



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 AM UTC

PDB ID : 3GG5 / pdb_00003gg5
Title : Replacement of Val3 in Human Thymidylate Synthase Affects Its Kinetic Properties and Intracellular Stability
Authors : Huang, X.; Gibson, L.M.; Bell, B.J.; Lovelace, L.L.; Lebioda, L.
Deposited on : 2009-02-27
Resolution : 2.77 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

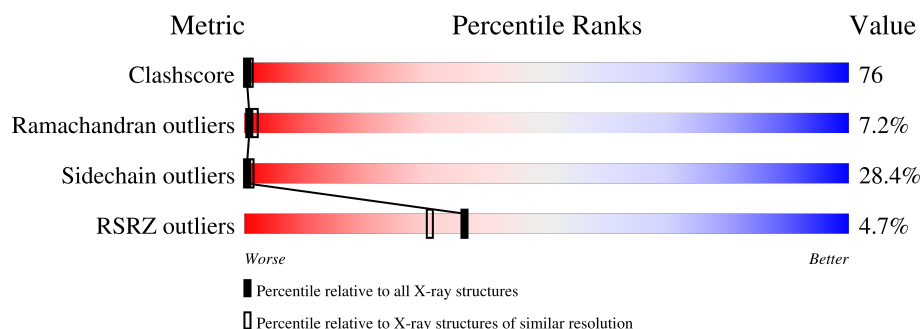
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	313	8% 30% 35% 17% 10%
1	B	313	5% 10% 23% 43% 13% 10%
1	C	313	4% 8% 30% 37% 16% 10%
1	D	313	6% 6% 24% 41% 19% 10%

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
2	SO4	A	616	-	X	-	-
3	PO4	B	616	-	X	X	-
3	PO4	D	616	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9174 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.

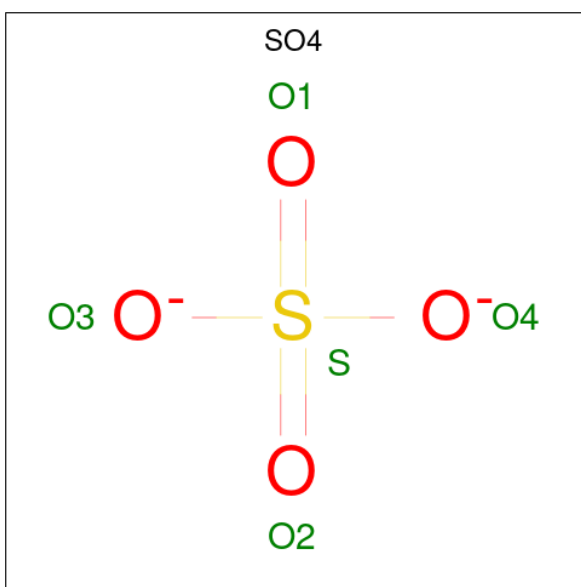
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			
1	B	281	Total	C	N	O	S	0	0	0
			2270	1451	397	411	11			
1	C	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			
1	D	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			

There are 4 discrepancies between the modelled and reference sequences:

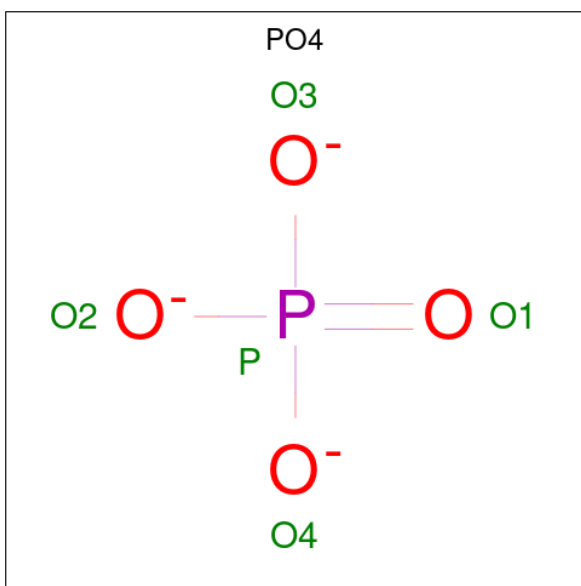
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	TYR	VAL	engineered mutation	UNP P04818
B	3	TYR	VAL	engineered mutation	UNP P04818
C	3	TYR	VAL	engineered mutation	UNP P04818
D	3	TYR	VAL	engineered mutation	UNP P04818

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

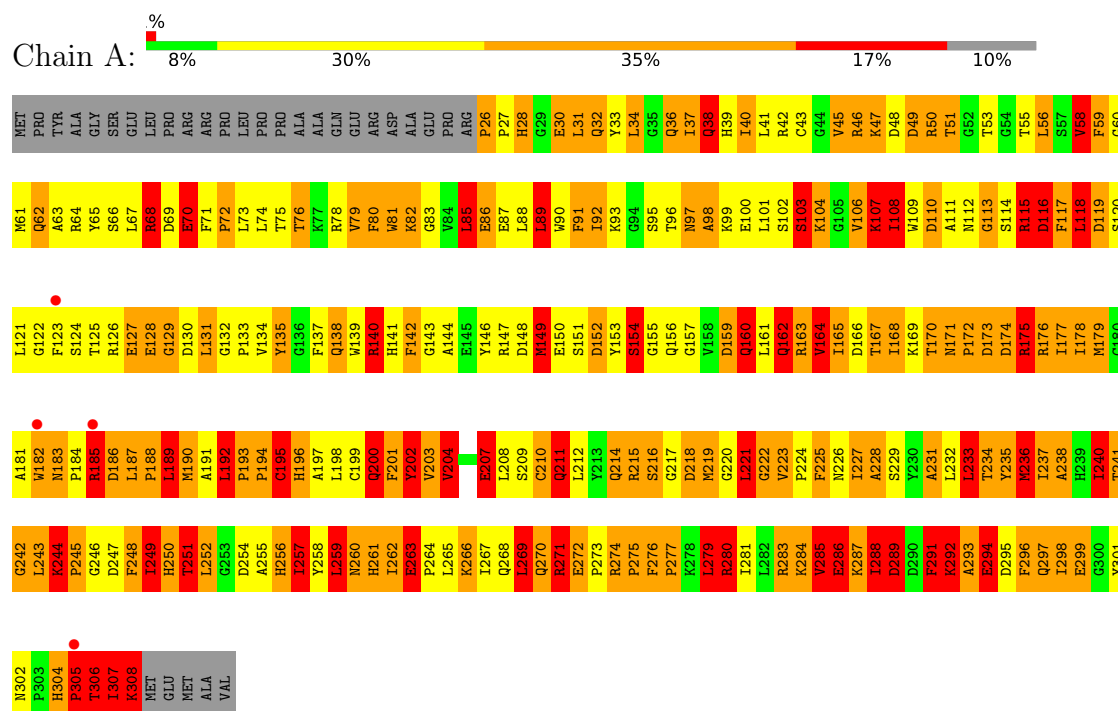
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	7	Total 7	O 7	0	0
4	C	5	Total 5	O 5	0	0
4	D	5	Total 5	O 5	0	0

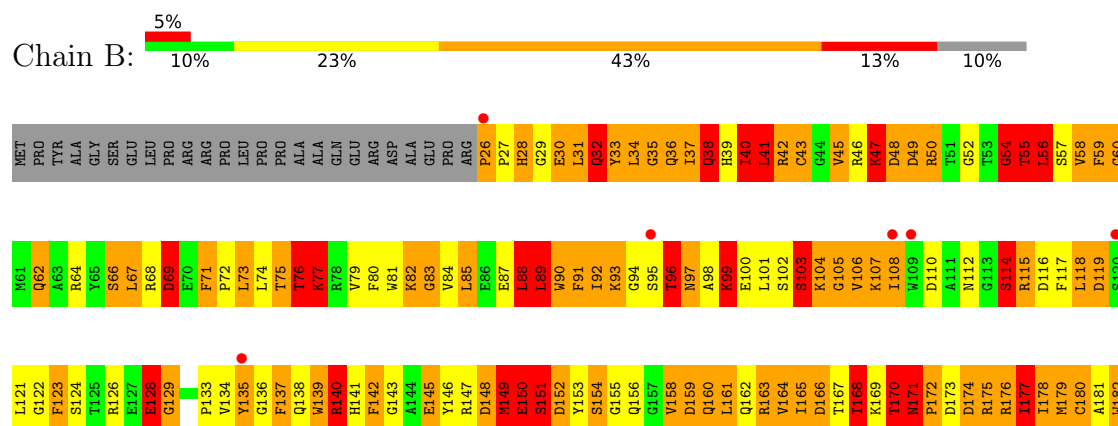
3 Residue-property plots

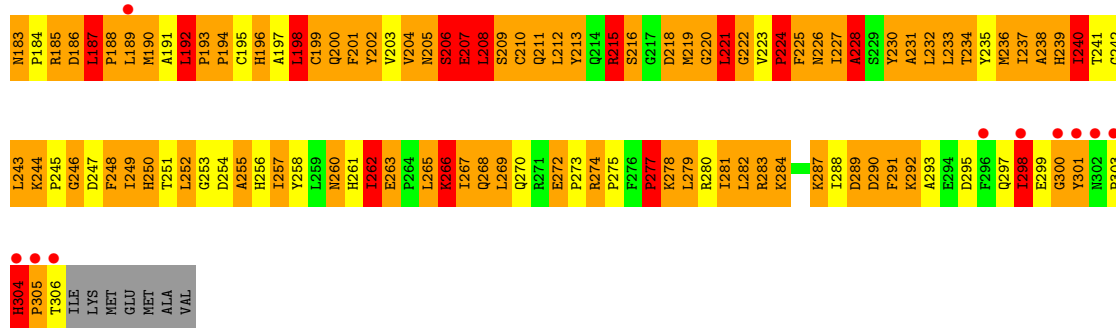
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

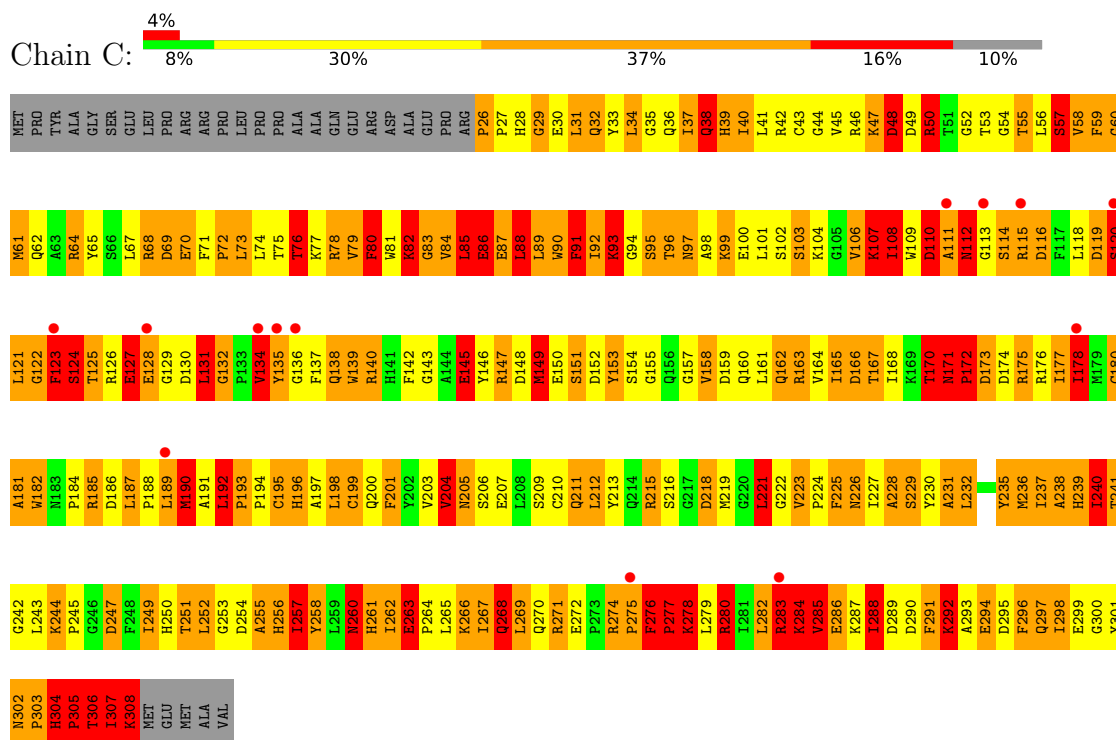


• Molecule 1: Thymidylate synthase

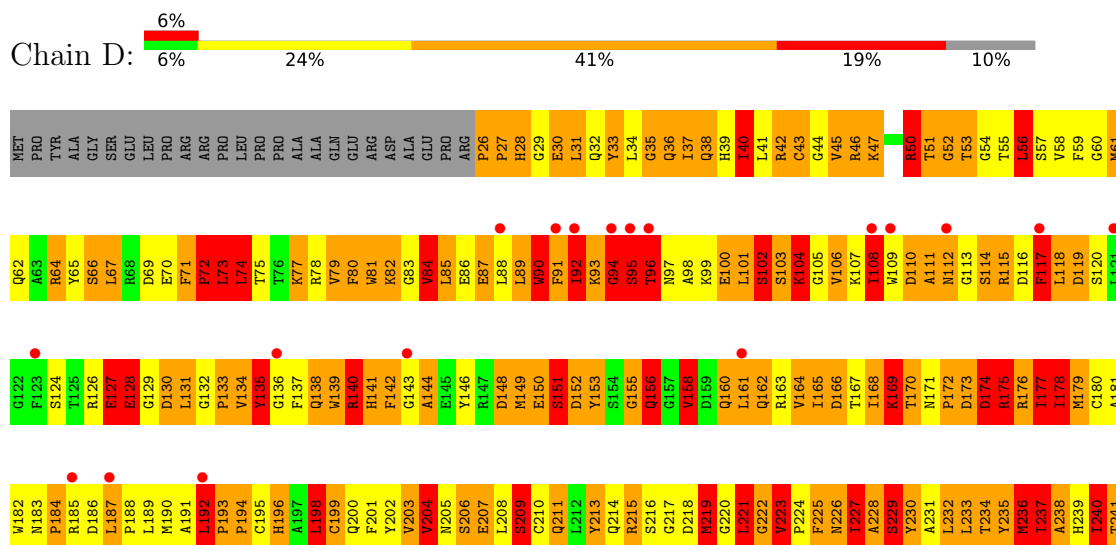


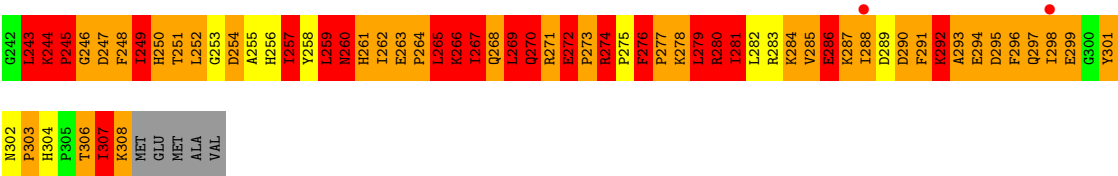


• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.56Å 94.86Å 130.86Å 90.00° 122.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.77 50.00 – 2.77	Depositor EDS
% Data completeness (in resolution range)	89.3 (50.00-2.77) 80.2 (50.00-2.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.254 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9174	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: SO4, PO4

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	3.23	239/2347 (10.2%)	2.97	227/3175 (7.1%)
1	B	2.83	179/2330 (7.7%)	2.55	181/3153 (5.7%)
1	C	2.95	212/2347 (9.0%)	2.87	236/3175 (7.4%)
1	D	2.77	187/2347 (8.0%)	2.68	232/3175 (7.3%)
All	All	2.95	817/9371 (8.7%)	2.77	876/12678 (6.9%)

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	6
1	B	0	6
1	C	0	10
1	D	0	4
All	All	0	26

