	0.42
1:A:47:ILE:HD12	1:A:60:PHE:HD2	1.82	0.42
1:A:99:VAL:HG12	1:A:120:MET:O	2.19	0.42
1:A:166:THR:OG1	1:B:103:ALA:HB2	2.20	0.42
1:B:42:GLU:CD	1:B:62:ARG:CD	2.91	0.42
1:D:47:ILE:HG21	1:D:49:ILE:CD1	2.50	0.42
1:B:22:PRO:HA	1:B:64:VAL:CG2	2.49	0.42
1:B:40:PHE:CA	5:B:1008:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:PHE:HB2	1:D:171:VAL:O	2.19	0.42
1:C:32:ILE:HG22	1:C:33:PRO:HD2	2.02	0.42
1:D:12:PHE:CD2	1:D:40:PHE:CZ	3.08	0.42
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.68	0.42
1:D:8:ARG:HH11	1:D:8:ARG:HD2	1.53	0.42
1:A:55:PHE:HE2	1:A:172:GLN:HG2	1.85	0.42
1:B:18:PHE:CD2	1:B:142:PRO:HG3	2.55	0.42
1:A:120:MET:HE3	5:B:1005:HOH:O	2.19	0.41
1:B:146:LYS:NZ	1:C:132:LEU:HD23	2.35	0.41
1:C:129:GLY:O	1:C:130:MET:HE2	2.19	0.41
1:C:145:TYR:CE2	1:C:152:VAL:CG2	3.03	0.41
1:D:37:ARG:HG2	1:D:38:GLU:N	2.21	0.41
1:D:82:VAL:O	1:D:82:VAL:CG2	2.68	0.41
1:A:107:MET:HG2	1:A:109:ILE:HD11	2.01	0.41
1:D:89:ARG:NH2	1:D:138:ASP:OD2	2.54	0.41
1:B:55:PHE:CD2	1:B:171:VAL:C	2.99	0.41
1:C:126:ASN:ND2	5:C:1043:HOH:O	2.54	0.41
1:D:85:ILE:HD11	1:D:143:TYR:CE1	2.55	0.41
1:D:162:LYS:CE	5:D:1023:HOH:O	2.69	0.41
1:A:36:VAL:HG23	1:A:37:ARG:N	2.31	0.41
1:A:148:ASN:HB3	1:A:149:ASN:H	1.60	0.41
1:B:36:VAL:HG23	1:B:36:VAL:C	2.44	0.41
1:C:44:ILE:O	1:C:46:SER:N	2.54	0.41
1:C:107:MET:HE2	1:D:105:ALA:HB2	2.02	0.41
1:D:146:LYS:HZ1	1:D:149:ASN:HA	1.85	0.41
1:D:147:ARG:HB2	1:D:152:VAL:HG11	2.02	0.41
1:A:73:LEU:HA	1:A:153:VAL:O	2.21	0.41
1:B:86:LEU:HB2	1:B:142:PRO:HG2	2.03	0.41
1:D:11:ARG:O	1:D:12:PHE:HB2	2.19	0.41
1:A:124:GLY:HA2	1:D:82:VAL:CG2	2.50	0.41
1:D:38:GLU:HA	1:D:42:GLU:O	2.20	0.41
1:D:85:ILE:HG23	1:D:143:TYR:CE2	2.56	0.41
1:D:162:LYS:CG	5:D:1023:HOH:O	2.69	0.41
1:D:168:VAL:HG12	1:D:169:CYS:N	2.35	0.41
1:A:1:ALA:CB	1:A:2:PRO:CD	2.84	0.41
1:A:55:PHE:HB2	1:A:170:ALA:HB1	2.02	0.41
1:B:65:ARG:HG2	1:B:68:LEU:HD11	2.03	0.41
1:C:100:ARG:CG	1:C:100:ARG:NH2	2.75	0.41
1:A:33:PRO:C	1:A:34:THR:OG1	2.62	0.40
1:B:126:ASN:O	1:B:128:LYS:NZ	2.54	0.40
1:D:36:VAL:CG1	1:D:36:VAL:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ARG:CG	5:D:1027:HOH:O	2.64	0.40
1:D:147:ARG:HB2	1:D:152:VAL:CG1	2.51	0.40
1:A:32:ILE:CB	1:A:33:PRO:N	2.77	0.40
1:B:113:LEU:C	1:B:113:LEU:CD2	2.95	0.40
1:A:19:TRP:HB3	1:A:68:LEU:CD1	2.51	0.40
1:B:101:MET:HE3	1:B:118:SER:O	2.21	0.40
1:B:2:PRO:CB	1:C:130:MET:HG2	2.28	0.40
1:B:94:LEU:N	1:B:94:LEU:CD1	2.83	0.40
1:D:65:ARG:HH21	1:D:68:LEU:HD21	1.86	0.40