All (817) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	GLN	C-O	29.12	1.60	1.23
1	C	114	SER	CA-C	-22.26	1.23	1.52
1	B	58	VAL	C-O	18.38	1.42	1.24
1	A	185	ARG	CZ-NH2	16.67	1.55	1.33
1	A	185	ARG	NE-CZ	-16.14	1.15	1.33
1	A	203	VAL	C-O	-15.82	1.06	1.23
1	A	200	GLN	N-CA	-15.07	1.26	1.45
1	A	79	VAL	CA-CB	-14.37	1.34	1.54
1	A	202	TYR	C-N	14.12	1.50	1.33
1	A	203	VAL	CA-CB	-13.81	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	ILE	CA-C	13.59	1.70	1.52
1	B	114	SER	N-CA	12.80	1.61	1.46
1	D	296	PHE	CA-C	-12.75	1.37	1.52
1	C	162	GLN	CA-C	-12.71	1.36	1.52
1	A	203	VAL	N-CA	12.70	1.62	1.46
1	B	249	ILE	CA-CB	-12.55	1.39	1.54
1	A	175	ARG	NE-CZ	12.39	1.46	1.33
1	B	227	ILE	CA-CB	-12.18	1.37	1.54
1	A	235	TYR	C-O	12.12	1.38	1.24
1	C	307	ILE	N-CA	12.09	1.61	1.46
1	A	201	PHE	CE2-CZ	12.03	1.74	1.38
1	A	203	VAL	CA-C	11.85	1.67	1.52
1	B	237	ILE	CA-CB	-11.79	1.39	1.54
1	B	197	ALA	CA-CB	-11.78	1.34	1.53
1	B	207	GLU	N-CA	-11.68	1.31	1.45
1	D	215	ARG	N-CA	11.67	1.60	1.46
1	C	239	HIS	N-CA	-11.65	1.31	1.46
1	D	134	VAL	CA-C	11.56	1.67	1.52
1	A	216	SER	C-O	-11.52	1.10	1.23
1	A	192	LEU	N-CA	11.41	1.56	1.45
1	A	178	ILE	CA-CB	-11.29	1.39	1.54
1	A	38	GLN	CG-CD	11.19	1.80	1.52
1	D	229	SER	C-O	11.14	1.36	1.24
1	C	111	ALA	N-CA	11.10	1.60	1.46
1	C	38	GLN	CG-CD	11.00	1.79	1.52
1	A	85	LEU	C-O	10.91	1.36	1.24
1	A	72	PRO	CA-C	-10.88	1.43	1.53
1	A	175	ARG	CZ-NH2	10.87	1.47	1.33
1	C	70	GLU	CA-C	-10.82	1.39	1.52
1	C	238	ALA	CA-CB	-10.78	1.34	1.53
1	A	306	THR	CA-C	10.75	1.66	1.52
1	C	106	VAL	CA-C	10.74	1.62	1.53
1	A	306	THR	C-O	10.72	1.37	1.24
1	B	27	PRO	N-CA	10.69	1.61	1.47
1	B	174	ASP	C-O	10.64	1.36	1.23
1	C	112	ASN	CA-C	10.38	1.66	1.52
1	B	108	ILE	CA-CB	10.34	1.70	1.54
1	A	185	ARG	CG-CD	10.30	1.83	1.52
1	B	235	TYR	N-CA	10.21	1.59	1.46
1	C	292	LYS	CD-CE	10.18	1.82	1.52
1	D	156	GLN	CA-C	10.13	1.65	1.53
1	C	251	THR	N-CA	-10.05	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	269	LEU	N-CA	-10.04	1.33	1.46
1	A	43	CYS	CA-C	-10.04	1.39	1.52
1	B	178	ILE	CA-CB	-9.99	1.41	1.54
1	A	216	SER	CA-C	-9.90	1.41	1.52
1	B	177	ILE	CA-CB	-9.89	1.42	1.53
1	C	110	ASP	CA-C	9.79	1.65	1.52
1	A	249	ILE	CA-CB	-9.70	1.42	1.54
1	A	37	ILE	CA-CB	-9.67	1.42	1.54
1	D	166	ASP	CA-C	-9.57	1.39	1.52
1	A	45	VAL	CA-CB	-9.55	1.40	1.54
1	C	284	LYS	CA-C	9.55	1.65	1.53
1	D	89	LEU	N-CA	9.52	1.57	1.46
1	C	110	ASP	C-N	9.47	1.47	1.33
1	C	240	ILE	C-O	-9.46	1.11	1.24
1	D	39	HIS	N-CA	-9.41	1.35	1.46
1	A	61	MET	C-O	9.40	1.35	1.23
1	B	142	PHE	CA-C	9.38	1.65	1.52
1	C	307	ILE	CA-C	9.34	1.64	1.52
1	B	251	THR	CA-C	-9.32	1.41	1.52
1	A	193	PRO	C-O	-9.29	1.17	1.25
1	A	305	PRO	CA-C	9.28	1.65	1.52
1	C	292	LYS	CE-NZ	9.29	1.77	1.49
1	D	252	LEU	CA-C	-9.22	1.41	1.52
1	A	203	VAL	CB-CG2	-9.20	1.22	1.52
1	B	219	MET	C-O	-9.19	1.13	1.24
1	A	177	ILE	C-O	9.17	1.35	1.24
1	A	178	ILE	N-CA	-9.15	1.35	1.46
1	C	292	LYS	CA-C	9.13	1.64	1.52
1	B	250	HIS	CA-C	-9.10	1.41	1.52
1	A	284	LYS	CG-CD	9.07	1.79	1.52
1	D	96	THR	C-N	-9.06	1.20	1.33
1	B	135	TYR	C-O	9.04	1.35	1.24
1	B	178	ILE	CA-C	-9.03	1.41	1.52
1	A	245	PRO	N-CA	9.01	1.58	1.47
1	A	63	ALA	CA-CB	-9.00	1.36	1.53
1	B	257	ILE	CA-CB	-8.99	1.43	1.54
1	D	306	THR	CA-C	8.99	1.64	1.52
1	C	232	LEU	C-O	8.99	1.35	1.24
1	B	37	ILE	CA-CB	-8.97	1.42	1.54
1	C	237	ILE	CA-CB	-8.97	1.42	1.54
1	C	167	THR	CA-CB	-8.95	1.37	1.53
1	A	202	TYR	C-O	-8.91	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	PHE	N-CA	-8.89	1.35	1.46
1	C	123	PHE	C-N	-8.88	1.21	1.33
1	C	280	ARG	CG-CD	8.87	1.79	1.52
1	A	91	PHE	CA-C	-8.85	1.41	1.52
1	C	162	GLN	C-N	-8.84	1.21	1.33
1	B	196	HIS	N-CA	-8.83	1.34	1.46
1	A	172	PRO	N-CA	-8.83	1.35	1.47
1	D	263	GLU	N-CA	8.81	1.54	1.46
1	B	255	ALA	CA-CB	-8.80	1.40	1.53
1	A	231	ALA	CA-CB	-8.80	1.38	1.53
1	D	279	LEU	C-O	8.80	1.34	1.23
1	C	149	MET	SD-CE	8.73	2.01	1.79
1	C	263	GLU	C-O	8.73	1.32	1.24
1	B	267	ILE	CA-C	8.71	1.63	1.52
1	D	209	SER	CA-C	-8.71	1.41	1.52
1	D	170	THR	C-O	-8.67	1.13	1.24
1	D	44	GLY	C-O	-8.67	1.15	1.23
1	A	210	CYS	C-O	-8.63	1.12	1.23
1	A	227	ILE	CA-CB	-8.62	1.44	1.54
1	A	252	LEU	N-CA	-8.60	1.35	1.45
1	B	228	ALA	C-O	8.59	1.34	1.24
1	C	201	PHE	CA-C	-8.58	1.41	1.53
1	D	70	GLU	N-CA	8.58	1.56	1.46
1	C	204	VAL	CA-C	8.52	1.63	1.52
1	D	307	ILE	CG1-CD1	8.52	1.84	1.51
1	A	277	PRO	CA-C	8.51	1.62	1.52
1	D	51	THR	CA-CB	8.51	1.66	1.53
1	B	242	GLY	C-O	-8.50	1.13	1.24
1	D	295	ASP	C-O	8.46	1.31	1.24
1	A	262	ILE	CA-CB	-8.46	1.44	1.54
1	A	75	THR	CA-C	8.44	1.64	1.52
1	C	209	SER	CA-C	-8.43	1.42	1.52
1	B	244	LYS	CG-CD	8.40	1.77	1.52
1	B	304	HIS	CA-CB	8.38	1.66	1.53
1	D	307	ILE	CA-CB	8.38	1.65	1.54
1	D	47	LYS	CD-CE	8.35	1.77	1.52
1	B	114	SER	CA-CB	-8.35	1.40	1.53
1	A	296	PHE	CA-C	-8.34	1.42	1.52
1	B	176	ARG	N-CA	-8.33	1.39	1.47
1	B	159	ASP	C-O	8.32	1.34	1.24
1	A	174	ASP	C-O	8.31	1.33	1.23
1	A	197	ALA	CA-CB	-8.29	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	SER	C-N	-8.26	1.24	1.33
1	D	66	SER	C-O	-8.21	1.14	1.24
1	A	174	ASP	N-CA	-8.21	1.35	1.46
1	A	28	HIS	CA-C	8.19	1.63	1.52
1	C	59	PHE	C-O	-8.18	1.14	1.23
1	D	36	GLN	N-CA	-8.17	1.36	1.46
1	A	176	ARG	C-O	-8.15	1.14	1.23
1	A	223	VAL	CA-CB	-8.14	1.43	1.54
1	C	307	ILE	CA-CB	8.13	1.65	1.54
1	A	79	VAL	CA-C	8.13	1.61	1.53
1	C	32	GLN	CA-C	-8.13	1.41	1.52
1	A	200	GLN	CD-NE2	-8.13	1.16	1.33
1	A	201	PHE	CA-C	-8.11	1.42	1.52
1	A	185	ARG	CZ-NH1	-8.10	1.21	1.32
1	D	279	LEU	CA-C	8.09	1.62	1.52
1	A	58	VAL	N-CA	-8.07	1.36	1.46
1	A	297	GLN	CA-C	-8.06	1.42	1.52
1	C	244	LYS	CA-C	8.06	1.63	1.52
1	A	65	TYR	CA-C	8.05	1.62	1.52
1	C	165	ILE	C-O	8.04	1.33	1.24
1	C	197	ALA	CA-CB	-8.05	1.40	1.53
1	C	275	PRO	CA-C	-8.02	1.41	1.52
1	D	96	THR	CA-CB	-8.02	1.42	1.53
1	B	234	THR	N-CA	-8.00	1.36	1.46
1	C	209	SER	C-O	8.00	1.34	1.23
1	B	304	HIS	N-CA	7.99	1.57	1.46
1	B	170	THR	CA-C	-7.98	1.42	1.52
1	A	274	ARG	C-O	-7.97	1.13	1.23
1	A	201	PHE	CA-CB	-7.97	1.41	1.53
1	A	257	ILE	CA-CB	-7.96	1.44	1.54
1	D	61	MET	C-O	7.95	1.33	1.23
1	D	240	ILE	CA-C	-7.93	1.43	1.52
1	A	283	ARG	CA-C	-7.92	1.42	1.52
1	A	177	ILE	N-CA	-7.91	1.36	1.46
1	B	200	GLN	N-CA	7.90	1.55	1.46
1	B	50	ARG	NE-CZ	7.89	1.41	1.33
1	B	252	LEU	C-O	7.88	1.33	1.23
1	A	247	ASP	CA-C	-7.86	1.43	1.52
1	D	295	ASP	CA-C	7.85	1.64	1.52
1	C	175	ARG	N-CA	-7.84	1.34	1.45
1	A	212	LEU	C-O	-7.84	1.14	1.24
1	C	223	VAL	C-O	-7.83	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	VAL	CA-CB	-7.83	1.44	1.54
1	C	280	ARG	CZ-NH2	7.83	1.43	1.33
1	D	41	LEU	C-O	-7.83	1.15	1.24
1	C	230	TYR	CA-C	-7.82	1.42	1.52
1	A	97	ASN	CA-C	-7.79	1.43	1.52
1	C	204	VAL	CA-CB	-7.75	1.44	1.54
1	D	292	LYS	CA-C	-7.75	1.42	1.52
1	C	173	ASP	CA-C	-7.69	1.42	1.52
1	D	273	PRO	CA-C	7.69	1.62	1.52
1	B	76	THR	CA-CB	7.67	1.66	1.53
1	D	93	LYS	C-N	-7.67	1.22	1.33
1	D	232	LEU	C-O	7.66	1.32	1.24
1	B	114	SER	CA-C	7.66	1.61	1.52
1	C	90	TRP	N-CA	-7.64	1.36	1.46
1	C	69	ASP	CB-CG	-7.62	1.33	1.52
1	A	250	HIS	CA-C	-7.61	1.43	1.52
1	A	41	LEU	N-CA	7.61	1.55	1.46
1	A	175	ARG	CA-CB	7.60	1.64	1.53
1	B	33	TYR	N-CA	-7.60	1.37	1.46
1	B	254	ASP	CA-CB	-7.60	1.43	1.52
1	A	32	GLN	CA-C	7.59	1.62	1.52
1	D	266	LYS	CB-CG	7.59	1.75	1.52
1	B	176	ARG	C-O	-7.57	1.18	1.23
1	A	51	THR	N-CA	-7.56	1.37	1.46
1	D	167	THR	CA-CB	-7.56	1.41	1.53
1	C	250	HIS	CA-CB	-7.55	1.43	1.53
1	D	33	TYR	C-O	7.54	1.32	1.24
1	B	164	VAL	CA-C	7.53	1.62	1.52
1	D	259	LEU	CA-CB	-7.53	1.41	1.53
1	B	253	GLY	N-CA	7.51	1.56	1.45
1	A	297	GLN	N-CA	-7.50	1.37	1.46
1	A	165	ILE	C-O	7.50	1.32	1.24
1	B	56	LEU	N-CA	7.48	1.55	1.46
1	B	134	VAL	CA-CB	7.46	1.64	1.54
1	A	75	THR	C-O	7.46	1.33	1.24
1	B	107	LYS	CD-CE	7.45	1.74	1.52
1	A	183	ASN	C-N	7.44	1.43	1.34
1	C	37	ILE	N-CA	-7.44	1.37	1.46
1	B	42	ARG	N-CA	-7.44	1.37	1.46
1	C	40	ILE	N-CA	-7.43	1.36	1.46
1	C	249	ILE	CG1-CD1	-7.42	1.22	1.51
1	C	263	GLU	CA-CB	-7.42	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	VAL	CA-CB	-7.41	1.44	1.54
1	D	234	THR	C-O	7.40	1.32	1.24
1	D	228	ALA	C-O	7.40	1.33	1.24
1	A	277	PRO	C-O	7.39	1.33	1.23
1	C	292	LYS	CG-CD	7.39	1.74	1.52
1	A	170	THR	CA-C	7.38	1.61	1.52
1	A	223	VAL	CA-C	7.38	1.60	1.52
1	C	210	CYS	N-CA	-7.38	1.36	1.45
1	A	219	MET	CA-C	-7.37	1.42	1.52
1	A	48	ASP	C-O	-7.37	1.14	1.23
1	D	95	SER	CA-C	-7.37	1.43	1.52
1	D	231	ALA	CA-C	-7.36	1.43	1.52
1	B	146	TYR	CA-CB	-7.36	1.42	1.53
1	B	76	THR	C-O	-7.34	1.14	1.24
1	B	107	LYS	N-CA	-7.33	1.37	1.46
1	A	48	ASP	N-CA	7.32	1.55	1.45
1	B	67	LEU	CA-C	-7.31	1.43	1.52
1	A	203	VAL	C-N	-7.31	1.23	1.33
1	D	175	ARG	N-CA	-7.31	1.36	1.46
1	C	55	THR	N-CA	7.29	1.56	1.46
1	B	291	PHE	C-N	-7.28	1.24	1.33
1	B	212	LEU	CA-CB	-7.28	1.42	1.53
1	A	165	ILE	CA-CB	-7.26	1.46	1.54
1	B	36	GLN	CD-OE1	7.25	1.37	1.23
1	A	302	ASN	N-CA	7.25	1.55	1.46
1	B	90	TRP	C-O	7.24	1.32	1.24
1	A	106	VAL	CA-CB	7.23	1.64	1.54
1	B	58	VAL	CA-C	7.23	1.61	1.52
1	C	182	TRP	N-CA	-7.22	1.37	1.46
1	B	194	PRO	CA-CB	-7.21	1.44	1.53
1	C	230	TYR	C-O	-7.21	1.15	1.24
1	C	168	ILE	CA-C	-7.21	1.42	1.52
1	B	42	ARG	CB-CG	7.21	1.74	1.52
1	A	92	ILE	CA-CB	-7.21	1.46	1.54
1	C	36	GLN	N-CA	-7.20	1.37	1.46
1	C	37	ILE	CA-C	7.20	1.61	1.52
1	B	237	ILE	CA-C	7.19	1.61	1.52
1	D	306	THR	N-CA	7.19	1.55	1.46
1	C	59	PHE	CA-C	-7.19	1.44	1.53
1	C	251	THR	CA-CB	-7.19	1.37	1.53
1	D	166	ASP	CA-CB	-7.18	1.41	1.53
1	A	60	GLY	CA-C	-7.18	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	53	THR	N-CA	7.17	1.55	1.46
1	A	175	ARG	CG-CD	7.16	1.74	1.52
1	C	231	ALA	C-O	-7.16	1.15	1.24
1	B	200	GLN	C-O	7.16	1.33	1.24
1	B	208	LEU	CG-CD2	-7.13	1.29	1.52
1	B	150	GLU	CA-C	7.12	1.62	1.52
1	B	209	SER	CA-C	-7.10	1.43	1.52
1	D	201	PHE	C-O	7.09	1.32	1.23
1	B	69	ASP	CA-C	7.08	1.62	1.52
1	B	92	ILE	C-O	7.08	1.32	1.24
1	A	280	ARG	N-CA	-7.08	1.37	1.45
1	C	61	MET	CA-C	-7.08	1.44	1.52
1	A	284	LYS	CB-CG	7.07	1.73	1.52
1	B	178	ILE	N-CA	-7.06	1.37	1.46
1	A	219	MET	CB-CG	-7.05	1.31	1.52
1	D	225	PHE	N-CA	-7.04	1.37	1.46
1	C	44	GLY	C-O	-7.04	1.13	1.23
1	C	38	GLN	CD-NE2	7.04	1.48	1.33
1	D	275	PRO	C-O	7.04	1.33	1.24
1	C	58	VAL	C-O	7.03	1.30	1.24
1	B	89	LEU	N-CA	-7.03	1.37	1.46
1	B	146	TYR	N-CA	-7.02	1.37	1.46
1	C	65	TYR	CD1-CE1	7.01	1.59	1.38
1	C	163	ARG	N-CA	-7.01	1.36	1.46
1	C	124	SER	N-CA	-6.99	1.37	1.46
1	D	161	LEU	CA-C	6.99	1.62	1.52
1	A	294	GLU	CD-OE2	6.99	1.38	1.25
1	B	62	GLN	CD-NE2	6.99	1.48	1.33
1	D	241	THR	CA-C	-6.99	1.44	1.52
1	A	255	ALA	N-CA	-6.97	1.37	1.46
1	C	107	LYS	CG-CD	6.97	1.73	1.52
1	C	60	GLY	N-CA	6.96	1.55	1.45
1	D	247	ASP	CG-OD2	6.95	1.38	1.25
1	D	30	GLU	CA-C	-6.94	1.43	1.52
1	D	140	ARG	N-CA	6.94	1.55	1.46
1	A	195	CYS	CA-C	-6.93	1.43	1.52
1	A	177	ILE	CA-C	6.93	1.60	1.52
1	D	120	SER	CA-C	6.92	1.62	1.52
1	A	47	LYS	N-CA	-6.91	1.38	1.46
1	B	54	GLY	C-O	-6.90	1.12	1.23
1	D	91	PHE	CA-C	-6.89	1.43	1.52
1	A	271	ARG	CA-C	6.87	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	ASP	C-O	-6.87	1.16	1.24
1	C	172	PRO	N-CA	-6.86	1.38	1.47
1	A	201	PHE	CG-CD1	6.86	1.53	1.38
1	C	235	TYR	C-O	6.84	1.32	1.24
1	A	284	LYS	CD-CE	6.83	1.73	1.52
1	D	141	HIS	CA-C	-6.83	1.43	1.52
1	B	56	LEU	C-O	6.82	1.32	1.23
1	B	234	THR	CA-C	-6.82	1.44	1.52
1	D	176	ARG	CA-C	6.82	1.62	1.52
1	D	299	GLU	N-CA	6.80	1.54	1.46
1	A	221	LEU	CG-CD2	6.80	1.75	1.52
1	D	249	ILE	N-CA	-6.79	1.37	1.46
1	C	38	GLN	CB-CG	6.79	1.72	1.52
1	A	53	THR	N-CA	6.79	1.54	1.46
1	C	57	SER	N-CA	-6.79	1.37	1.45
1	A	159	ASP	C-O	6.78	1.32	1.23
1	D	243	LEU	C-O	6.78	1.32	1.23
1	A	285	VAL	CA-CB	6.77	1.64	1.54
1	C	53	THR	CA-CB	-6.77	1.43	1.53
1	C	306	THR	CA-C	6.77	1.61	1.52
1	D	211	GLN	CA-C	-6.76	1.44	1.52
1	C	82	LYS	C-O	-6.75	1.16	1.24
1	A	154	SER	CA-C	6.75	1.61	1.52
1	A	236	MET	CA-C	-6.75	1.44	1.52
1	D	260	ASN	N-CA	6.74	1.54	1.46
1	A	73	LEU	C-O	-6.74	1.15	1.24
1	A	37	ILE	C-O	6.74	1.32	1.24
1	C	221	LEU	CG-CD1	6.74	1.74	1.52
1	C	57	SER	CA-C	6.73	1.60	1.52
1	A	53	THR	C-O	6.72	1.31	1.23
1	B	172	PRO	C-O	6.72	1.32	1.24
1	C	37	ILE	C-O	6.72	1.31	1.24
1	D	237	ILE	N-CA	6.72	1.54	1.46
1	A	191	ALA	CA-CB	-6.71	1.42	1.53
1	D	62	GLN	CA-C	-6.71	1.44	1.52
1	A	251	THR	C-O	6.69	1.31	1.24
1	C	108	ILE	C-O	-6.69	1.16	1.24
1	B	199	CYS	C-O	6.69	1.32	1.23
1	A	63	ALA	C-O	6.68	1.32	1.23
1	A	193	PRO	CA-C	-6.68	1.48	1.51
1	B	183	ASN	CG-OD1	6.67	1.36	1.23
1	B	204	VAL	CA-C	-6.67	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ILE	CA-CB	6.66	1.63	1.54
1	B	255	ALA	N-CA	-6.65	1.37	1.46
1	B	216	SER	N-CA	-6.64	1.38	1.46
1	D	281	ILE	CA-CB	6.63	1.62	1.54
1	A	117	PHE	CA-C	-6.62	1.44	1.52
1	B	174	ASP	N-CA	-6.62	1.37	1.46
1	A	78	ARG	N-CA	6.61	1.54	1.46
1	D	71	PHE	N-CA	-6.60	1.38	1.46
1	A	91	PHE	N-CA	6.60	1.54	1.46
1	C	262	ILE	CA-CB	-6.59	1.46	1.54
1	B	161	LEU	C-O	6.59	1.31	1.24
1	C	201	PHE	C-O	6.59	1.32	1.23
1	D	235	TYR	CZ-OH	6.59	1.51	1.38
1	A	79	VAL	CB-CG1	-6.59	1.30	1.52
1	C	215	ARG	C-O	6.59	1.32	1.24
1	D	164	VAL	CA-C	-6.58	1.44	1.52
1	B	256	HIS	CA-C	-6.58	1.44	1.52
1	C	240	ILE	CA-CB	6.58	1.65	1.54
1	B	95	SER	CA-C	-6.57	1.44	1.52
1	C	299	GLU	CG-CD	6.57	1.68	1.52
1	A	286	GLU	N-CA	6.56	1.52	1.46
1	D	41	LEU	CA-C	-6.55	1.44	1.52
1	D	192	LEU	CG-CD2	6.55	1.74	1.52
1	D	199	CYS	N-CA	6.55	1.54	1.46
1	D	53	THR	CA-CB	6.55	1.64	1.53
1	D	160	GLN	CA-CB	-6.54	1.43	1.53
1	A	262	ILE	CA-C	-6.53	1.44	1.52
1	B	58	VAL	CA-CB	6.53	1.64	1.54
1	C	280	ARG	CD-NE	6.52	1.55	1.46
1	A	286	GLU	CG-CD	6.52	1.68	1.52
1	B	55	THR	CA-C	-6.52	1.44	1.52
1	C	128	GLU	CA-C	6.52	1.60	1.52
1	A	204	VAL	C-O	6.51	1.31	1.24
1	B	90	TRP	CA-CB	-6.51	1.43	1.53
1	A	250	HIS	CA-CB	-6.49	1.44	1.53
1	B	28	HIS	CA-C	6.49	1.61	1.53
1	C	26	PRO	N-CA	6.48	1.56	1.47
1	A	187	LEU	CA-C	-6.48	1.44	1.52
1	A	294	GLU	CD-OE1	6.48	1.37	1.25
1	C	93	LYS	N-CA	6.48	1.54	1.46
1	D	44	GLY	N-CA	6.47	1.52	1.45
1	A	225	PHE	CE2-CZ	6.47	1.58	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	26	PRO	CB-CG	6.47	1.81	1.49
1	B	230	TYR	CZ-OH	6.46	1.51	1.38
1	D	59	PHE	CA-CB	-6.46	1.43	1.53
1	B	140	ARG	C-O	-6.45	1.15	1.24
1	D	221	LEU	N-CA	6.45	1.54	1.46
1	A	185	ARG	CD-NE	-6.44	1.37	1.46
1	C	283	ARG	CA-C	6.44	1.61	1.52
1	D	38	GLN	CD-OE1	6.43	1.35	1.23
1	D	224	PRO	CA-CB	-6.42	1.44	1.53
1	A	30	GLU	CA-CB	-6.40	1.42	1.53
1	C	97	ASN	CA-CB	-6.39	1.44	1.53
1	A	248	PHE	C-O	-6.39	1.16	1.24
1	C	277	PRO	N-CA	6.39	1.55	1.47
1	A	124	SER	N-CA	6.38	1.54	1.46
1	C	226	ASN	CA-CB	-6.38	1.43	1.53
1	B	192	LEU	CG-CD2	6.38	1.73	1.52
1	C	244	LYS	CE-NZ	6.37	1.68	1.49
1	C	236	MET	CA-CB	-6.36	1.43	1.53
1	D	270	GLN	N-CA	6.36	1.54	1.46
1	D	31	LEU	CA-C	6.36	1.61	1.52
1	D	204	VAL	CB-CG2	-6.36	1.31	1.52
1	C	165	ILE	CA-CB	-6.35	1.46	1.54
1	D	151	SER	CA-C	6.35	1.61	1.52
1	D	114	SER	N-CA	6.35	1.53	1.45
1	A	110	ASP	CA-C	-6.35	1.44	1.52
1	A	171	ASN	N-CA	6.33	1.55	1.46
1	C	163	ARG	CA-C	-6.33	1.44	1.52
1	D	266	LYS	N-CA	6.33	1.54	1.46
1	A	240	ILE	N-CA	-6.33	1.38	1.46
1	B	88	LEU	CA-C	6.32	1.60	1.52
1	D	244	LYS	CA-C	6.32	1.60	1.52
1	A	70	GLU	C-N	-6.31	1.20	1.33
1	A	179	MET	CA-CB	-6.30	1.44	1.53
1	B	92	ILE	CG1-CD1	-6.30	1.27	1.51
1	A	78	ARG	CD-NE	6.29	1.55	1.46
1	C	168	ILE	CA-CB	-6.29	1.45	1.54
1	C	33	TYR	CA-CB	-6.29	1.42	1.53
1	D	164	VAL	C-O	-6.29	1.16	1.24
1	D	204	VAL	CA-C	-6.29	1.44	1.52
1	C	42	ARG	CG-CD	6.28	1.71	1.52
1	A	48	ASP	CG-OD1	6.28	1.37	1.25
1	D	98	ALA	CA-CB	-6.28	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	LYS	C-O	6.27	1.31	1.24
1	A	262	ILE	CG1-CD1	-6.26	1.27	1.51
1	B	40	ILE	CA-CB	-6.26	1.47	1.54
1	A	171	ASN	C-N	-6.25	1.27	1.34
1	D	227	ILE	C-O	6.25	1.31	1.24
1	A	286	GLU	CB-CG	6.25	1.71	1.52
1	B	79	VAL	C-O	6.24	1.32	1.24
1	D	207	GLU	CD-OE2	6.24	1.37	1.25
1	C	177	ILE	C-O	6.24	1.31	1.24
1	C	147	ARG	CA-C	6.23	1.57	1.52
1	A	214	GLN	CA-C	-6.22	1.45	1.52
1	D	290	ASP	N-CA	6.22	1.53	1.46
1	C	34	LEU	CG-CD1	6.22	1.73	1.52
1	C	36	GLN	CA-CB	-6.21	1.43	1.53
1	C	47	LYS	C-O	6.21	1.31	1.23
1	C	171	ASN	CA-C	-6.20	1.45	1.52
1	D	39	HIS	CA-CB	-6.20	1.43	1.53
1	A	174	ASP	CA-CB	-6.20	1.43	1.53
1	D	207	GLU	N-CA	-6.20	1.38	1.46
1	D	106	VAL	CA-CB	6.19	1.60	1.53
1	A	175	ARG	CZ-NH1	6.19	1.41	1.32
1	C	71	PHE	N-CA	-6.19	1.38	1.46
1	D	108	ILE	N-CA	6.19	1.54	1.46
1	A	236	MET	N-CA	-6.18	1.38	1.46
1	D	43	CYS	CB-SG	6.18	2.01	1.81
1	A	42	ARG	C-O	-6.18	1.15	1.24
1	A	171	ASN	CA-C	-6.17	1.45	1.52
1	D	278	LYS	C-O	-6.17	1.15	1.23
1	C	182	TRP	CA-CB	-6.16	1.45	1.53
1	D	267	ILE	CA-CB	6.16	1.62	1.54
1	D	245	PRO	CB-CG	6.15	1.80	1.49
1	A	228	ALA	C-O	-6.15	1.16	1.24
1	A	183	ASN	CA-CB	-6.14	1.44	1.53
1	A	144	ALA	CA-C	-6.14	1.45	1.52
1	D	223	VAL	N-CA	-6.13	1.39	1.46
1	A	26	PRO	CB-CG	6.13	1.80	1.49
1	C	249	ILE	N-CA	-6.12	1.38	1.46
1	A	166	ASP	CA-CB	-6.11	1.44	1.53
1	C	262	ILE	N-CA	-6.11	1.39	1.46
1	C	280	ARG	NE-CZ	6.11	1.39	1.33
1	A	131	LEU	CG-CD2	-6.10	1.32	1.52
1	D	172	PRO	C-O	-6.09	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	124	SER	C-N	-6.09	1.25	1.33
1	D	180	CYS	C-O	-6.09	1.16	1.24
1	B	250	HIS	C-O	6.09	1.31	1.24
1	D	211	GLN	CA-CB	-6.08	1.44	1.53
1	B	168	ILE	CA-CB	-6.08	1.47	1.54
1	C	166	ASP	C-O	-6.07	1.17	1.24
1	C	276	PHE	CA-C	6.06	1.59	1.53
1	A	217	GLY	N-CA	-6.06	1.36	1.45
1	C	26	PRO	CA-C	6.06	1.65	1.52
1	C	96	THR	C-O	6.06	1.30	1.23
1	D	273	PRO	N-CA	6.05	1.54	1.47
1	B	221	LEU	N-CA	-6.04	1.38	1.46
1	C	216	SER	CA-C	-6.04	1.45	1.52
1	B	169	LYS	CA-C	-6.04	1.45	1.52
1	C	199	CYS	N-CA	6.04	1.53	1.45
1	A	175	ARG	CB-CG	6.04	1.70	1.52
1	B	201	PHE	CA-CB	-6.04	1.44	1.53
1	A	221	LEU	C-O	6.03	1.32	1.23
1	A	247	ASP	CA-CB	-6.03	1.44	1.53
1	C	153	TYR	CB-CG	6.03	1.65	1.51
1	C	267	ILE	CA-CB	6.03	1.61	1.54
1	A	108	ILE	CA-C	-6.02	1.45	1.53
1	A	98	ALA	CA-CB	-6.01	1.43	1.53
1	D	258	TYR	CA-C	-6.01	1.44	1.53
1	D	100	GLU	CA-C	6.01	1.60	1.52
1	D	244	LYS	C-O	6.00	1.31	1.24
1	C	49	ASP	C-O	-6.00	1.16	1.23
1	B	287	LYS	CB-CG	6.00	1.70	1.52
1	C	73	LEU	C-O	6.00	1.30	1.23
1	D	256	HIS	CB-CG	-5.99	1.41	1.50
1	D	296	PHE	CA-CB	-5.99	1.44	1.53
1	A	254	ASP	C-O	-5.99	1.15	1.23
1	A	200	GLN	CB-CG	5.98	1.70	1.52
1	A	256	HIS	C-O	-5.98	1.16	1.23
1	C	84	VAL	CA-C	-5.98	1.45	1.52
1	B	210	CYS	CA-CB	-5.98	1.43	1.53
1	B	151	SER	CA-C	5.97	1.60	1.52
1	D	96	THR	CA-C	-5.97	1.45	1.53
1	C	249	ILE	CA-CB	-5.96	1.46	1.54
1	A	162	GLN	CB-CG	5.96	1.70	1.52
1	C	145	GLU	CA-C	5.95	1.60	1.52
1	C	84	VAL	CA-CB	-5.95	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	275	PRO	CA-C	5.95	1.60	1.52
1	A	209	SER	C-O	-5.94	1.16	1.23
1	A	78	ARG	CZ-NH1	5.94	1.41	1.32
1	B	177	ILE	CB-CG2	5.94	1.72	1.52
1	C	124	SER	CA-C	-5.93	1.44	1.52
1	D	227	ILE	CA-C	5.93	1.60	1.52
1	D	92	ILE	CA-CB	-5.93	1.48	1.54
1	C	187	LEU	CA-C	-5.93	1.45	1.52
1	B	177	ILE	CB-CG1	-5.92	1.41	1.53
1	A	30	GLU	C-O	5.92	1.31	1.24
1	C	162	GLN	N-CA	-5.91	1.39	1.46
1	A	86	GLU	C-O	5.91	1.31	1.24
1	D	237	ILE	CA-C	5.91	1.60	1.52
1	A	193	PRO	C-N	-5.91	1.26	1.33
1	A	168	ILE	CB-CG1	5.90	1.65	1.53
1	B	175	ARG	CZ-NH1	5.90	1.41	1.32
1	C	260	ASN	C-O	-5.89	1.16	1.24
1	B	166	ASP	CG-OD1	5.89	1.36	1.25
1	D	192	LEU	CB-CG	5.89	1.65	1.53
1	C	301	TYR	N-CA	5.88	1.53	1.46
1	C	41	LEU	CG-CD2	-5.88	1.33	1.52
1	A	285	VAL	CA-C	5.87	1.60	1.52
1	D	40	ILE	C-O	5.87	1.31	1.24
1	D	90	TRP	CB-CG	-5.87	1.32	1.50
1	B	249	ILE	N-CA	-5.87	1.39	1.46
1	D	151	SER	CA-CB	5.87	1.63	1.53
1	D	259	LEU	N-CA	-5.86	1.39	1.46
1	A	292	LYS	CB-CG	5.85	1.70	1.52
1	C	308	LYS	CA-C	5.85	1.65	1.52
1	A	254	ASP	CB-CG	5.85	1.66	1.52
1	C	178	ILE	CG1-CD1	-5.85	1.28	1.51