All (7) 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)
5:A:1011:HOH:O	5:C:1016:HOH:O[6_655]	1.64	0.56
5:A:1010:HOH:O	5:C:1017:HOH:O[6_655]	1.88	0.32
1:C:130:MET:SD	3:A:301:TLA:O41[6_555]	2.01	0.19
1:A:47:ILE:O	5:C:1017:HOH:O[6_655]	2.04	0.16
1:A:62:ARG:NH1	5:C:1033:HOH:O[5_554]	2.08	0.12
1:A:37:ARG:CD	5:C:1040:HOH:O[5_554]	2.10	0.10
1:A:37:ARG:CG	5:C:1040:HOH:O[5_554]	2.15	0.05

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	171/173 (99%)	143 (84%)	17 (10%)	11 (6%)	1	3
1	B	171/173 (99%)	133 (78%)	29 (17%)	9 (5%)	1	5
1	C	171/173 (99%)	142 (83%)	20 (12%)	9 (5%)	1	5
1	D	171/173 (99%)	131 (77%)	28 (16%)	12 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	684/692 (99%)	549 (80%)	94 (14%)	41 (6%)	1 3

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	109	ILE
1	C	36	VAL
1	C	124	GLY
1	C	148	ASN
1	D	35	GLY
1	D	109	ILE
1	A	36	VAL
1	A	37	ARG
1	A	91	SER
1	A	131	ASP
1	A	148	ASN
1	B	4	THR
1	B	40	PHE
1	B	62	ARG
1	B	112	ARG
1	B	124	GLY
1	C	129	GLY
1	D	34	THR
1	D	63	LYS
1	D	145	TYR
1	A	92	GLY
1	A	110	GLN
1	B	147	ARG
1	C	163	SER
1	D	12	PHE
1	D	22	PRO
1	D	105	ALA
1	B	3	PRO
1	B	91	SER
1	C	34	THR
1	C	45	GLU
1	A	147	ARG
1	D	36	VAL
1	B	49	ILE
1	C	111	GLY
1	D	49	ILE

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Mol	Chain	Res	Type
1	C	21	SER
1	D	43	PRO
1	D	44	ILE
1	A	32	ILE

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	138/138 (100%)	84 (61%)	54 (39%)	0	0
1	B	138/138 (100%)	83 (60%)	55 (40%)	0	0
1	C	138/138 (100%)	81 (59%)	57 (41%)	0	0
1	D	138/138 (100%)	85 (62%)	53 (38%)	0	0
All	All	552/552 (100%)	333 (60%)	219 (40%)	0	0

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ARG
1	A	14	SER
1	A	20	VAL
1	A	21	SER
1	A	22	PRO
1	A	23	THR
1	A	26	ILE
1	A	28	THR
1	A	32	ILE
1	A	38	GLU
1	A	39	PHE
1	A	42	GLU
1	A	44	ILE
1	A	45	GLU
1	A	47	ILE
1	A	51	ARG

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	63	LYS
1	A	69	THR
1	A	73	LEU
1	A	75	GLU
1	A	79	GLU
1	A	81	VAL
1	A	84	SER
1	A	85	ILE
1	A	89	ARG
1	A	90	ASP
1	A	99	VAL
1	A	100	ARG
1	A	104	ILE
1	A	106	SER
1	A	107	MET
1	A	108	LYS
1	A	110	GLN
1	A	112	ARG
1	A	113	LEU
1	A	121	LEU
1	A	122	LEU
1	A	123	THR
1	A	130	MET
1	A	131	ASP
1	A	132	LEU
1	A	135	LEU
1	A	136	PRO
1	A	139	CYS
1	A	142	PRO
1	A	147	ARG
1	A	149	ASN
1	A	151	TRP
1	A	153	VAL
1	A	162	LYS
1	A	163	SER
1	A	172	GLN
1	B	5	LEU
1	B	7	SER
1	B	8	ARG
1	B	9	VAL
1	B	10	VAL