1	D	249	ILE	CA-CB	-5.85	1.46	1.54
1	D	307	ILE	N-CA	5.85	1.53	1.46
1	A	293	ALA	C-O	-5.84	1.16	1.24
1	B	146	TYR	CA-C	-5.84	1.45	1.52
1	C	254	ASP	N-CA	-5.84	1.39	1.46
1	B	238	ALA	CA-CB	5.83	1.62	1.53
1	A	244	LYS	CE-NZ	5.83	1.66	1.49
1	B	243	LEU	CG-CD2	5.83	1.71	1.52
1	A	174	ASP	CA-C	5.83	1.60	1.52
1	C	211	GLN	C-O	-5.83	1.17	1.23
1	D	259	LEU	CG-CD1	5.81	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	GLU	CA-CB	-5.81	1.43	1.53
1	B	178	ILE	CB-CG2	-5.81	1.33	1.52
1	C	127	GLU	CA-C	-5.80	1.45	1.52
1	B	48	ASP	CG-OD1	5.80	1.36	1.25
1	A	279	LEU	CG-CD2	5.79	1.71	1.52
1	A	78	ARG	C-O	-5.78	1.17	1.24
1	B	145	GLU	CD-OE1	5.77	1.36	1.25
1	D	153	TYR	CA-C	-5.77	1.44	1.52
1	A	279	LEU	CA-CB	-5.77	1.45	1.53
1	B	118	LEU	N-CA	5.76	1.53	1.46
1	C	254	ASP	CA-CB	-5.76	1.45	1.52
1	C	128	GLU	N-CA	5.76	1.53	1.46
1	B	149	MET	CA-C	5.75	1.60	1.52
1	C	31	LEU	CA-CB	-5.75	1.44	1.53
1	A	255	ALA	CA-C	5.75	1.59	1.52
1	A	304	HIS	N-CA	5.75	1.54	1.46
1	B	247	ASP	C-O	5.75	1.30	1.23
1	D	234	THR	CA-C	5.73	1.60	1.52
1	A	197	ALA	N-CA	-5.73	1.39	1.46
1	A	63	ALA	N-CA	5.72	1.52	1.45
1	D	255	ALA	CA-C	5.71	1.60	1.52
1	B	35	GLY	C-O	-5.71	1.16	1.23
1	B	287	LYS	CA-C	5.71	1.60	1.52
1	C	106	VAL	CA-CB	5.71	1.59	1.53
1	C	37	ILE	CG1-CD1	-5.71	1.29	1.51
1	D	201	PHE	CE1-CZ	-5.71	1.21	1.38
1	D	272	GLU	N-CA	5.71	1.54	1.46
1	B	216	SER	C-O	5.71	1.31	1.23
1	B	304	HIS	CA-C	5.71	1.60	1.52
1	D	96	THR	N-CA	-5.70	1.39	1.46
1	B	226	ASN	CA-CB	-5.68	1.44	1.53
1	D	31	LEU	CG-CD2	-5.68	1.33	1.52
1	B	89	LEU	C-O	5.68	1.31	1.24
1	D	52	GLY	C-N	5.67	1.41	1.33
1	D	179	MET	CB-CG	-5.65	1.35	1.52
1	B	42	ARG	CG-CD	5.65	1.69	1.52
1	C	176	ARG	CA-C	-5.65	1.45	1.52
1	C	65	TYR	CB-CG	-5.64	1.39	1.51
1	B	73	LEU	N-CA	5.64	1.52	1.46
1	C	247	ASP	C-O	-5.64	1.16	1.23
1	B	287	LYS	CG-CD	5.64	1.69	1.52
1	D	267	ILE	CA-C	-5.63	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	135	TYR	CA-C	5.63	1.60	1.52
1	C	205	ASN	CA-CB	-5.62	1.45	1.53
1	A	42	ARG	NE-CZ	5.61	1.39	1.33
1	A	181	ALA	CA-CB	-5.61	1.44	1.53
1	B	171	ASN	CG-ND2	5.61	1.45	1.33
1	A	108	ILE	CG1-CD1	5.61	1.73	1.51
1	B	221	LEU	CG-CD1	5.61	1.71	1.52
1	B	105	GLY	CA-C	5.61	1.59	1.51
1	D	216	SER	CA-C	-5.60	1.45	1.52
1	D	141	HIS	N-CA	-5.60	1.39	1.46
1	D	263	GLU	CA-C	-5.60	1.46	1.52
1	C	54	GLY	C-O	-5.60	1.15	1.23
1	C	251	THR	CB-OG1	-5.59	1.34	1.43
1	B	202	TYR	CD1-CE1	5.58	1.55	1.38
1	B	161	LEU	CA-C	-5.58	1.46	1.52
1	B	62	GLN	CA-CB	-5.58	1.44	1.53
1	C	50	ARG	CD-NE	5.58	1.54	1.46
1	C	244	LYS	C-N	5.58	1.40	1.33
1	B	244	LYS	CB-CG	5.58	1.69	1.52
1	A	200	GLN	C-N	-5.58	1.25	1.33
1	C	263	GLU	CA-C	-5.57	1.46	1.52
1	D	286	GLU	CA-CB	5.57	1.62	1.53
1	B	266	LYS	CD-CE	5.57	1.69	1.52
1	C	280	ARG	C-O	5.57	1.30	1.23
1	D	248	PHE	CA-CB	-5.57	1.44	1.53
1	C	247	ASP	CB-CG	-5.57	1.38	1.52
1	D	223	VAL	C-O	5.56	1.31	1.24
1	D	160	GLN	CA-C	-5.56	1.45	1.52
1	A	263	GLU	CG-CD	5.56	1.66	1.52
1	B	183	ASN	N-CA	-5.56	1.38	1.46
1	B	248	PHE	CA-CB	-5.56	1.45	1.53
1	B	137	PHE	CA-CB	5.55	1.62	1.53
1	D	192	LEU	CG-CD1	5.55	1.70	1.52
1	D	144	ALA	N-CA	5.55	1.52	1.46
1	B	298	ILE	CA-CB	-5.55	1.46	1.54
1	C	289	ASP	C-O	5.55	1.31	1.24
1	B	204	VAL	C-O	5.54	1.30	1.23
1	A	234	THR	C-O	-5.54	1.17	1.24
1	B	192	LEU	CG-CD1	5.53	1.70	1.52
1	C	35	GLY	N-CA	-5.53	1.37	1.45
1	D	245	PRO	CG-CD	-5.53	1.31	1.50
1	A	116	ASP	CB-CG	5.53	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	LEU	CG-CD2	5.53	1.70	1.52
1	D	181	ALA	N-CA	5.52	1.52	1.46
1	B	139	TRP	CA-CB	-5.51	1.44	1.53
1	B	32	GLN	CA-C	5.51	1.60	1.52
1	B	263	GLU	CG-CD	5.51	1.65	1.52
1	D	33	TYR	N-CA	-5.51	1.39	1.46
1	C	165	ILE	CB-CG2	-5.50	1.34	1.52
1	B	227	ILE	C-O	5.49	1.30	1.24
1	A	116	ASP	CA-C	5.48	1.60	1.52
1	B	213	TYR	CA-CB	-5.48	1.46	1.53
1	C	303	PRO	CA-C	-5.48	1.46	1.52
1	D	128	GLU	CA-C	5.48	1.60	1.52
1	B	255	ALA	C-O	5.48	1.30	1.24
1	B	60	GLY	C-O	-5.47	1.16	1.23
1	A	183	ASN	N-CA	-5.47	1.40	1.46
1	C	177	ILE	CB-CG2	-5.47	1.34	1.52
1	C	221	LEU	CG-CD2	5.46	1.70	1.52
1	C	282	LEU	CA-C	5.46	1.59	1.52
1	B	189	LEU	N-CA	-5.46	1.39	1.46
1	A	183	ASN	CA-C	5.45	1.59	1.52
1	C	62	GLN	C-O	-5.45	1.17	1.23
1	D	201	PHE	CG-CD2	-5.45	1.27	1.38
1	A	211	GLN	N-CA	-5.44	1.39	1.46
1	D	225	PHE	C-O	5.44	1.30	1.24
1	B	104	LYS	CA-CB	5.44	1.61	1.53
1	D	178	ILE	CA-CB	-5.44	1.47	1.54
1	D	108	ILE	CA-C	5.43	1.59	1.52
1	A	236	MET	SD-CE	5.43	1.93	1.79
1	B	185	ARG	N-CA	5.43	1.52	1.46
1	A	243	LEU	CA-CB	-5.42	1.44	1.53
1	B	108	ILE	CG1-CD1	5.42	1.72	1.51
1	B	191	ALA	CA-C	-5.41	1.45	1.52
1	D	283	ARG	N-CA	-5.41	1.39	1.45
1	D	37	ILE	C-O	5.41	1.30	1.24
1	A	89	LEU	N-CA	-5.40	1.39	1.46
1	A	204	VAL	C-N	5.40	1.41	1.33
1	C	229	SER	N-CA	-5.40	1.39	1.46
1	C	69	ASP	CA-CB	-5.39	1.45	1.53
1	C	176	ARG	C-O	-5.39	1.15	1.23
1	C	291	PHE	CD2-CE2	5.39	1.54	1.38
1	D	187	LEU	N-CA	5.38	1.53	1.46
1	C	235	TYR	CB-CG	5.38	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	HIS	N-CA	-5.38	1.40	1.46
1	C	285	VAL	N-CA	5.38	1.53	1.46
1	C	166	ASP	CG-OD1	5.38	1.35	1.25
1	B	225	PHE	CA-C	5.38	1.59	1.52
1	B	188	PRO	CG-CD	5.37	1.69	1.50
1	C	278	LYS	N-CA	5.37	1.52	1.46
1	A	228	ALA	N-CA	5.37	1.52	1.46
1	A	291	PHE	CA-C	-5.36	1.45	1.52
1	D	39	HIS	C-O	-5.36	1.18	1.24
1	A	201	PHE	CB-CG	-5.36	1.38	1.50
1	C	69	ASP	CA-C	5.36	1.61	1.52
1	D	134	VAL	N-CA	5.36	1.53	1.46
1	A	47	LYS	C-O	5.35	1.30	1.23
1	A	215	ARG	CG-CD	-5.35	1.36	1.52
1	B	105	GLY	N-CA	5.35	1.53	1.45
1	A	191	ALA	C-N	5.34	1.39	1.33
1	A	179	MET	C-N	-5.34	1.26	1.33
1	A	272	GLU	N-CA	5.34	1.53	1.46
1	D	205	ASN	CG-OD1	5.34	1.33	1.23
1	A	227	ILE	C-O	-5.33	1.18	1.24
1	A	42	ARG	CZ-NH1	5.33	1.40	1.32
1	D	230	TYR	CA-C	-5.33	1.45	1.52
1	B	59	PHE	CD2-CE2	5.32	1.54	1.38
1	B	96	THR	CA-CB	5.32	1.61	1.54
1	B	138	GLN	N-CA	-5.32	1.39	1.46
1	D	202	TYR	CA-CB	-5.31	1.44	1.53
1	C	270	GLN	CA-CB	5.31	1.62	1.53
1	A	49	ASP	C-O	5.30	1.29	1.23
1	A	26	PRO	CA-C	5.30	1.64	1.52
1	D	161	LEU	N-CA	-5.30	1.39	1.46
1	C	42	ARG	N-CA	5.29	1.52	1.46
1	A	219	MET	C-O	-5.29	1.17	1.24
1	A	228	ALA	CA-CB	-5.29	1.45	1.53
1	C	211	GLN	CA-C	-5.29	1.46	1.52
1	C	256	HIS	C-O	-5.29	1.17	1.23
1	C	204	VAL	C-O	5.28	1.30	1.24
1	C	247	ASP	CA-CB	-5.28	1.43	1.53
1	C	257	ILE	CB-CG1	-5.28	1.42	1.53
1	C	288	ILE	CA-CB	5.28	1.61	1.54
1	D	228	ALA	CA-C	5.28	1.59	1.52
1	A	177	ILE	CB-CG1	-5.28	1.42	1.53
1	C	245	PRO	C-O	5.28	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	LYS	CD-CE	5.27	1.68	1.52
1	D	108	ILE	CG1-CD1	5.27	1.72	1.51
1	A	68	ARG	CA-CB	-5.26	1.44	1.53
1	C	135	TYR	CD1-CE1	5.26	1.54	1.38
1	C	219	MET	C-O	-5.26	1.17	1.24
1	C	166	ASP	CG-OD2	5.26	1.35	1.25
1	C	221	LEU	CA-C	-5.26	1.46	1.53
1	C	255	ALA	N-CA	-5.25	1.39	1.46
1	A	185	ARG	CB-CG	5.25	1.68	1.52
1	A	236	MET	CA-CB	-5.25	1.45	1.53
1	D	234	THR	C-N	5.25	1.40	1.33
1	D	251	THR	N-CA	-5.24	1.39	1.45
1	D	57	SER	CA-C	-5.24	1.45	1.52
1	A	307	ILE	C-N	5.24	1.40	1.33
1	A	123	PHE	CA-CB	5.23	1.60	1.52
1	C	114	SER	CA-CB	-5.23	1.44	1.53
1	D	192	LEU	N-CA	5.23	1.53	1.46
1	C	116	ASP	N-CA	5.23	1.52	1.46
1	C	49	ASP	N-CA	-5.22	1.39	1.45
1	C	65	TYR	C-O	5.22	1.29	1.24
1	D	195	CYS	C-O	5.22	1.30	1.24
1	A	242	GLY	CA-C	5.21	1.56	1.51
1	D	77	LYS	CB-CG	5.21	1.68	1.52
1	A	164	VAL	C-O	5.20	1.29	1.24
1	B	190	MET	C-O	5.20	1.30	1.23
1	D	196	HIS	C-O	-5.20	1.16	1.23
1	C	120	SER	N-CA	5.20	1.52	1.46
1	A	229	SER	N-CA	-5.19	1.40	1.46
1	A	131	LEU	CG-CD1	-5.19	1.35	1.52
1	C	201	PHE	C-N	-5.19	1.27	1.33
1	D	307	ILE	CA-C	5.19	1.59	1.52
1	A	164	VAL	N-CA	-5.18	1.40	1.46
1	C	304	HIS	CA-C	-5.18	1.46	1.52
1	D	254	ASP	C-O	-5.18	1.16	1.23
1	B	38	GLN	C-O	-5.18	1.17	1.24
1	C	119	ASP	CA-C	5.17	1.60	1.52
1	B	128	GLU	N-CA	5.17	1.52	1.46
1	B	145	GLU	CD-OE2	5.17	1.35	1.25
1	D	146	TYR	C-O	5.16	1.29	1.23
1	B	42	ARG	CD-NE	5.16	1.53	1.46
1	B	266	LYS	CE-NZ	5.16	1.64	1.49
1	D	194	PRO	CA-CB	-5.16	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLN	CD-NE2	5.15	1.44	1.33
1	C	77	LYS	CG-CD	5.15	1.67	1.52
1	A	207	GLU	CA-C	-5.14	1.46	1.52
1	C	111	ALA	CA-C	5.14	1.59	1.52
1	A	259	LEU	CA-CB	-5.14	1.44	1.53
1	B	263	GLU	N-CA	5.14	1.51	1.46
1	A	276	PHE	CA-C	-5.13	1.48	1.53
1	C	308	LYS	CD-CE	5.13	1.67	1.52
1	C	266	LYS	N-CA	5.13	1.52	1.46
1	D	169	LYS	CA-C	-5.13	1.46	1.52
1	A	137	PHE	CD2-CE2	5.12	1.54	1.38
1	C	231	ALA	CA-CB	-5.12	1.45	1.53
1	A	96	THR	CA-CB	5.12	1.61	1.53
1	B	176	ARG	CA-C	-5.12	1.48	1.52
1	D	211	GLN	CG-CD	5.12	1.64	1.52
1	A	160	GLN	N-CA	-5.11	1.39	1.46
1	B	260	ASN	CB-CG	5.11	1.64	1.52
1	D	139	TRP	N-CA	-5.11	1.40	1.46
1	B	58	VAL	CB-CG2	-5.11	1.35	1.52
1	C	167	THR	CA-C	-5.11	1.45	1.52
1	D	203	VAL	CA-C	-5.11	1.46	1.52
1	B	193	PRO	N-CA	5.10	1.53	1.46
1	A	308	LYS	N-CA	5.09	1.55	1.46
1	A	37	ILE	CB-CG1	-5.09	1.43	1.53
1	C	42	ARG	NE-CZ	5.08	1.38	1.33
1	A	307	ILE	CG1-CD1	5.08	1.71	1.51
1	B	226	ASN	C-O	5.08	1.30	1.24
1	C	27	PRO	CG-CD	5.07	1.68	1.50
1	A	68	ARG	C-N	-5.07	1.26	1.33
1	A	46	ARG	CZ-NH1	5.06	1.39	1.32
1	C	285	VAL	CB-CG1	5.06	1.69	1.52
1	B	226	ASN	CA-C	-5.05	1.45	1.52
1	D	164	VAL	CA-CB	-5.05	1.47	1.54
1	D	295	ASP	N-CA	5.05	1.53	1.46
1	A	283	ARG	N-CA	-5.04	1.39	1.46
1	A	58	VAL	CA-CB	-5.04	1.46	1.55
1	C	254	ASP	CB-CG	5.04	1.64	1.52
1	D	104	LYS	CE-NZ	5.04	1.64	1.49
1	B	224	PRO	C-O	5.04	1.30	1.24
1	B	174	ASP	CA-C	5.03	1.58	1.52
1	C	242	GLY	CA-C	-5.03	1.46	1.51
1	B	151	SER	CA-CB	5.02	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	268	GLN	CB-CG	-5.02	1.37	1.52
1	D	50	ARG	NE-CZ	5.01	1.38	1.33
1	D	90	TRP	CA-CB	-5.01	1.45	1.53
1	D	167	THR	CA-C	-5.01	1.46	1.52
1	C	82	LYS	CA-C	-5.01	1.46	1.52
1	D	82	LYS	N-CA	-5.01	1.40	1.46
1	D	151	SER	N-CA	5.01	1.52	1.46
1	D	148	ASP	CA-CB	-5.01	1.47	1.53
1	B	218	ASP	CA-C	5.00	1.59	1.52