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Mol	Chain	Res	Type
1	B	11	ARG
1	B	20	VAL
1	B	23	THR
1	B	24	VAL
1	B	25	PHE
1	B	31	VAL
1	B	34	THR
1	B	36	VAL
1	B	37	ARG
1	B	38	GLU
1	B	39	PHE
1	B	42	GLU
1	B	44	ILE
1	B	45	GLU
1	B	47	ILE
1	B	51	ARG
1	B	59	ARG
1	B	61	SER
1	B	65	ARG
1	B	69	THR
1	B	73	LEU
1	B	79	GLU
1	B	85	ILE
1	B	86	LEU
1	B	89	ARG
1	B	91	SER
1	B	101	MET
1	B	104	ILE
1	B	106	SER
1	B	107	MET
1	B	108	LYS
1	B	110	GLN
1	B	112	ARG
1	B	113	LEU
1	B	117	GLN
1	B	120	MET
1	B	121	LEU
1	B	128	LYS
1	B	130	MET
1	B	131	ASP
1	B	132	LEU
1	B	134	THR

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Mol	Chain	Res	Type
1	B	146	LYS
1	B	147	ARG
1	B	151	TRP
1	B	152	VAL
1	B	154	CYS
1	B	156	VAL
1	B	162	LYS
1	B	169	CYS
1	C	3	PRO
1	C	10	VAL
1	C	11	ARG
1	C	20	VAL
1	C	26	ILE
1	C	31	VAL
1	C	34	THR
1	C	37	ARG
1	C	38	GLU
1	C	39	PHE
1	C	42	GLU
1	C	43	PRO
1	C	44	ILE
1	C	45	GLU
1	C	47	ILE
1	C	49	ILE
1	C	54	GLU
1	C	59	ARG
1	C	62	ARG
1	C	63	LYS
1	C	65	ARG
1	C	68	LEU
1	C	69	THR
1	C	71	MET
1	C	73	LEU
1	C	74	GLU
1	C	75	GLU
1	C	78	PRO
1	C	79	GLU
1	C	85	ILE
1	C	86	LEU
1	C	93	GLU
1	C	99	VAL
1	C	100	ARG

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Mol	Chain	Res	Type
1	C	104	ILE
1	C	106	SER
1	C	107	MET
1	C	108	LYS
1	C	110	GLN
1	C	112	ARG
1	C	113	LEU
1	C	122	LEU
1	C	123	THR
1	C	130	MET
1	C	132	LEU
1	C	135	LEU
1	C	146	LYS
1	C	147	ARG
1	C	148	ASN
1	C	149	ASN
1	C	151	TRP
1	C	152	VAL
1	C	153	VAL
1	C	154	CYS
1	C	162	LYS
1	C	166	THR
1	C	167	VAL
1	D	10	VAL
1	D	14	SER
1	D	20	VAL
1	D	21	SER
1	D	24	VAL
1	D	28	THR
1	D	30	HIS
1	D	31	VAL
1	D	32	ILE
1	D	34	THR
1	D	36	VAL
1	D	37	ARG
1	D	38	GLU
1	D	39	PHE
1	D	42	GLU
1	D	43	PRO
1	D	44	ILE
1	D	46	SER
1	D	49	ILE

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Mol	Chain	Res	Type
1	D	54	GLU
1	D	59	ARG
1	D	60	PHE
1	D	61	SER
1	D	64	VAL
1	D	65	ARG
1	D	67	ASP
1	D	68	LEU
1	D	69	THR
1	D	73	LEU
1	D	81	VAL
1	D	82	VAL
1	D	85	ILE
1	D	86	LEU
1	D	88	LYS
1	D	89	ARG
1	D	99	VAL
1	D	104	ILE
1	D	106	SER
1	D	107	MET
1	D	108	LYS
1	D	113	LEU
1	D	117	GLN
1	D	121	LEU
1	D	122	LEU
1	D	128	LYS
1	D	131	ASP
1	D	132	LEU
1	D	146	LYS
1	D	151	TRP
1	D	152	VAL
1	D	161	THR
1	D	162	LYS
1	D	172	GLN