All (876) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH1	28.98	150.48	121.50
1	A	185	ARG	NE-CZ-NH2	-28.57	93.49	119.20
1	C	123	PHE	O-C-N	23.89	154.36	122.59
1	A	185	ARG	CD-NE-CZ	23.02	156.63	124.40
1	D	281	ILE	N-CA-C	-21.75	76.98	108.53
1	C	171	ASN	CA-C-N	21.61	146.85	119.84
1	C	171	ASN	C-N-CA	21.61	146.85	119.84
1	A	306	THR	N-CA-C	20.84	142.10	108.96
1	A	70	GLU	O-C-N	-20.42	95.03	121.78
1	A	171	ASN	CA-C-N	18.24	138.84	119.87
1	A	171	ASN	C-N-CA	18.24	138.84	119.87
1	A	192	LEU	CA-C-N	16.19	131.48	119.66
1	A	192	LEU	C-N-CA	16.19	131.48	119.66
1	A	68	ARG	O-C-N	15.90	143.73	122.59
1	C	123	PHE	CA-C-N	15.45	151.05	121.54
1	C	123	PHE	C-N-CA	15.45	151.05	121.54
1	A	175	ARG	N-CA-C	-15.03	94.25	112.59
1	C	122	GLY	O-C-N	14.91	142.08	122.70
1	C	106	VAL	CB-CA-C	14.35	125.72	111.23
1	A	176	ARG	N-CA-C	14.24	127.52	110.44
1	C	283	ARG	O-C-N	-13.82	102.79	122.41
1	A	307	ILE	N-CA-C	13.80	129.87	108.89
1	D	235	TYR	N-CA-C	-13.64	96.41	111.28
1	B	114	SER	O-C-N	13.61	139.35	123.29
1	D	274	ARG	CA-C-N	-13.34	103.16	119.84
1	D	274	ARG	C-N-CA	-13.34	103.16	119.84
1	C	70	GLU	N-CA-C	-13.28	88.88	109.85
1	A	227	ILE	N-CA-C	-13.06	98.25	110.53
1	A	298	ILE	CB-CA-C	-12.73	93.03	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	CYS	CA-CB-SG	-12.72	85.14	114.40
1	C	287	LYS	N-CA-C	-12.62	89.95	109.52
1	A	165	ILE	N-CA-C	12.36	123.08	110.23
1	C	69	ASP	N-CA-C	12.29	127.70	112.47
1	D	92	ILE	O-C-N	-12.04	103.13	122.16
1	B	267	ILE	N-CA-C	11.90	121.84	110.30
1	C	108	ILE	CA-C-N	-11.84	103.44	122.26
1	C	108	ILE	C-N-CA	-11.84	103.44	122.26
1	D	175	ARG	NE-CZ-NH2	11.73	129.75	119.20
1	B	71	PHE	CA-C-N	-11.68	105.24	119.84
1	B	71	PHE	C-N-CA	-11.68	105.24	119.84
1	D	296	PHE	N-CA-C	-11.35	89.73	108.34
1	B	170	THR	CB-CA-C	-11.30	92.72	110.81
1	C	108	ILE	N-CA-C	-11.28	96.95	111.05
1	A	182	TRP	O-C-N	11.28	137.48	122.82
1	C	121	LEU	CA-C-N	-11.18	99.49	121.41
1	C	121	LEU	C-N-CA	-11.18	99.49	121.41
1	C	306	THR	N-CA-C	11.17	134.59	110.80
1	A	138	GLN	N-CA-C	-11.12	99.10	112.89
1	C	178	ILE	N-CA-C	11.11	124.89	109.45
1	D	124	SER	N-CA-C	-11.05	99.83	113.97
1	D	193	PRO	CA-C-N	-11.02	108.46	120.14
1	D	193	PRO	C-N-CA	-11.02	108.46	120.14
1	A	26	PRO	CA-C-N	10.94	133.51	119.84
1	A	26	PRO	C-N-CA	10.94	133.51	119.84
1	A	305	PRO	CB-CA-C	10.88	129.51	111.56
1	D	215	ARG	N-CA-C	10.83	124.10	111.11
1	A	202	TYR	CA-C-O	-10.65	109.83	121.33
1	A	200	GLN	N-CA-C	-10.61	93.08	109.52
1	A	175	ARG	CA-CB-CG	10.54	135.18	114.10
1	A	259	LEU	N-CA-C	10.51	124.01	111.82
1	A	121	LEU	N-CA-C	-10.45	100.53	113.38
1	A	202	TYR	CA-C-N	-10.43	105.88	122.25
1	A	202	TYR	C-N-CA	-10.43	105.88	122.25
1	A	203	VAL	CB-CA-C	-10.38	92.09	111.30
1	C	244	LYS	N-CA-C	10.38	122.69	109.72
1	A	199	CYS	CA-C-N	-10.37	106.31	122.59
1	A	199	CYS	C-N-CA	-10.37	106.31	122.59
1	B	92	ILE	N-CA-C	-10.34	100.28	110.72
1	A	76	THR	N-CA-C	-10.32	100.71	113.20
1	B	40	ILE	CB-CA-C	-10.24	98.59	111.70
1	A	175	ARG	CB-CA-C	10.21	127.46	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	TYR	N-CA-C	10.18	126.27	108.56
1	C	64	ARG	NE-CZ-NH2	10.17	128.35	119.20
1	A	89	LEU	N-CA-C	-10.16	100.21	111.28
1	A	79	VAL	CB-CA-C	-10.15	100.42	111.59
1	D	272	GLU	CA-C-N	-10.15	109.60	119.85
1	D	272	GLU	C-N-CA	-10.15	109.60	119.85
1	C	166	ASP	N-CA-C	10.12	121.90	111.07
1	D	219	MET	CA-C-O	10.06	131.48	119.61
1	B	145	GLU	CA-C-N	-10.04	107.14	121.50
1	B	145	GLU	C-N-CA	-10.04	107.14	121.50
1	D	94	GLY	O-C-N	10.01	135.72	122.70
1	A	304	HIS	CA-C-N	-9.98	107.37	119.84
1	A	304	HIS	C-N-CA	-9.98	107.37	119.84
1	C	123	PHE	CA-CB-CG	9.97	123.77	113.80
1	C	97	ASN	N-CA-C	9.96	124.76	108.52
1	C	39	HIS	N-CA-C	-9.96	99.44	111.69
1	C	198	LEU	N-CA-C	9.94	123.11	108.60
1	C	283	ARG	CA-C-N	-9.93	104.65	122.12
1	C	283	ARG	C-N-CA	-9.93	104.65	122.12
1	C	96	THR	N-CA-C	-9.83	99.61	114.16
1	B	169	LYS	N-CA-C	-9.81	100.14	111.03
1	B	225	PHE	N-CA-C	9.77	122.84	111.11
1	C	110	ASP	O-C-N	-9.68	111.97	122.03
1	C	114	SER	O-C-N	9.59	134.84	122.95
1	A	187	LEU	CA-C-N	-9.46	108.01	119.84
1	A	187	LEU	C-N-CA	-9.46	108.01	119.84
1	D	92	ILE	CB-CA-C	-9.39	100.75	111.55
1	B	82	LYS	N-CA-C	-9.37	100.94	111.71
1	D	40	ILE	N-CA-C	-9.34	99.37	111.05
1	D	117	PHE	N-CA-C	-9.27	101.15	111.07
1	D	179	MET	CA-C-N	-9.27	110.45	122.77
1	D	179	MET	C-N-CA	-9.27	110.45	122.77
1	C	178	ILE	CG1-CB-CG2	-9.26	82.91	110.70
1	C	271	ARG	N-CA-C	-9.16	98.44	110.53
1	A	79	VAL	N-CA-CB	-9.14	96.20	111.38
1	D	39	HIS	CA-C-O	-9.07	111.19	120.90
1	C	304	HIS	CA-C-N	-9.07	108.51	119.84
1	C	304	HIS	C-N-CA	-9.07	108.51	119.84
1	A	219	MET	CB-CA-C	-9.06	93.88	110.63
1	A	218	ASP	CB-CA-C	-9.05	97.36	111.83
1	A	269	LEU	N-CA-C	-9.03	102.45	113.19
1	B	168	ILE	N-CA-C	9.01	119.00	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	THR	N-CA-C	-8.99	101.85	113.17
1	C	84	VAL	CB-CA-C	-8.98	100.25	112.02
1	D	51	THR	N-CA-C	-8.98	100.98	113.37
1	A	68	ARG	CA-C-N	8.96	135.09	122.36
1	A	68	ARG	C-N-CA	8.96	135.09	122.36
1	C	76	THR	N-CA-C	-8.94	102.51	113.41
1	B	118	LEU	N-CA-C	8.94	120.79	111.14
1	A	244	LYS	N-CA-C	8.88	121.27	110.07
1	C	113	GLY	O-C-N	8.86	133.45	122.29
1	A	91	PHE	CB-CA-C	-8.85	94.51	110.70
1	C	306	THR	CB-CA-C	-8.81	92.89	110.42
1	B	244	LYS	N-CA-C	8.80	123.60	110.32
1	A	200	GLN	CA-C-O	-8.78	111.17	121.44
1	A	169	LYS	N-CA-C	8.77	123.24	112.54
1	D	111	ALA	N-CA-C	-8.75	101.29	112.93
1	A	63	ALA	CA-C-N	8.75	135.53	123.11
1	A	63	ALA	C-N-CA	8.75	135.53	123.11
1	D	291	PHE	CA-C-N	-8.74	109.15	122.09
1	D	291	PHE	C-N-CA	-8.74	109.15	122.09
1	D	222	GLY	N-CA-C	-8.70	92.56	113.18
1	A	203	VAL	O-C-N	-8.65	113.06	123.09
1	A	40	ILE	N-CA-C	-8.64	102.00	110.72
1	B	282	LEU	N-CA-C	8.64	123.82	113.28
1	A	261	HIS	N-CA-C	8.62	123.22	112.87
1	C	75	THR	N-CA-C	8.59	123.57	112.41
1	B	41	LEU	CA-C-N	-8.52	109.12	122.49
1	B	41	LEU	C-N-CA	-8.52	109.12	122.49
1	B	301	TYR	N-CA-CB	-8.48	99.12	110.57
1	C	78	ARG	N-CA-C	8.47	123.01	110.30
1	B	128	GLU	N-CA-C	8.46	122.70	109.07
1	D	257	ILE	CB-CA-C	-8.42	96.14	110.71
1	A	42	ARG	N-CA-C	-8.42	103.01	113.28
1	D	37	ILE	CB-CA-C	-8.41	101.02	112.04
1	D	53	THR	N-CA-CB	8.41	122.56	109.69
1	B	206	SER	CA-C-N	-8.38	108.73	122.81
1	B	206	SER	C-N-CA	-8.38	108.73	122.81
1	A	288	ILE	CB-CA-C	-8.34	98.76	112.26
1	D	56	LEU	O-C-N	-8.33	113.52	123.10
1	A	203	VAL	CA-C-O	8.31	129.80	120.90
1	C	173	ASP	N-CA-C	-8.29	102.95	113.72
1	B	206	SER	CA-CB-OG	-8.28	94.54	111.10
1	A	103	SER	N-CA-C	-8.27	102.29	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	ILE	N-CA-C	8.27	119.76	108.84
1	D	93	LYS	O-C-N	8.23	131.58	122.20
1	B	163	ARG	CB-CG-CD	-8.20	92.43	111.30
1	A	197	ALA	N-CA-C	-8.19	102.31	111.82
1	D	131	LEU	N-CA-C	8.19	123.44	112.30
1	B	58	VAL	CA-C-O	8.15	129.80	120.67
1	C	75	THR	CB-CA-C	-8.15	97.82	111.02
1	D	192	LEU	CA-CB-CG	8.10	144.66	116.30
1	D	187	LEU	CA-C-N	-8.05	109.78	119.84
1	D	187	LEU	C-N-CA	-8.05	109.78	119.84
1	A	173	ASP	CA-C-N	-8.03	109.57	121.05
1	A	173	ASP	C-N-CA	-8.03	109.57	121.05
1	C	185	ARG	CA-C-N	-8.01	108.79	122.56
1	C	185	ARG	C-N-CA	-8.01	108.79	122.56
1	B	46	ARG	N-CA-C	-8.00	96.19	109.46
1	B	151	SER	N-CA-C	7.99	121.27	108.41
1	C	307	ILE	N-CA-C	7.97	125.93	109.34
1	B	50	ARG	N-CA-C	-7.97	102.82	112.54
1	C	256	HIS	N-CA-C	7.96	120.96	108.79
1	B	204	VAL	N-CA-C	-7.95	97.85	108.35
1	C	226	ASN	N-CA-C	7.95	120.65	111.11
1	D	207	GLU	CA-C-N	-7.89	111.84	122.72
1	D	207	GLU	C-N-CA	-7.89	111.84	122.72
1	C	241	THR	N-CA-C	-7.88	101.82	112.94
1	C	97	ASN	CB-CA-C	-7.87	97.28	110.19
1	B	50	ARG	NE-CZ-NH1	7.87	129.37	121.50
1	C	260	ASN	N-CA-C	-7.87	103.41	113.16
1	B	83	GLY	N-CA-C	-7.86	102.98	112.49
1	D	250	HIS	CA-C-N	-7.85	110.48	122.81
1	D	250	HIS	C-N-CA	-7.85	110.48	122.81
1	D	276	PHE	CB-CA-C	-7.84	97.81	108.87
1	D	306	THR	N-CA-C	7.84	127.51	110.80
1	C	58	VAL	CG1-CB-CG2	-7.84	93.56	110.80
1	C	158	VAL	N-CA-C	7.83	119.22	108.89
1	D	250	HIS	N-CA-C	7.83	122.20	109.76
1	A	80	PHE	N-CA-CB	-7.82	100.02	110.57
1	A	122	GLY	N-CA-C	-7.77	101.56	114.76
1	C	175	ARG	N-CA-C	-7.73	101.67	113.89
1	C	106	VAL	CA-C-O	7.72	129.27	121.09
1	A	171	ASN	N-CA-CB	7.71	124.10	110.37
1	D	243	LEU	CA-CB-CG	-7.70	89.35	116.30
1	A	36	GLN	N-CA-C	-7.70	102.22	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	THR	N-CA-C	7.69	122.41	112.26
1	B	234	THR	CA-C-O	-7.68	112.94	121.00
1	B	237	ILE	CB-CA-C	7.68	122.09	112.04
1	C	162	GLN	O-C-N	7.68	130.29	122.08
1	D	279	LEU	N-CA-C	7.67	122.11	109.06
1	C	297	GLN	N-CA-C	7.67	121.33	108.13
1	D	56	LEU	N-CA-CB	-7.67	98.14	110.63
1	C	199	CYS	CA-CB-SG	-7.64	96.83	114.40
1	C	89	LEU	N-CA-C	-7.63	102.96	111.28
1	A	185	ARG	CG-CD-NE	-7.62	95.24	112.00
1	D	210	CYS	N-CA-C	7.59	121.73	108.75
1	A	203	VAL	CA-CB-CG2	-7.59	97.50	110.40
1	A	42	ARG	CD-NE-CZ	7.58	135.02	124.40
1	D	155	GLY	N-CA-C	7.55	127.59	114.76
1	B	177	ILE	N-CA-CB	-7.54	102.03	111.31
1	A	305	PRO	CA-C-O	7.54	134.32	120.60
1	D	254	ASP	CB-CA-C	7.54	123.84	111.41
1	D	270	GLN	N-CA-C	7.53	120.58	111.40
1	C	79	VAL	CB-CA-C	-7.52	100.85	111.38
1	C	171	ASN	N-CA-C	7.51	126.40	109.81
1	A	34	LEU	N-CA-C	-7.51	102.79	110.97
1	D	46	ARG	N-CA-C	-7.48	99.96	110.50
1	A	112	ASN	N-CA-C	-7.45	103.50	112.59
1	B	55	THR	N-CA-C	-7.45	94.93	110.80
1	C	64	ARG	NE-CZ-NH1	-7.44	114.06	121.50
1	D	168	ILE	CB-CA-C	-7.44	102.30	112.04
1	D	152	ASP	CA-C-N	-7.43	110.57	122.23
1	D	152	ASP	C-N-CA	-7.43	110.57	122.23
1	B	161	LEU	CB-CA-C	-7.42	99.45	110.95
1	A	75	THR	N-CA-C	7.41	121.57	112.23
1	D	130	ASP	N-CA-C	-7.39	99.09	110.10
1	C	197	ALA	N-CA-C	-7.38	103.17	111.07
1	D	134	VAL	N-CA-C	7.37	124.66	109.34
1	D	297	GLN	CB-CA-C	7.33	121.32	110.62
1	A	203	VAL	CA-CB-CG1	7.33	122.86	110.40
1	D	91	PHE	CA-C-N	-7.32	113.72	122.35
1	D	91	PHE	C-N-CA	-7.32	113.72	122.35
1	B	230	TYR	N-CA-C	7.31	119.24	111.28
1	A	256	HIS	N-CA-C	7.29	121.02	109.50
1	B	265	LEU	N-CA-C	-7.29	103.05	112.23
1	D	266	LYS	CA-CB-CG	7.29	128.67	114.10
1	B	176	ARG	CA-C-N	-7.26	113.28	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ARG	C-N-CA	-7.26	113.28	122.43
1	A	167	THR	CA-C-N	-7.25	111.25	120.60
1	A	167	THR	C-N-CA	-7.25	111.25	120.60
1	C	79	VAL	CA-C-N	-7.25	112.19	122.41
1	C	79	VAL	C-N-CA	-7.25	112.19	122.41
1	A	237	ILE	N-CA-C	7.24	121.15	111.44
1	A	221	LEU	CB-CG-CD2	7.24	132.41	110.70
1	C	132	GLY	CA-C-N	7.23	128.87	119.84
1	C	132	GLY	C-N-CA	7.23	128.87	119.84
1	D	73	LEU	N-CA-C	-7.22	97.47	109.24
1	B	187	LEU	CA-C-N	-7.21	110.83	119.84
1	B	187	LEU	C-N-CA	-7.21	110.83	119.84
1	A	42	ARG	NE-CZ-NH2	-7.20	112.72	119.20
1	D	263	GLU	O-C-N	7.19	126.06	120.38
1	B	205	ASN	CA-C-N	-7.19	112.36	125.66
1	B	205	ASN	C-N-CA	-7.19	112.36	125.66
1	C	103	SER	N-CA-CB	-7.19	99.28	110.06
1	C	267	ILE	CB-CA-C	-7.18	102.61	112.02
1	A	32	GLN	CA-CB-CG	7.16	128.43	114.10
1	D	175	ARG	NE-CZ-NH1	-7.16	114.34	121.50
1	B	99	LYS	N-CA-C	-7.13	104.39	113.23
1	A	143	GLY	N-CA-C	-7.13	105.95	113.58
1	C	145	GLU	N-CA-C	7.12	119.41	109.15
1	B	207	GLU	N-CA-C	-7.11	98.62	109.85
1	A	182	TRP	CB-CA-C	-7.10	98.92	110.77
1	C	268	GLN	CA-C-O	7.09	128.12	120.10
1	B	37	ILE	CB-CA-C	-7.09	99.67	111.29
1	D	61	MET	CA-CB-CG	-7.07	99.97	114.10
1	D	180	CYS	N-CA-C	7.06	120.24	108.73
1	A	202	TYR	O-C-N	-7.06	115.20	123.25
1	B	198	LEU	CA-C-O	-7.03	113.16	120.89
1	B	240	ILE	CB-CA-C	-7.01	101.29	112.16
1	C	195	CYS	N-CA-C	7.01	119.96	111.40
1	C	199	CYS	N-CA-C	-7.01	98.51	108.96
1	C	236	MET	CA-C-N	-7.00	110.47	120.42
1	C	236	MET	C-N-CA	-7.00	110.47	120.42
1	B	220	GLY	N-CA-C	7.00	121.11	112.64
1	D	138	GLN	CA-C-N	6.98	129.97	120.54
1	D	138	GLN	C-N-CA	6.98	129.97	120.54
1	A	238	ALA	N-CA-C	-6.98	103.75	111.36
1	B	176	ARG	CG-CD-NE	6.97	127.33	112.00
1	D	203	VAL	CA-C-N	-6.96	109.44	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	VAL	C-N-CA	-6.96	109.44	121.97
1	B	236	MET	CA-C-N	-6.96	110.79	120.74
1	B	236	MET	C-N-CA	-6.96	110.79	120.74
1	D	207	GLU	CG-CD-OE1	-6.95	102.41	118.40
1	A	203	VAL	CG1-CB-CG2	-6.95	95.51	110.80
1	A	284	LYS	CG-CD-CE	6.95	127.27	111.30
1	B	142	PHE	N-CA-C	6.94	119.79	109.59
1	C	69	ASP	CB-CA-C	-6.93	100.46	111.48
1	C	53	THR	CA-C-N	-6.91	112.73	120.53
1	C	53	THR	C-N-CA	-6.91	112.73	120.53
1	C	163	ARG	N-CA-C	-6.90	104.73	113.01
1	B	252	LEU	N-CA-C	6.90	121.07	109.76
1	B	183	ASN	CA-C-O	-6.89	114.22	119.32
1	A	173	ASP	N-CA-C	-6.88	104.50	113.17
1	A	56	LEU	N-CA-CB	-6.87	99.76	110.55
1	B	277	PRO	CB-CA-C	-6.85	100.26	111.56
1	C	58	VAL	CA-C-N	-6.85	113.09	122.95
1	C	58	VAL	C-N-CA	-6.85	113.09	122.95
1	C	251	THR	OG1-CB-CG2	-6.85	95.61	109.30
1	A	292	LYS	CA-C-O	6.84	128.95	120.54
1	D	70	GLU	N-CA-C	6.84	118.91	108.52
1	A	175	ARG	NH1-CZ-NH2	-6.83	110.42	119.30
1	A	201	PHE	N-CA-C	6.82	120.25	109.81
1	B	47	LYS	CA-CB-CG	6.80	127.70	114.10
1	C	48	ASP	N-CA-C	6.80	120.60	109.72
1	C	70	GLU	CA-C-O	-6.76	113.56	121.46
1	C	106	VAL	N-CA-C	6.76	116.62	106.42
1	C	131	LEU	N-CA-C	-6.76	105.07	113.38
1	A	70	GLU	N-CA-C	-6.75	99.72	109.31
1	D	297	GLN	CA-C-N	6.75	131.30	121.18
1	D	297	GLN	C-N-CA	6.75	131.30	121.18
1	A	176	ARG	NE-CZ-NH1	-6.75	114.75	121.50
1	C	89	LEU	CA-C-N	-6.74	110.57	120.28
1	C	89	LEU	C-N-CA	-6.74	110.57	120.28
1	A	175	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	D	56	LEU	CA-C-N	-6.74	108.69	121.63
1	D	56	LEU	C-N-CA	-6.74	108.69	121.63
1	D	266	LYS	N-CA-CB	6.73	120.16	110.06
1	C	240	ILE	O-C-N	-6.73	114.39	122.06
1	D	40	ILE	CB-CA-C	-6.72	101.74	112.16
1	A	165	ILE	CB-CA-C	-6.72	103.10	111.70
1	C	225	PHE	CA-C-N	-6.72	111.47	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	PHE	C-N-CA	-6.72	111.47	120.54
1	C	113	GLY	CA-C-N	6.70	130.27	120.82
1	C	113	GLY	C-N-CA	6.70	130.27	120.82
1	D	104	LYS	CD-CE-NZ	6.70	133.34	111.90
1	B	176	ARG	N-CA-C	-6.70	103.83	113.21
1	B	168	ILE	CB-CA-C	-6.69	103.25	112.02
1	D	44	GLY	N-CA-C	6.69	119.19	111.36
1	A	87	GLU	N-CA-C	-6.68	104.39	112.54
1	C	124	SER	N-CA-C	6.68	125.02	110.80
1	A	149	MET	CA-C-N	-6.67	110.83	121.44
1	A	149	MET	C-N-CA	-6.67	110.83	121.44
1	A	50	ARG	CD-NE-CZ	6.67	133.73	124.40
1	D	39	HIS	N-CA-C	6.66	119.11	111.11
1	B	117	PHE	CA-C-N	6.66	129.50	120.44
1	B	117	PHE	C-N-CA	6.66	129.50	120.44
1	C	29	GLY	O-C-N	-6.64	114.06	122.70
1	A	117	PHE	N-CA-C	-6.64	104.12	111.36
1	C	250	HIS	CA-C-N	-6.63	112.99	122.94
1	C	250	HIS	C-N-CA	-6.63	112.99	122.94
1	B	69	ASP	CA-C-N	-6.63	111.68	122.81
1	B	69	ASP	C-N-CA	-6.63	111.68	122.81
1	B	58	VAL	CA-C-N	-6.62	113.71	123.11
1	B	58	VAL	C-N-CA	-6.62	113.71	123.11
1	C	135	TYR	CA-CB-CG	6.62	125.81	113.90
1	A	182	TRP	N-CA-C	6.61	118.92	108.67
1	D	108	ILE	CA-C-N	-6.61	112.08	122.65
1	D	108	ILE	C-N-CA	-6.61	112.08	122.65
1	D	187	LEU	N-CA-C	6.60	124.41	109.81
1	B	250	HIS	CA-C-N	-6.60	113.70	123.00
1	B	250	HIS	C-N-CA	-6.60	113.70	123.00
1	D	75	THR	N-CA-C	-6.60	104.86	113.17
1	B	28	HIS	N-CA-C	6.60	119.07	110.43
1	C	269	LEU	N-CA-C	-6.59	104.17	111.82
1	D	140	ARG	CA-CB-CG	6.58	127.27	114.10
1	C	236	MET	N-CA-C	6.58	118.24	111.14
1	D	74	LEU	CB-CG-CD1	-6.57	90.99	110.70
1	B	180	CYS	CA-CB-SG	-6.55	99.32	114.40
1	A	201	PHE	CA-C-N	-6.54	110.44	121.75
1	A	201	PHE	C-N-CA	-6.54	110.44	121.75
1	B	56	LEU	N-CA-C	-6.54	99.87	110.20
1	B	232	LEU	CA-C-N	-6.52	111.73	120.54
1	B	232	LEU	C-N-CA	-6.52	111.73	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	MET	CA-C-N	-6.52	111.02	121.58
1	D	61	MET	C-N-CA	-6.52	111.02	121.58
1	A	173	ASP	CB-CA-C	-6.52	99.21	110.09
1	C	198	LEU	CB-CG-CD1	-6.51	91.17	110.70
1	B	66	SER	CA-C-N	-6.50	112.28	122.49
1	B	66	SER	C-N-CA	-6.50	112.28	122.49
1	B	164	VAL	N-CA-CB	-6.50	102.95	110.55
1	B	129	GLY	N-CA-C	-6.50	105.95	115.63
1	B	235	TYR	N-CA-CB	6.49	121.47	110.49
1	D	116	ASP	N-CA-C	6.49	121.48	112.45
1	A	212	LEU	N-CA-C	6.48	119.97	109.40
1	A	194	PRO	CA-C-N	-6.46	112.42	122.37
1	A	194	PRO	C-N-CA	-6.46	112.42	122.37
1	C	40	ILE	N-CA-C	-6.46	102.78	111.44
1	B	199	CYS	N-CA-C	6.45	119.52	109.52
1	B	56	LEU	CA-C-N	-6.45	111.28	122.37
1	B	56	LEU	C-N-CA	-6.45	111.28	122.37
1	C	230	TYR	CA-C-N	-6.44	109.56	120.58
1	C	230	TYR	C-N-CA	-6.44	109.56	120.58
1	A	169	LYS	CB-CG-CD	-6.44	96.49	111.30
1	A	221	LEU	N-CA-C	6.44	120.50	111.30
1	C	91	PHE	CB-CA-C	-6.44	96.74	110.32
1	D	209	SER	CA-CB-OG	6.43	123.97	111.10
1	C	192	LEU	CA-C-N	6.43	127.00	120.38
1	C	192	LEU	C-N-CA	6.43	127.00	120.38
1	B	190	MET	CB-CG-SD	-6.42	93.44	112.70
1	C	204	VAL	N-CA-C	6.41	122.67	109.34
1	B	170	THR	N-CA-CB	6.40	119.48	109.94
1	A	37	ILE	CA-C-O	-6.40	114.07	120.85
1	C	254	ASP	CA-C-N	-6.40	113.17	122.19
1	C	254	ASP	C-N-CA	-6.40	113.17	122.19
1	D	42	ARG	CB-CA-C	-6.40	98.39	110.67
1	B	183	ASN	CB-CA-C	-6.38	100.20	109.38
1	C	240	ILE	CA-C-N	-6.35	112.58	122.37
1	C	240	ILE	C-N-CA	-6.35	112.58	122.37
1	B	34	LEU	CA-CB-CG	-6.35	94.08	116.30
1	B	42	ARG	CB-CA-C	6.34	121.30	111.02
1	C	192	LEU	CB-CA-C	6.34	117.89	109.65
1	A	203	VAL	N-CA-CB	6.32	121.73	111.36
1	D	138	GLN	CA-CB-CG	-6.32	101.45	114.10
1	D	249	ILE	N-CA-CB	-6.32	104.12	112.34
1	A	220	GLY	CA-C-N	-6.31	112.58	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	GLY	C-N-CA	-6.31	112.58	123.25
1	C	272	GLU	CB-CA-C	-6.31	102.02	109.47
1	D	74	LEU	N-CA-C	6.31	119.82	110.48
1	D	98	ALA	N-CA-C	-6.31	105.29	112.87
1	D	240	ILE	CA-C-N	-6.31	111.60	122.14
1	D	240	ILE	C-N-CA	-6.31	111.60	122.14
1	D	265	LEU	N-CA-C	6.31	124.24	110.80
1	A	129	GLY	N-CA-C	6.30	123.40	115.21
1	A	167	THR	N-CA-C	6.30	118.95	111.33
1	D	67	LEU	CA-C-N	-6.29	114.17	123.11
1	D	67	LEU	C-N-CA	-6.29	114.17	123.11
1	D	283	ARG	NE-CZ-NH1	-6.28	115.22	121.50
1	B	261	HIS	N-CA-C	6.28	120.41	112.87
1	A	289	ASP	N-CA-C	-6.28	105.38	113.16
1	B	249	ILE	CB-CA-C	-6.28	101.79	110.96
1	B	291	PHE	N-CA-C	6.27	118.40	110.24
1	A	91	PHE	N-CA-C	-6.27	103.98	111.69
1	A	87	GLU	CA-C-N	-6.26	108.30	121.64
1	A	87	GLU	C-N-CA	-6.26	108.30	121.64
1	D	266	LYS	CA-C-N	6.26	129.04	120.46
1	D	266	LYS	C-N-CA	6.26	129.04	120.46
1	C	301	TYR	CB-CA-C	-6.26	97.96	110.42
1	B	250	HIS	CB-CA-C	-6.26	99.76	110.22
1	D	217	GLY	CA-C-N	-6.26	113.21	122.41
1	D	217	GLY	C-N-CA	-6.26	113.21	122.41
1	B	171	ASN	CA-C-N	6.26	127.17	120.47
1	B	171	ASN	C-N-CA	6.26	127.17	120.47
1	C	257	ILE	CA-CB-CG2	6.25	121.13	110.50
1	A	294	GLU	CB-CA-C	-6.25	99.07	110.63
1	C	124	SER	N-CA-CB	-6.25	99.94	110.49
1	C	276	PHE	CA-C-N	6.24	127.64	119.84
1	C	276	PHE	C-N-CA	6.24	127.64	119.84
1	A	297	GLN	N-CA-C	-6.24	98.08	108.32
1	B	244	LYS	CA-CB-CG	6.24	126.58	114.10
1	A	137	PHE	N-CA-C	-6.24	106.21	113.88
1	D	189	LEU	CA-CB-CG	-6.21	94.56	116.30
1	D	103	SER	N-CA-CB	-6.21	100.38	109.82
1	A	286	GLU	CA-C-N	-6.21	112.88	122.87
1	A	286	GLU	C-N-CA	-6.21	112.88	122.87
1	B	241	THR	CB-CA-C	-6.20	99.21	109.99
1	C	80	PHE	CB-CA-C	6.20	121.47	112.05
1	C	205	ASN	CA-CB-CG	-6.20	106.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	GLY	CA-C-N	6.19	129.66	120.87
1	A	113	GLY	C-N-CA	6.19	129.66	120.87
1	C	262	ILE	N-CA-C	6.19	116.94	110.62
1	D	108	ILE	N-CA-C	6.19	122.22	109.34
1	B	298	ILE	CB-CA-C	-6.18	104.79	111.59
1	C	231	ALA	CA-C-O	-6.18	113.38	120.24
1	B	239	HIS	N-CA-C	6.18	117.70	110.97
1	B	91	PHE	N-CA-C	6.17	118.80	111.33
1	B	197	ALA	CA-C-N	-6.17	109.79	121.63
1	B	197	ALA	C-N-CA	-6.17	109.79	121.63
1	C	83	GLY	CA-C-N	-6.16	112.67	120.56
1	C	83	GLY	C-N-CA	-6.16	112.67	120.56
1	D	192	LEU	CB-CG-CD2	6.16	129.19	110.70
1	B	177	ILE	CG1-CB-CG2	6.16	129.19	110.70
1	D	177	ILE	CB-CA-C	-6.16	101.19	111.29
1	D	299	GLU	CA-CB-CG	6.16	126.42	114.10
1	C	134	VAL	CB-CA-C	6.15	121.38	111.29
1	D	90	TRP	CA-CB-CG	-6.15	101.91	113.60
1	C	231	ALA	N-CA-C	-6.15	104.13	111.69
1	D	274	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	A	144	ALA	CA-C-N	6.14	130.20	121.42
1	A	144	ALA	C-N-CA	6.14	130.20	121.42
1	C	247	ASP	CB-CA-C	-6.14	97.74	109.66
1	D	39	HIS	CA-C-N	6.13	130.15	120.47
1	D	39	HIS	C-N-CA	6.13	130.15	120.47
1	A	221	LEU	CB-CG-CD1	-6.12	92.33	110.70
1	A	263	GLU	CA-CB-CG	-6.11	101.88	114.10
1	B	49	ASP	N-CA-C	6.10	118.72	109.63
1	D	102	SER	CA-C-N	6.10	129.27	120.79
1	D	102	SER	C-N-CA	6.10	129.27	120.79
1	C	274	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	D	34	LEU	CA-C-O	6.09	126.96	119.05
1	A	225	PHE	CB-CA-C	-6.08	101.25	110.92
1	D	262	ILE	CB-CG1-CD1	6.08	126.57	113.80
1	C	294	GLU	CA-CB-CG	-6.08	101.94	114.10
1	B	48	ASP	CA-C-O	-6.07	114.49	121.47
1	A	201	PHE	CZ-CE2-CD2	-6.07	109.08	120.00
1	D	198	LEU	CB-CG-CD1	-6.06	92.53	110.70
1	D	285	VAL	N-CA-C	6.06	121.94	109.34
1	B	246	GLY	CA-C-N	-6.05	111.95	122.37
1	B	246	GLY	C-N-CA	-6.05	111.95	122.37
1	C	52	GLY	CA-C-N	-6.05	113.65	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	GLY	C-N-CA	-6.05	113.65	122.19
1	A	85	LEU	O-C-N	6.05	128.55	122.08
1	A	284	LYS	CA-C-N	6.05	132.01	122.33
1	A	284	LYS	C-N-CA	6.05	132.01	122.33
1	A	50	ARG	NE-CZ-NH2	-6.05	113.76	119.20
1	B	155	GLY	CA-C-N	-6.05	113.13	122.87
1	B	155	GLY	C-N-CA	-6.05	113.13	122.87
1	C	252	LEU	CA-CB-CG	-6.02	95.24	116.30
1	D	45	VAL	CB-CA-C	-6.01	102.72	111.68
1	D	177	ILE	N-CA-CB	6.00	121.14	111.23
1	B	248	PHE	CB-CA-C	-6.00	101.01	110.79
1	D	93	LYS	N-CA-C	-6.00	104.07	111.75
1	D	301	TYR	CA-C-N	-5.99	115.90	123.15
1	D	301	TYR	C-N-CA	-5.99	115.90	123.15
1	A	244	LYS	CA-C-O	5.99	125.22	120.19
1	B	283	ARG	N-CA-C	-5.98	98.06	110.80
1	D	155	GLY	CA-C-N	-5.97	114.35	122.95
1	D	155	GLY	C-N-CA	-5.97	114.35	122.95
1	D	240	ILE	CB-CG1-CD1	-5.97	101.27	113.80
1	B	180	CYS	CA-C-O	-5.97	113.75	120.43
1	A	297	GLN	O-C-N	5.96	130.21	123.42
1	C	247	ASP	CA-C-N	-5.96	114.78	123.00
1	C	247	ASP	C-N-CA	-5.96	114.78	123.00
1	D	142	PHE	N-CA-C	-5.96	101.95	110.59
1	B	182	TRP	N-CA-C	-5.95	97.47	108.24
1	B	190	MET	N-CA-C	5.95	119.24	109.72
1	A	203	VAL	N-CA-C	-5.94	100.50	108.35
1	B	254	ASP	CA-C-N	-5.94	113.81	122.19
1	B	254	ASP	C-N-CA	-5.94	113.81	122.19
1	A	51	THR	N-CA-C	-5.94	105.34	112.59
1	B	233	LEU	CA-CB-CG	-5.93	95.55	116.30
1	D	61	MET	N-CA-CB	-5.93	102.20	111.56
1	D	151	SER	CA-CB-OG	5.92	122.95	111.10
1	D	169	LYS	O-C-N	5.92	128.48	122.09
1	C	181	ALA	N-CA-C	-5.92	107.05	114.56
1	C	187	LEU	O-C-N	5.91	125.05	120.38
1	D	108	ILE	CB-CG1-CD1	5.91	126.22	113.80
1	B	73	LEU	CA-C-N	-5.91	110.21	120.97
1	B	73	LEU	C-N-CA	-5.91	110.21	120.97
1	C	86	GLU	CA-C-O	5.91	126.76	119.79
1	D	249	ILE	CB-CA-C	-5.90	103.68	110.41
1	A	296	PHE	CB-CA-C	-5.90	97.69	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	LYS	N-CA-C	-5.90	98.64	108.32
1	D	229	SER	O-C-N	5.90	128.16	122.03
1	C	274	ARG	CA-C-N	5.89	127.20	119.84
1	C	274	ARG	C-N-CA	5.89	127.20	119.84
1	D	95	SER	N-CA-C	-5.88	99.06	109.06
1	D	148	ASP	CB-CA-C	-5.88	99.96	112.78
1	B	198	LEU	CB-CG-CD2	-5.87	93.09	110.70
1	C	236	MET	CA-CB-CG	-5.87	102.36	114.10
1	D	235	TYR	N-CA-CB	5.87	118.75	110.12
1	C	242	GLY	N-CA-C	-5.87	103.20	113.76
1	B	181	ALA	CA-C-N	-5.86	114.14	122.41
1	B	181	ALA	C-N-CA	-5.86	114.14	122.41
1	C	45	VAL	CA-C-O	-5.86	113.96	121.40
1	C	292	LYS	N-CA-C	5.86	118.28	108.73
1	A	251	THR	CA-CB-OG1	-5.85	100.82	109.60
1	A	62	GLN	CA-CB-CG	-5.85	102.41	114.10
1	D	33	TYR	CA-C-N	-5.84	109.61	121.18
1	D	33	TYR	C-N-CA	-5.84	109.61	121.18
1	A	179	MET	N-CA-C	5.84	118.04	108.52
1	D	258	TYR	CA-C-N	-5.84	110.96	120.71
1	D	258	TYR	C-N-CA	-5.84	110.96	120.71
1	D	71	PHE	CA-C-O	5.84	124.14	119.59
1	A	106	VAL	CA-C-N	-5.84	113.28	122.79
1	A	106	VAL	C-N-CA	-5.84	113.28	122.79
1	C	54	GLY	CA-C-O	-5.84	114.49	122.31
1	D	206	SER	CA-C-N	-5.84	114.54	122.77
1	D	206	SER	C-N-CA	-5.84	114.54	122.77
1	D	283	ARG	N-CA-C	-5.84	100.18	109.23
1	A	231	ALA	N-CA-C	-5.83	105.06	111.82
1	D	35	GLY	N-CA-C	-5.83	105.44	112.49
1	A	175	ARG	N-CA-CB	-5.83	101.60	110.92
1	A	175	ARG	CB-CG-CD	5.82	124.68	111.30
1	C	221	LEU	N-CA-C	5.82	121.32	112.54
1	A	274	ARG	N-CA-C	5.81	118.14	110.36
1	C	28	HIS	CB-CA-C	5.81	119.19	109.89
1	D	175	ARG	CA-CB-CG	5.80	125.71	114.10
1	B	114	SER	CB-CA-C	5.79	119.75	109.72
1	C	300	GLY	N-CA-C	-5.79	106.75	115.32
1	A	70	GLU	CA-C-N	5.79	135.93	121.80
1	A	70	GLU	C-N-CA	5.79	135.93	121.80
1	C	146	TYR	CB-CA-C	-5.79	100.41	109.84
1	A	210	CYS	CA-C-O	-5.79	114.34	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	SER	CA-C-O	-5.78	114.33	120.92
1	D	295	ASP	N-CA-C	5.77	117.22	110.41
1	C	187	LEU	N-CA-C	-5.77	104.62	112.35
1	D	58	VAL	CA-C-N	-5.77	115.04	123.00
1	D	58	VAL	C-N-CA	-5.77	115.04	123.00
1	C	80	PHE	N-CA-C	5.76	118.67	108.24
1	C	172	PRO	N-CA-CB	-5.76	97.20	103.25
1	B	194	PRO	CB-CA-C	-5.76	102.73	110.85
1	D	53	THR	N-CA-C	5.76	118.68	110.10