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

Mol	Chain	Res	Type
1	A	172	GLN
1	B	57	GLN
1	B	149	ASN
1	B	165	ASN

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Mol	Chain	Res	Type
1	C	149	ASN
1	C	172	GLN
1	D	30	HIS
1	D	117	GLN
1	D	157	HIS
1	D	172	GLN

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](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	TAR	A	300	-	9,9,9	3.70	3 (33%)	12,12,12	3.10	8 (66%)
3	TLA	A	301	-	9,9,9	5.41	5 (55%)	12,12,12	4.71	6 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TAR	A	300	-	-	3/12/12/12	-
3	TLA	A	301	-	-	2/12/12/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	TLA	C2-C1	10.64	1.67	1.52
3	A	301	TLA	C3-C2	9.19	1.82	1.53
4	A	300	TAR	O3-C3	7.63	1.57	1.42
3	A	301	TLA	O2-C2	6.91	1.55	1.42
4	A	300	TAR	O2-C2	6.33	1.54	1.42
4	A	300	TAR	O41-C4	-3.49	1.19	1.30
3	A	301	TLA	O41-C4	-3.01	1.21	1.30
3	A	301	TLA	O4-C4	2.03	1.28	1.22

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	TLA	O2-C2-C3	-8.25	93.38	110.17
3	A	301	TLA	O2-C2-C1	-7.54	94.57	110.69
4	A	300	TAR	C2-C3-C4	6.80	124.89	109.82
3	A	301	TLA	O3-C3-C2	6.61	123.63	110.17
3	A	301	TLA	O3-C3-C4	-6.56	96.68	110.69
3	A	301	TLA	C3-C2-C1	5.99	123.10	109.82
4	A	300	TAR	O11-C1-C2	4.47	125.73	113.31
4	A	300	TAR	O3-C3-C4	3.12	117.36	110.69
4	A	300	TAR	O2-C2-C3	3.00	116.27	110.17
3	A	301	TLA	O11-C1-O1	-2.81	117.71	124.08
4	A	300	TAR	O41-C4-C3	2.58	120.48	113.31
4	A	300	TAR	O11-C1-O1	-2.49	118.43	124.08
4	A	300	TAR	O1-C1-C2	-2.39	115.25	121.62
4	A	300	TAR	O2-C2-C1	2.20	115.40	110.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	300	TAR	O2-C2-C3-O3
3	A	301	TLA	O2-C2-C3-O3
4	A	300	TAR	C1-C2-C3-O3
4	A	300	TAR	O2-C2-C3-C4
3	A	301	TLA	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	300	TAR	4	0
3	A	301	TLA	6	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:VAL	C	37:ARG	N	1.17

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

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

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, 95th 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 ²)	Q<0.9
1	A	173/173 (100%)	-1.01	0 100 100	23, 49, 101, 135	0
1	B	173/173 (100%)	-0.60	1 (0%) 85 80	33, 75, 129, 147	0
1	C	173/173 (100%)	-1.01	0 100 100	23, 51, 98, 135	0
1	D	173/173 (100%)	-0.80	0 100 100	33, 66, 120, 141	0
All	All	692/692 (100%)	-0.85	1 (0%) 92 90	23, 60, 117, 147	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	PRO	3.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TLA	A	301	10/10	0.84	0.09	152,162,165,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TAR	A	300	10/10	0.93	0.06	68,107,112,113	0
2	HG	A	1001	1/1	0.98	0.11	81,81,81,81	1
2	HG	C	1005	1/1	0.98	0.08	60,60,60,60	1
2	HG	A	1002	1/1	0.99	0.06	65,65,65,65	1
2	HG	C	1006	1/1	0.99	0.08	75,75,75,75	1
2	HG	D	1007	1/1	0.99	0.09	64,64,64,64	1
2	HG	D	1008	1/1	0.99	0.06	96,96,96,96	1
2	HG	B	1003	1/1	0.99	0.09	69,69,69,69	1
2	HG	B	1004	1/1	0.99	0.10	118,118,118,118	1

6.5 Other polymers [i](#)

There are no such residues in this entry.