1	C	110	ASP	CA-C-N	5.75	132.52	121.54
1	C	110	ASP	C-N-CA	5.75	132.52	121.54
1	C	278	LYS	CA-CB-CG	-5.75	102.61	114.10
1	C	180	CYS	N-CA-C	5.74	118.77	110.28
1	C	283	ARG	CA-C-O	5.72	125.99	119.18
1	A	47	LYS	CD-CE-NZ	5.72	130.21	111.90
1	D	204	VAL	CA-C-O	-5.72	113.63	120.78
1	C	171	ASN	C-N-CD	-5.72	101.55	125.00
1	A	121	LEU	CA-C-O	5.72	125.67	119.15
1	C	255	ALA	N-CA-C	-5.72	99.97	109.46
1	D	28	HIS	N-CA-C	5.72	118.48	109.96
1	A	91	PHE	N-CA-CB	5.71	118.71	110.20
1	B	33	TYR	N-CA-CB	-5.71	101.57	109.91
1	D	47	LYS	N-CA-C	-5.71	99.29	108.55
1	C	252	LEU	CB-CA-C	-5.71	98.07	109.33
1	A	159	ASP	CB-CA-C	-5.70	103.38	111.76
1	D	166	ASP	CA-CB-CG	-5.70	106.90	112.60
1	D	209	SER	CB-CA-C	-5.70	97.97	111.65
1	A	65	TYR	N-CA-C	5.70	118.01	108.73
1	D	92	ILE	CA-C-N	5.70	128.70	120.38
1	D	92	ILE	C-N-CA	5.70	128.70	120.38
1	A	196	HIS	N-CA-CB	-5.69	101.08	110.53
1	D	57	SER	N-CA-CB	-5.69	101.43	111.39
1	A	252	LEU	N-CA-CB	-5.69	101.98	111.20
1	B	250	HIS	N-CA-C	5.69	118.00	108.96
1	B	62	GLN	CB-CA-C	-5.69	99.62	109.86
1	B	89	LEU	O-C-N	5.68	128.86	122.22
1	D	268	GLN	CA-CB-CG	-5.67	102.75	114.10
1	A	208	LEU	CA-C-N	-5.66	113.31	122.82
1	A	208	LEU	C-N-CA	-5.66	113.31	122.82
1	A	68	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	C	110	ASP	N-CA-CB	5.66	118.17	109.91
1	D	169	LYS	CA-C-O	-5.66	114.87	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	SER	CA-C-O	-5.65	114.47	120.92
1	D	253	GLY	N-CA-C	-5.65	99.78	113.18
1	A	37	ILE	CA-CB-CG1	-5.65	100.80	110.40
1	C	78	ARG	CA-C-N	-5.64	114.49	122.34
1	C	78	ARG	C-N-CA	-5.64	114.49	122.34
1	D	298	ILE	CB-CA-C	-5.64	103.77	111.33
1	C	196	HIS	CB-CA-C	5.64	120.71	111.41
1	A	177	ILE	N-CA-C	-5.63	98.85	106.85
1	B	237	ILE	N-CA-CB	-5.63	102.42	110.52
1	D	127	GLU	N-CA-CB	5.63	119.34	110.39
1	B	165	ILE	CB-CA-C	5.62	119.73	112.14
1	D	149	MET	N-CA-C	5.62	122.77	110.80
1	C	212	LEU	N-CA-C	5.62	118.56	109.40
1	B	262	ILE	CB-CA-C	-5.61	102.08	111.29
1	D	195	CYS	N-CA-C	5.61	119.85	112.89
1	C	241	THR	CA-C-O	5.61	126.10	119.48
1	D	156	GLN	N-CA-C	5.60	119.41	107.70
1	D	174	ASP	CA-C-N	-5.60	110.84	121.54
1	D	174	ASP	C-N-CA	-5.60	110.84	121.54
1	B	57	SER	CA-C-N	-5.59	115.16	122.94
1	B	57	SER	C-N-CA	-5.59	115.16	122.94
1	B	226	ASN	N-CA-C	-5.59	105.95	112.89
1	B	47	LYS	CD-CE-NZ	5.59	129.79	111.90
1	C	55	THR	CB-CA-C	-5.59	98.23	111.65
1	B	75	THR	N-CA-CB	5.59	119.94	110.49
1	D	47	LYS	N-CA-CB	5.58	120.86	110.99
1	D	280	ARG	CA-C-O	5.57	126.38	120.36
1	C	263	GLU	O-C-N	5.57	124.11	120.27
1	C	306	THR	CA-C-N	5.57	132.00	121.97
1	C	306	THR	C-N-CA	5.57	132.00	121.97
1	D	152	ASP	N-CA-C	-5.57	101.20	110.17
1	B	274	ARG	O-C-N	5.57	125.15	121.14
1	B	178	ILE	CA-CB-CG2	-5.57	101.04	110.50
1	A	240	ILE	CB-CA-C	-5.55	103.94	112.05
1	B	89	LEU	CB-CG-CD1	-5.55	94.05	110.70
1	A	200	GLN	N-CA-CB	-5.54	101.91	111.55
1	B	107	LYS	CB-CA-C	5.54	120.08	110.72
1	D	189	LEU	N-CA-C	5.54	121.01	113.37
1	D	252	LEU	CA-CB-CG	-5.54	96.92	116.30
1	A	125	THR	CB-CA-C	-5.53	101.10	110.88
1	D	166	ASP	O-C-N	5.52	128.50	122.20
1	B	243	LEU	CB-CG-CD1	-5.52	94.14	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	LEU	N-CA-CB	5.52	120.13	110.42
1	C	127	GLU	CA-C-N	-5.51	115.40	123.00
1	C	127	GLU	C-N-CA	-5.51	115.40	123.00
1	A	292	LYS	CA-CB-CG	5.50	125.11	114.10
1	D	72	PRO	CA-C-N	-5.50	115.13	122.72
1	D	72	PRO	C-N-CA	-5.50	115.13	122.72
1	C	139	TRP	N-CA-C	5.50	118.79	111.75
1	C	282	LEU	CB-CA-C	5.50	118.86	109.24
1	A	37	ILE	CA-C-N	-5.49	111.05	121.54
1	A	37	ILE	C-N-CA	-5.49	111.05	121.54
1	B	41	LEU	CB-CG-CD1	-5.49	94.23	110.70
1	C	215	ARG	NH1-CZ-NH2	5.49	126.44	119.30
1	A	58	VAL	CA-C-N	-5.48	114.85	123.13
1	A	58	VAL	C-N-CA	-5.48	114.85	123.13
1	A	240	ILE	CA-C-N	-5.48	113.49	122.54
1	A	240	ILE	C-N-CA	-5.48	113.49	122.54
1	C	190	MET	CG-SD-CE	5.48	112.96	100.90
1	B	118	LEU	CA-CB-CG	5.47	135.46	116.30
1	A	43	CYS	CB-CA-C	-5.47	99.53	110.42
1	A	79	VAL	N-CA-C	5.47	116.01	110.05
1	A	257	ILE	CA-CB-CG1	-5.47	101.10	110.40
1	D	284	LYS	N-CA-C	5.47	117.75	110.53
1	B	114	SER	N-CA-CB	-5.47	101.98	110.57
1	A	42	ARG	NE-CZ-NH1	5.46	126.97	121.50
1	D	241	THR	CA-C-N	-5.46	114.15	122.28
1	D	241	THR	C-N-CA	-5.46	114.15	122.28
1	A	174	ASP	N-CA-C	5.45	118.26	110.24
1	B	221	LEU	N-CA-CB	-5.45	101.27	110.49
1	D	222	GLY	CA-C-N	-5.45	112.04	122.13
1	D	222	GLY	C-N-CA	-5.45	112.04	122.13
1	B	77	LYS	CD-CE-NZ	5.45	129.35	111.90
1	B	182	TRP	CA-C-N	-5.45	114.03	121.61
1	B	182	TRP	C-N-CA	-5.45	114.03	121.61
1	B	58	VAL	N-CA-CB	5.45	120.38	111.44
1	A	274	ARG	CA-C-N	-5.44	113.04	119.84
1	A	274	ARG	C-N-CA	-5.44	113.04	119.84
1	A	32	GLN	N-CA-C	-5.44	105.25	111.07
1	B	89	LEU	CA-C-N	5.44	127.84	120.44
1	B	89	LEU	C-N-CA	5.44	127.84	120.44
1	A	112	ASN	CB-CA-C	-5.44	102.27	111.02
1	B	298	ILE	CA-C-O	-5.43	115.41	121.98
1	A	78	ARG	CB-CA-C	-5.42	102.35	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	ALA	N-CA-C	5.42	118.69	111.75
1	C	199	CYS	CA-C-O	-5.42	115.65	121.45
1	C	299	GLU	CA-CB-CG	5.42	124.94	114.10
1	D	178	ILE	CA-C-N	-5.42	115.17	122.86
1	D	178	ILE	C-N-CA	-5.42	115.17	122.86
1	C	29	GLY	CA-C-N	-5.42	111.93	120.60
1	C	29	GLY	C-N-CA	-5.42	111.93	120.60
1	A	59	PHE	N-CA-C	5.41	118.55	107.69
1	A	251	THR	O-C-N	5.41	129.63	123.31
1	C	306	THR	CA-C-O	-5.41	112.78	120.51
1	D	267	ILE	CB-CA-C	-5.40	104.85	112.14
1	D	173	ASP	O-C-N	-5.40	115.41	122.59
1	D	131	LEU	CA-CB-CG	5.40	135.19	116.30
1	C	43	CYS	CB-CA-C	-5.39	100.75	110.35
1	D	199	CYS	CB-CA-C	-5.39	100.59	110.62
1	D	209	SER	N-CA-C	5.39	116.46	108.86
1	C	88	LEU	CB-CA-C	-5.39	102.38	110.90
1	D	245	PRO	CB-CG-CD	-5.39	88.86	106.10
1	B	165	ILE	N-CA-C	-5.39	105.12	110.62
1	C	239	HIS	N-CA-C	-5.39	104.83	111.40
1	C	58	VAL	CA-CB-CG2	-5.38	101.25	110.40
1	C	173	ASP	CA-C-N	-5.38	111.78	120.87
1	C	173	ASP	C-N-CA	-5.38	111.78	120.87
1	C	69	ASP	CB-CG-OD2	-5.38	106.03	118.40
1	B	202	TYR	N-CA-C	-5.37	98.81	108.48
1	C	155	GLY	CA-C-N	-5.37	115.58	123.00
1	C	155	GLY	C-N-CA	-5.37	115.58	123.00
1	C	193	PRO	N-CA-C	5.37	117.25	110.70
1	B	76	THR	N-CA-CB	5.37	119.56	110.49
1	A	284	LYS	O-C-N	5.36	129.54	122.89
1	A	223	VAL	CA-C-N	-5.36	113.01	118.85
1	A	223	VAL	C-N-CA	-5.36	113.01	118.85
1	C	256	HIS	N-CA-CB	-5.36	103.25	111.56
1	C	296	PHE	N-CA-C	5.36	117.82	108.76
1	D	192	LEU	CA-C-N	-5.36	114.86	120.38
1	D	192	LEU	C-N-CA	-5.36	114.86	120.38
1	A	186	ASP	N-CA-C	5.35	119.81	113.28
1	A	201	PHE	CG-CD2-CE2	5.35	129.80	120.70
1	A	283	ARG	N-CA-C	-5.35	99.40	110.80
1	D	29	GLY	CA-C-N	-5.35	114.26	122.60
1	D	29	GLY	C-N-CA	-5.35	114.26	122.60
1	C	231	ALA	N-CA-CB	5.34	118.17	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	ARG	CA-C-N	-5.34	115.69	123.06
1	C	280	ARG	C-N-CA	-5.34	115.69	123.06
1	A	240	ILE	O-C-N	-5.33	116.51	121.90
1	B	191	ALA	O-C-N	5.33	129.69	122.59
1	B	279	LEU	CA-C-N	5.33	129.78	122.84
1	B	279	LEU	C-N-CA	5.33	129.78	122.84
1	A	28	HIS	N-CA-C	5.33	117.40	109.25
1	C	228	ALA	CA-C-N	-5.33	113.14	120.28
1	C	228	ALA	C-N-CA	-5.33	113.14	120.28
1	B	74	LEU	N-CA-CB	5.33	117.97	110.36
1	D	144	ALA	N-CA-C	5.32	117.41	108.73
1	A	43	CYS	CA-CB-SG	-5.32	102.17	114.40
1	C	305	PRO	N-CA-C	-5.31	101.52	112.47
1	D	277	PRO	CB-CA-C	-5.31	104.59	111.39
1	B	267	ILE	N-CA-CB	-5.31	104.83	110.62
1	C	64	ARG	CG-CD-NE	-5.31	100.32	112.00
1	C	261	HIS	N-CA-CB	5.31	118.79	110.46
1	A	164	VAL	N-CA-C	-5.30	105.16	110.30
1	C	128	GLU	N-CA-C	5.30	117.60	109.07
1	C	175	ARG	N-CA-CB	-5.29	103.33	110.95
1	C	258	TYR	O-C-N	-5.28	116.99	122.96
1	A	163	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	C	111	ALA	O-C-N	5.28	129.61	122.59
1	D	96	THR	CB-CA-C	-5.28	102.63	111.13
1	A	40	ILE	CB-CA-C	-5.27	104.95	112.22
1	A	252	LEU	N-CA-C	5.26	118.17	109.85
1	A	271	ARG	N-CA-C	5.26	117.50	110.35
1	B	198	LEU	CD1-CG-CD2	-5.26	99.23	110.80
1	D	77	LYS	CA-C-N	-5.25	113.98	122.81
1	D	77	LYS	C-N-CA	-5.25	113.98	122.81
1	D	103	SER	N-CA-C	5.25	117.43	111.02
1	C	85	LEU	CB-CA-C	5.25	120.75	110.67
1	A	63	ALA	N-CA-C	-5.25	101.56	109.85
1	C	153	TYR	CA-CB-CG	5.25	123.35	113.90
1	A	305	PRO	N-CA-C	5.25	123.28	112.47
1	B	92	ILE	CA-C-N	-5.25	111.81	122.31
1	B	92	ILE	C-N-CA	-5.25	111.81	122.31
1	C	46	ARG	N-CA-C	-5.24	102.53	110.24
1	C	215	ARG	CG-CD-NE	-5.24	100.46	112.00
1	B	40	ILE	CG1-CB-CG2	5.24	126.43	110.70
1	A	144	ALA	O-C-N	5.24	129.41	123.12
1	D	161	LEU	CA-CB-CG	-5.23	97.99	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	ARG	CD-NE-CZ	5.22	131.71	124.40
1	A	195	CYS	N-CA-C	-5.21	105.59	112.94
1	D	261	HIS	N-CA-C	-5.21	106.43	112.89
1	A	108	ILE	N-CA-C	-5.21	105.00	112.35
1	B	245	PRO	CB-CA-C	-5.21	105.07	111.64
1	D	59	PHE	N-CA-C	-5.21	100.68	109.07
1	C	275	PRO	CA-C-N	-5.21	113.57	120.65
1	C	275	PRO	C-N-CA	-5.21	113.57	120.65
1	D	160	GLN	CA-C-N	-5.20	113.02	120.82
1	D	160	GLN	C-N-CA	-5.20	113.02	120.82
1	C	125	THR	O-C-N	5.20	127.63	122.12
1	A	168	ILE	N-CA-CB	5.20	116.28	110.51
1	C	275	PRO	N-CA-C	5.20	123.18	112.47
1	D	95	SER	O-C-N	5.20	129.62	123.33
1	D	213	TYR	CA-C-N	-5.20	115.78	123.05
1	D	213	TYR	C-N-CA	-5.20	115.78	123.05
1	A	245	PRO	N-CA-C	5.19	118.64	110.80
1	A	286	GLU	N-CA-C	5.19	120.37	112.54
1	C	68	ARG	CD-NE-CZ	-5.18	117.15	124.40
1	A	179	MET	O-C-N	-5.17	117.17	123.27
1	B	26	PRO	CA-C-N	5.17	126.30	119.84
1	B	26	PRO	C-N-CA	5.17	126.30	119.84
1	D	251	THR	OG1-CB-CG2	-5.17	98.96	109.30
1	C	28	HIS	N-CA-CB	-5.17	102.15	109.85
1	C	240	ILE	CB-CA-C	-5.16	101.93	111.79
1	A	274	ARG	N-CA-CB	-5.16	103.75	109.74
1	D	290	ASP	N-CA-C	5.16	118.60	112.72
1	D	162	GLN	N-CA-C	-5.16	105.73	112.23
1	B	140	ARG	N-CA-C	-5.15	107.02	113.72
1	D	256	HIS	N-CA-C	5.15	116.90	109.07
1	B	281	ILE	CB-CA-C	-5.15	103.19	111.59
1	B	107	LYS	CD-CE-NZ	5.15	128.38	111.90
1	D	26	PRO	CA-C-N	5.14	126.27	119.84
1	D	26	PRO	C-N-CA	5.14	126.27	119.84
1	C	288	ILE	N-CA-C	-5.14	106.03	113.07
1	C	106	VAL	N-CA-CB	-5.12	107.53	112.65
1	B	266	LYS	CG-CD-CE	5.12	123.08	111.30
1	D	156	GLN	CB-CA-C	5.12	119.06	111.17
1	A	218	ASP	N-CA-CB	-5.12	103.21	110.58
1	C	297	GLN	CB-CA-C	-5.12	102.77	110.24
1	B	76	THR	CA-CB-CG2	5.11	119.19	110.50
1	B	206	SER	N-CA-C	5.11	123.50	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	GLU	CA-C-N	-5.11	115.72	122.56
1	C	70	GLU	C-N-CA	-5.11	115.72	122.56
1	D	252	LEU	N-CA-C	5.11	117.62	109.81
1	A	261	HIS	CA-C-N	-5.10	113.33	120.53
1	A	261	HIS	C-N-CA	-5.10	113.33	120.53
1	A	233	LEU	CB-CA-C	-5.10	100.27	110.42
1	C	76	THR	OG1-CB-CG2	-5.10	99.10	109.30
1	A	135	TYR	CA-CB-CG	-5.09	104.73	113.90
1	C	176	ARG	CB-CA-C	-5.09	102.75	111.46
1	B	258	TYR	CA-CB-CG	-5.08	104.75	113.90
1	D	274	ARG	C-N-CD	5.08	145.84	125.00
1	B	163	ARG	CA-CB-CG	-5.08	103.94	114.10
1	C	170	THR	N-CA-C	5.08	116.51	111.07
1	B	244	LYS	CB-CA-C	5.08	115.72	108.76
1	A	177	ILE	N-CA-CB	-5.08	105.58	111.83
1	B	178	ILE	CA-C-O	5.08	126.07	120.64
1	C	36	GLN	CB-CG-CD	-5.08	103.97	112.60
1	D	269	LEU	CA-CB-CG	5.08	134.07	116.30
1	A	223	VAL	CA-CB-CG1	-5.07	101.78	110.40
1	B	211	GLN	CA-CB-CG	-5.07	103.96	114.10
1	A	200	GLN	CA-C-N	-5.07	113.96	123.03
1	A	200	GLN	C-N-CA	-5.07	113.96	123.03
1	B	48	ASP	CB-CG-OD2	-5.06	106.76	118.40
1	D	232	LEU	CA-C-N	-5.06	112.99	120.28
1	D	232	LEU	C-N-CA	-5.06	112.99	120.28
1	A	269	LEU	CB-CA-C	5.06	120.08	110.27
1	D	177	ILE	CA-CB-CG1	5.06	119.00	110.40
1	D	249	ILE	CG1-CB-CG2	5.05	125.86	110.70
1	C	62	GLN	O-C-N	-5.05	116.42	123.34
1	A	197	ALA	N-CA-CB	-5.05	102.46	110.28
1	A	221	LEU	CA-C-O	-5.04	115.39	121.34
1	C	204	VAL	O-C-N	5.04	128.87	122.57
1	C	198	LEU	N-CA-CB	-5.04	103.70	111.46
1	D	173	ASP	N-CA-CB	-5.04	101.98	110.49
1	D	207	GLU	O-C-N	-5.04	117.38	123.27
1	C	32	GLN	CB-CA-C	-5.03	102.39	110.74
1	D	231	ALA	O-C-N	5.03	127.52	122.09
1	C	263	GLU	CA-C-N	-5.03	113.74	118.97
1	C	263	GLU	C-N-CA	-5.03	113.74	118.97
1	A	107	LYS	CB-CG-CD	5.03	122.86	111.30
1	C	173	ASP	CA-C-O	5.02	124.57	119.05
1	A	160	GLN	N-CA-C	-5.01	106.42	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	35	GLY	O-C-N	5.01	127.00	122.19
1	C	91	PHE	N-CA-C	5.01	118.49	112.38
1	B	215	ARG	CA-CB-CG	5.01	124.11	114.10
1	D	40	ILE	CG1-CB-CG2	-5.01	95.68	110.70
1	B	59	PHE	CD1-CG-CD2	-5.00	111.10	118.60
1	C	302	ASN	CB-CA-C	5.00	120.26	111.20
1	C	27	PRO	N-CA-CB	5.00	107.70	103.35

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	PRO	Peptide
1	A	200	GLN	Mainchain
1	A	202	TYR	Mainchain
1	A	286	GLU	Peptide
1	A	70	GLU	Peptide,Mainchain
1	B	114	SER	Peptide
1	B	123	PHE	Peptide
1	B	222	GLY	Peptide
1	B	304	HIS	Peptide
1	B	54	GLY	Peptide
1	B	69	ASP	Peptide
1	C	120	SER	Peptide
1	C	121	LEU	Peptide
1	C	127	GLU	Mainchain
1	C	138	GLN	Peptide
1	C	282	LEU	Peptide
1	C	283	ARG	Peptide
1	C	284	LYS	Peptide
1	C	285	VAL	Peptide
1	C	304	HIS	Peptide
1	C	92	ILE	Peptide
1	D	110	ASP	Peptide
1	D	174	ASP	Peptide
1	D	245	PRO	Peptide
1	D	92	ILE	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	2287	0	2258	324	0
1	B	2270	0	2233	369	0
1	C	2287	0	2258	325	0
1	D	2287	0	2259	410	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	B	5	0	0	7	0
3	D	5	0	0	4	0
4	A	6	0	0	0	0
4	B	7	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
All	All	9174	0	9008	1373	0

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 76.

All (1373) 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:201:PHE:CE2	1:A:201:PHE:CZ	1.74	1.64
1:B:107:LYS:CD	1:B:107:LYS:CE	1.74	1.64
1:B:244:LYS:CG	1:B:244:LYS:CD	1.77	1.62
1:D:266:LYS:CG	1:D:266:LYS:CB	1.75	1.62
1:A:221:LEU:CG	1:A:221:LEU:CD2	1.75	1.62
1:C:292:LYS:CD	1:C:292:LYS:CG	1.74	1.61
1:C:221:LEU:CG	1:C:221:LEU:CD1	1.74	1.60
1:D:47:LYS:CE	1:D:47:LYS:CD	1.77	1.59
1:C:280:ARG:CG	1:C:280:ARG:CD	1.79	1.56
1:A:284:LYS:CD	1:A:284:LYS:CG	1.79	1.56
1:A:38:GLN:CD	1:A:38:GLN:CG	1.80	1.55
1:C:292:LYS:CD	1:C:292:LYS:CE	1.83	1.55
1:C:38:GLN:CG	1:C:38:GLN:CD	1.79	1.54
1:C:244:LYS:CE	1:C:244:LYS:NZ	1.68	1.53
1:A:185:ARG:CD	1:A:185:ARG:CG	1.83	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ILE:CD1	1:D:307:ILE:CG1	1.85	1.53
1:B:73:LEU:HD23	1:B:301:TYR:CE1	1.43	1.50
1:D:43:CYS:CB	1:D:43:CYS:SG	2.01	1.47
1:C:26:PRO:CG	1:C:26:PRO:CB	1.82	1.46
1:C:292:LYS:CE	1:C:292:LYS:NZ	1.77	1.46
1:A:26:PRO:CG	1:A:26:PRO:CB	1.80	1.43
1:D:97:ASN:ND2	1:D:99:LYS:HB2	1.23	1.43
1:A:263:GLU:HB3	1:A:264:PRO:CD	1.43	1.41
1:C:115:ARG:NH2	1:C:128:GLU:HB3	1.26	1.40
1:D:188:PRO:CB	1:D:188:PRO:CG	1.74	1.39
1:B:73:LEU:HD23	1:B:301:TYR:CZ	1.61	1.34
1:D:245:PRO:CG	1:D:245:PRO:CB	1.80	1.28
1:C:160:GLN:O	1:C:164:VAL:HG23	1.10	1.28
1:D:308:LYS:HD2	1:D:308:LYS:C	1.63	1.21
1:C:115:ARG:HH21	1:C:128:GLU:CB	1.56	1.19
1:B:73:LEU:CD2	1:B:301:TYR:CZ	2.25	1.17
1:A:260:ASN:H	1:A:260:ASN:ND2	1.33	1.17
1:C:115:ARG:NH2	1:C:128:GLU:CB	2.07	1.17
1:B:32:GLN:HE21	1:B:32:GLN:HA	1.11	1.15
1:B:177:ILE:CG2	1:B:201:PHE:H	1.59	1.15
1:B:305:PRO:CB	1:B:306:THR:HA	1.63	1.15
1:A:260:ASN:HD22	1:A:260:ASN:N	1.38	1.15
1:C:240:ILE:HG22	1:C:241:THR:HG22	1.27	1.14
1:B:177:ILE:HG22	1:B:201:PHE:H	1.03	1.14
1:C:115:ARG:CZ	1:C:128:GLU:HB3	1.76	1.14
1:D:97:ASN:ND2	1:D:99:LYS:CB	2.09	1.14
1:B:160:GLN:HE22	1:B:180:CYS:N	1.45	1.13
1:B:287:LYS:HD3	1:B:288:ILE:H	0.97	1.13
1:A:263:GLU:CB	1:A:264:PRO:HD3	1.76	1.13
1:C:240:ILE:HG22	1:C:241:THR:CG2	1.80	1.11
1:B:287:LYS:HD3	1:B:288:ILE:N	1.65	1.11
1:C:119:ASP:HA	1:C:122:GLY:HA3	1.30	1.11
1:C:107:LYS:HA	1:C:110:ASP:OD1	1.51	1.10
1:A:176:ARG:HH12	1:B:193:PRO:HG2	1.04	1.09
1:A:50:ARG:HH11	1:B:176:ARG:NH2	1.48	1.09
1:B:287:LYS:CD	1:B:288:ILE:HG22	1.81	1.08
1:D:53:THR:HG22	1:D:54:GLY:O	1.53	1.08
1:C:160:GLN:O	1:C:164:VAL:CG2	2.00	1.08
1:B:215:ARG:HG2	1:B:215:ARG:HH11	1.17	1.07
1:C:148:ASP:OD2	1:C:151:SER:HB2	1.54	1.07
1:D:112:ASN:ND2	1:D:191:ALA:HB1	1.70	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:SER:OG	1:D:100:GLU:OE2	1.68	1.07
1:A:176:ARG:HH12	1:B:193:PRO:CG	1.66	1.07
1:D:183:ASN:HB3	1:D:186:ASP:HB2	1.34	1.06
1:C:50:ARG:HE	1:C:50:ARG:HA	0.98	1.06
1:D:198:LEU:HD12	1:D:198:LEU:C	1.76	1.06
1:D:204:VAL:O	1:D:207:GLU:HB2	1.54	1.06
1:B:97:ASN:HB2	1:B:149:MET:SD	1.95	1.06
1:D:115:ARG:HH21	1:D:127:GLU:HA	1.15	1.06
1:B:73:LEU:HD21	1:B:301:TYR:OH	1.55	1.05
1:D:176:ARG:HH12	3:D:616:PO4:P	1.80	1.05
1:A:74:LEU:CD1	1:A:224:PRO:HB3	1.85	1.05
1:A:74:LEU:HD12	1:A:224:PRO:CB	1.87	1.05
1:D:138:GLN:HA	1:D:138:GLN:OE1	1.57	1.05
1:B:160:GLN:NE2	1:B:180:CYS:H	1.55	1.04
1:A:67:LEU:O	1:A:69:ASP:N	1.89	1.04
1:A:257:ILE:HD11	1:A:262:ILE:HG13	1.34	1.04
1:B:85:LEU:HD12	1:B:85:LEU:O	1.56	1.04
1:B:73:LEU:CD2	1:B:301:TYR:CE1	2.39	1.03
1:C:292:LYS:O	1:C:295:ASP:N	1.91	1.03
1:A:288:ILE:O	1:A:288:ILE:HG13	1.54	1.03
1:B:32:GLN:HA	1:B:32:GLN:NE2	1.73	1.03
1:D:133:PRO:C	1:D:190:MET:HE2	1.83	1.03
1:A:292:LYS:HE3	1:A:292:LYS:HA	1.32	1.02
1:D:280:ARG:HD2	1:D:299:GLU:OE2	1.58	1.02
1:C:263:GLU:OE1	1:C:263:GLU:HA	1.23	1.02
1:D:133:PRO:O	1:D:190:MET:HE2	1.60	1.02
1:B:32:GLN:HE21	1:B:32:GLN:CA	1.72	1.01
1:A:195:CYS:O	1:A:214:GLN:HA	1.60	1.01
1:B:100:GLU:O	1:B:103:SER:HB2	1.61	1.01
1:B:119:ASP:OD1	1:B:122:GLY:HA2	1.60	1.01
1:B:287:LYS:CD	1:B:288:ILE:H	1.73	1.01
1:C:72:PRO:HA	1:C:276:PHE:CE1	1.96	1.01
1:C:203:VAL:O	1:C:204:VAL:HG23	1.58	1.00
1:B:305:PRO:HB2	1:B:306:THR:HA	1.42	1.00
1:C:260:ASN:H	1:C:260:ASN:ND2	1.48	1.00
1:C:263:GLU:OE1	1:C:266:LYS:HD3	1.61	1.00
1:B:76:THR:O	1:B:305:PRO:HD3	1.63	0.98
1:C:50:ARG:HA	1:C:50:ARG:NE	1.77	0.98
1:A:240:ILE:HD11	1:A:288:ILE:HA	1.43	0.98
1:A:221:LEU:CD2	1:A:221:LEU:HG	1.92	0.97
1:D:135:TYR:C	1:D:137:PHE:H	1.73	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:HD3	1:B:288:ILE:HG22	1.45	0.97
1:D:235:TYR:O	1:D:238:ALA:HB3	1.63	0.97
1:C:76:THR:HB	1:C:268:GLN:HE21	1.26	0.97
1:A:176:ARG:NH1	1:B:193:PRO:CG	2.26	0.97
1:C:257:ILE:HD11	1:C:262:ILE:HG13	1.47	0.97
1:C:119:ASP:HA	1:C:122:GLY:CA	1.96	0.96
1:C:263:GLU:OE1	1:C:263:GLU:CA	2.13	0.95
1:C:50:ARG:HE	1:C:50:ARG:CA	1.78	0.95
1:D:209:SER:HB3	1:D:247:ASP:O	1.65	0.95
1:D:40:ILE:HG21	1:D:257:ILE:HG13	1.44	0.95
1:D:286:GLU:OE1	1:D:286:GLU:HA	1.65	0.95
1:B:73:LEU:CD2	1:B:301:TYR:OH	2.13	0.95
1:B:148:ASP:OD1	1:B:150:GLU:N	2.00	0.95
1:C:92:ILE:O	1:C:140:ARG:NH1	2.00	0.94
1:D:112:ASN:HD22	1:D:191:ALA:HB1	1.28	0.94
1:A:257:ILE:CD1	1:A:262:ILE:HG13	1.98	0.94
1:B:29:GLY:O	1:B:32:GLN:HB2	1.67	0.94
1:B:287:LYS:HG3	1:B:289:ASP:OD1	1.67	0.94
1:B:287:LYS:HD2	1:B:288:ILE:HG22	1.50	0.93
1:C:260:ASN:H	1:C:260:ASN:HD22	0.97	0.93
1:B:299:GLU:O	1:B:300:GLY:C	2.10	0.93
1:D:97:ASN:HD22	1:D:99:LYS:HB2	1.18	0.93
1:D:149:MET:HG3	1:D:150:GLU:H	1.33	0.93
1:D:144:ALA:HB2	1:D:156:GLN:O	1.67	0.93
1:C:143:GLY:HA2	1:D:185:ARG:NH2	1.84	0.93
1:D:198:LEU:C	1:D:198:LEU:CD1	2.42	0.92
1:D:26:PRO:N	1:D:27:PRO:HD2	1.81	0.92
1:B:301:TYR:O	1:B:303:PRO:HD3	1.70	0.92
1:B:161:LEU:O	1:B:164:VAL:HB	1.69	0.91
1:B:299:GLU:O	1:B:301:TYR:N	2.03	0.91
1:C:119:ASP:CA	1:C:122:GLY:HA3	2.00	0.91
1:A:176:ARG:NH1	1:B:193:PRO:HG2	1.82	0.91
1:A:263:GLU:CB	1:A:264:PRO:CD	2.26	0.90
1:D:78:ARG:NH1	1:D:303:PRO:HG2	1.86	0.90
1:A:72:PRO:HA	1:A:276:PHE:CE1	2.06	0.90
1:C:97:ASN:HB2	1:C:149:MET:SD	2.10	0.90
1:B:39:HIS:O	1:B:43:CYS:HB2	1.70	0.89
1:B:283:ARG:HG2	1:B:284:LYS:H	1.38	0.89
1:B:143:GLY:HA2	1:B:185:ARG:HH22	1.33	0.89
1:B:177:ILE:HG22	1:B:201:PHE:N	1.86	0.89
1:D:176:ARG:NH1	3:D:616:PO4:P	2.44	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLY:CA	1:D:185:ARG:NH2	2.36	0.89
1:D:101:LEU:HD23	1:D:102:SER:N	1.87	0.89
1:A:187:LEU:HA	1:A:190:MET:HE3	1.53	0.89
1:A:68:ARG:HH21	1:A:246:GLY:HA2	1.36	0.89
1:C:204:VAL:HG11	1:D:45:VAL:HG21	1.55	0.89
1:D:160:GLN:O	1:D:164:VAL:HG23	1.74	0.88
1:D:292:LYS:O	1:D:295:ASP:OD2	1.90	0.88
1:D:112:ASN:HD22	1:D:191:ALA:CB	1.85	0.88
1:D:223:VAL:O	1:D:227:ILE:HG12	1.72	0.88
1:A:187:LEU:HA	1:A:190:MET:CE	2.04	0.88
1:C:186:ASP:O	1:C:190:MET:HG2	1.74	0.87
1:B:110:ASP:O	1:B:112:ASN:N	2.06	0.87
1:D:133:PRO:O	1:D:190:MET:CE	2.22	0.87
1:B:177:ILE:CG2	1:B:177:ILE:O	2.21	0.87
1:A:279:LEU:HD12	1:A:280:ARG:N	1.89	0.87
1:D:203:VAL:CG2	1:D:208:LEU:HD13	2.04	0.87
1:C:69:ASP:OD1	1:C:69:ASP:C	2.17	0.87
1:C:130:ASP:HB2	1:C:149:MET:HG2	1.56	0.87
1:D:108:ILE:O	1:D:108:ILE:HG13	1.72	0.87
1:B:115:ARG:HD3	1:B:128:GLU:OE2	1.74	0.87
1:C:198:LEU:C	1:C:198:LEU:HD12	2.00	0.87
1:B:139:TRP:CE2	1:B:179:MET:HE3	2.10	0.86
1:C:221:LEU:CD1	1:C:221:LEU:HG	2.06	0.86
1:A:185:ARG:CG	1:A:185:ARG:NE	2.38	0.86
1:C:101:LEU:O	1:C:104:LYS:HB2	1.75	0.86
1:C:119:ASP:C	1:C:122:GLY:HA3	2.01	0.86
1:B:176:ARG:NH1	3:B:616:PO4:O3	2.09	0.86
1:A:102:SER:HB2	1:A:110:ASP:OD2	1.75	0.85
1:D:37:ILE:CG2	1:D:269:LEU:HD21	2.07	0.85
1:A:187:LEU:HD23	1:A:190:MET:HE3	1.56	0.85
1:B:177:ILE:HG22	1:B:177:ILE:O	1.72	0.85
1:B:176:ARG:NH1	3:B:616:PO4:P	2.49	0.85
1:B:289:ASP:OD1	1:B:289:ASP:N	2.09	0.85
1:D:176:ARG:NH1	3:D:616:PO4:O4	2.09	0.85
1:B:211:GLN:HG3	1:B:249:ILE:HB	1.55	0.85
1:B:304:HIS:HB2	1:B:305:PRO:HA	1.59	0.85
1:D:67:LEU:HB2	1:D:245:PRO:HB2	1.57	0.84
1:A:70:GLU:OE1	1:A:276:PHE:HD2	1.60	0.84
1:B:273:PRO:HA	1:B:304:HIS:CE1	2.13	0.84
1:C:184:PRO:O	1:C:185:ARG:C	2.17	0.83
1:B:172:PRO:CB	1:B:203:VAL:HG11	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:PRO:CB	1:B:306:THR:CA	2.55	0.83
1:D:150:GLU:N	1:D:150:GLU:OE1	2.12	0.83
1:C:239:HIS:HE1	1:C:284:LYS:HG3	1.42	0.83
1:D:196:HIS:CE1	1:D:226:ASN:ND2	2.47	0.83
1:C:239:HIS:CE1	1:C:284:LYS:HG3	2.14	0.83
1:D:301:TYR:CZ	1:D:303:PRO:HG3	2.13	0.82
1:A:68:ARG:HH21	1:A:246:GLY:CA	1.90	0.82
1:B:102:SER:O	1:B:105:GLY:N	2.12	0.82
1:D:37:ILE:HG21	1:D:269:LEU:HD21	1.61	0.82
1:B:152:ASP:OD2	1:B:154:SER:HB3	1.80	0.82
1:C:260:ASN:HD22	1:C:260:ASN:N	1.76	0.82
1:D:115:ARG:NH2	1:D:127:GLU:HA	1.93	0.82
1:A:183:ASN:HB3	1:A:186:ASP:HB2	1.61	0.82
1:D:73:LEU:HD12	1:D:228:ALA:HB2	1.59	0.81
1:A:67:LEU:C	1:A:69:ASP:H	1.80	0.81
1:B:186:ASP:O	1:B:190:MET:HE3	1.80	0.81
1:A:85:LEU:C	1:A:85:LEU:HD12	2.06	0.81
1:B:177:ILE:CG2	1:B:201:PHE:N	2.42	0.81
1:D:80:PHE:O	1:D:83:GLY:N	2.12	0.81
1:A:85:LEU:HD12	1:A:85:LEU:O	1.79	0.81
1:A:85:LEU:HD11	1:A:89:LEU:HD11	1.63	0.81
1:B:283:ARG:CG	1:B:284:LYS:H	1.94	0.81
1:C:184:PRO:HA	1:C:187:LEU:CD1	2.11	0.81
1:C:139:TRP:C	1:C:140:ARG:HD2	2.05	0.81
1:B:184:PRO:HA	1:B:187:LEU:HD12	1.63	0.81
1:D:232:LEU:O	1:D:235:TYR:N	2.14	0.81
1:A:292:LYS:HE3	1:A:292:LYS:CA	2.10	0.80
1:B:165:ILE:HG21	1:B:287:LYS:NZ	1.96	0.80
1:B:215:ARG:HG2	1:B:215:ARG:NH1	1.90	0.80
1:D:37:ILE:HG21	1:D:269:LEU:CD2	2.11	0.80
1:A:30:GLU:HG3	1:A:74:LEU:HD22	1.63	0.80
1:C:240:ILE:CG2	1:C:241:THR:HG22	2.08	0.80
1:C:32:GLN:HE22	1:C:64:ARG:H	1.26	0.80
1:A:263:GLU:HB3	1:A:264:PRO:HD3	0.80	0.80
1:B:100:GLU:O	1:B:103:SER:CB	2.28	0.80
1:A:50:ARG:HH11	1:B:176:ARG:HH21	1.27	0.80
1:D:97:ASN:CG	1:D:99:LYS:HB2	2.07	0.80
1:B:37:ILE:HG22	1:B:38:GLN:N	1.94	0.80
1:D:196:HIS:NE2	1:D:226:ASN:ND2	2.29	0.80
1:C:140:ARG:O	1:C:159:ASP:HA	1.82	0.80
1:B:73:LEU:HD21	1:B:301:TYR:CZ	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:HB	1:C:268:GLN:NE2	1.96	0.80
1:A:56:LEU:HD13	1:A:259:LEU:HD23	1.63	0.79
1:A:279:LEU:O	1:A:280:ARG:NH1	2.15	0.79
1:A:99:LYS:HG3	1:A:129:GLY:HA3	1.65	0.79
1:A:176:ARG:NH1	1:B:193:PRO:HG3	1.96	0.79
1:B:292:LYS:N	1:B:295:ASP:OD1	2.14	0.79
1:D:86:GLU:OE2	1:D:104:LYS:NZ	2.15	0.79
1:C:30:GLU:OE1	1:C:76:THR:OG1	2.00	0.79
1:C:143:GLY:HA2	1:D:185:ARG:HH21	1.47	0.79
1:B:239:HIS:HD1	1:B:281:ILE:HD13	1.47	0.79
1:C:130:ASP:CB	1:C:149:MET:HG2	2.13	0.78
1:B:305:PRO:HB3	1:B:306:THR:HA	1.63	0.78
1:D:135:TYR:O	1:D:137:PHE:N	2.15	0.78
1:D:213:TYR:C	1:D:213:TYR:CD2	2.60	0.78
1:B:176:ARG:HH12	3:B:616:PO4:P	2.05	0.78
1:B:305:PRO:HB2	1:B:306:THR:CA	2.11	0.78
1:C:260:ASN:ND2	1:C:260:ASN:N	2.28	0.78
1:C:140:ARG:HD2	1:C:140:ARG:N	1.98	0.78
1:B:73:LEU:HD23	1:B:301:TYR:HE1	1.45	0.78
1:C:88:LEU:O	1:C:91:PHE:HB2	1.83	0.78
1:A:269:LEU:O	1:A:269:LEU:HD12	1.84	0.78
1:A:307:ILE:O	1:A:308:LYS:NZ	2.14	0.77
1:B:151:SER:O	1:B:153:TYR:CD1	2.36	0.77
1:C:91:PHE:CE1	1:C:135:TYR:HB2	2.19	0.77
1:C:204:VAL:CG2	1:D:47:LYS:HD2	2.14	0.77
1:C:147:ARG:N	1:C:153:TYR:OH	2.17	0.77
1:B:135:TYR:HE1	1:B:196:HIS:HB2	1.50	0.77
1:C:145:GLU:OE1	1:C:185:ARG:NH2	2.17	0.77
1:C:48:ASP:N	1:C:48:ASP:OD2	2.13	0.77
1:A:307:ILE:HD12	1:A:308:LYS:H	1.47	0.77
1:A:184:PRO:O	1:A:188:PRO:HD3	1.85	0.77
1:A:176:ARG:CZ	1:B:193:PRO:HG3	2.15	0.77
1:C:239:HIS:NE2	1:C:284:LYS:HB2	1.99	0.77
1:D:164:VAL:HG13	1:D:177:ILE:HG22	1.67	0.77
1:A:67:LEU:O	1:A:69:ASP:CA	2.33	0.76
1:C:178:ILE:HG22	1:C:199:CYS:O	1.84	0.76
1:D:73:LEU:HD12	1:D:228:ALA:CB	2.14	0.76
1:D:183:ASN:CB	1:D:186:ASP:HB2	2.13	0.76
1:C:76:THR:CB	1:C:268:GLN:HE21	1.98	0.76
1:C:274:ARG:HD2	1:C:304:HIS:CD2	2.21	0.76
1:D:308:LYS:C	1:D:308:LYS:CD	2.46	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HB2	1:C:188:PRO:HD3	1.67	0.76
1:A:85:LEU:HD12	1:A:89:LEU:HD12	1.68	0.75
1:D:94:GLY:HA3	1:D:136:GLY:O	1.85	0.75
1:A:67:LEU:O	1:A:69:ASP:HA	1.86	0.75
1:A:130:ASP:CG	1:A:149:MET:HG2	2.10	0.75
1:A:135:TYR:CE1	1:A:194:PRO:HB3	2.21	0.75
1:A:187:LEU:O	1:A:189:LEU:N	2.19	0.75
1:D:296:PHE:O	1:D:297:GLN:HG3	1.86	0.75
1:A:97:ASN:ND2	1:A:149:MET:HE1	2.01	0.75
1:C:283:ARG:HG2	1:C:285:VAL:CG2	2.16	0.75
1:D:79:VAL:HG11	1:D:225:PHE:HA	1.67	0.75
1:B:139:TRP:CD2	1:B:179:MET:HE3	2.22	0.74
1:C:32:GLN:HE22	1:C:64:ARG:N	1.85	0.74
1:B:172:PRO:HB3	1:B:203:VAL:HG11	1.67	0.74
1:C:213:TYR:HD2	1:D:213:TYR:HD1	1.35	0.74
1:B:28:HIS:ND1	1:B:29:GLY:N	2.34	0.74
1:B:288:ILE:O	1:B:291:PHE:HD2	1.70	0.74
1:B:163:ARG:HA	1:B:166:ASP:OD1	1.87	0.74
1:A:67:LEU:C	1:A:69:ASP:N	2.41	0.74
1:A:74:LEU:HD12	1:A:224:PRO:HB3	0.91	0.74
1:D:97:ASN:HD21	1:D:99:LYS:CG	2.00	0.74
1:A:259:LEU:O	1:A:260:ASN:C	2.29	0.74
1:C:199:CYS:HA	1:C:211:GLN:O	1.88	0.74
1:C:257:ILE:HG13	1:C:257:ILE:O	1.82	0.74
1:C:185:ARG:O	1:C:188:PRO:HD2	1.87	0.73
1:D:280:ARG:HD2	1:D:299:GLU:CD	2.12	0.73
1:B:143:GLY:HA2	1:B:185:ARG:NH2	2.02	0.73
1:D:112:ASN:ND2	1:D:191:ALA:CB	2.46	0.73
1:B:47:LYS:O	1:B:55:THR:HB	1.88	0.73
1:D:97:ASN:HD21	1:D:99:LYS:HG3	1.53	0.73
1:D:220:GLY:C	1:D:221:LEU:HG	2.13	0.73
1:B:287:LYS:HD3	1:B:288:ILE:CG2	2.17	0.73
1:D:115:ARG:HG2	1:D:128:GLU:OE1	1.88	0.73
1:D:203:VAL:HG22	1:D:208:LEU:HD13	1.70	0.73
1:C:192:LEU:HD13	1:C:192:LEU:O	1.88	0.73
1:B:231:ALA:O	1:B:234:THR:N	2.22	0.72
1:D:80:PHE:CE1	1:D:82:LYS:HB2	2.24	0.72
1:D:203:VAL:HA	1:D:207:GLU:O	1.89	0.72
1:A:192:LEU:HD12	1:A:192:LEU:N	2.04	0.72
1:D:270:GLN:HA	1:D:270:GLN:OE1	1.88	0.72
1:B:32:GLN:NE2	1:B:32:GLN:CA	2.41	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HG23	1:C:200:GLN:HB2	1.70	0.72
1:C:148:ASP:OD2	1:C:151:SER:CB	2.35	0.72
1:A:185:ARG:NH2	1:A:185:ARG:HB3	2.04	0.72
1:D:101:LEU:C	1:D:103:SER:N	2.45	0.72
1:D:239:HIS:ND1	1:D:281:ILE:HD13	2.04	0.72
1:A:50:ARG:NH1	1:B:176:ARG:NH2	2.33	0.72
1:C:292:LYS:N	1:C:295:ASP:OD1	2.23	0.72
1:B:172:PRO:HB2	1:B:203:VAL:CG1	2.20	0.72
1:A:149:MET:O	1:A:150:GLU:HG3	1.88	0.72
1:B:75:THR:O	1:B:77:LYS:N	2.23	0.72
1:C:271:ARG:HH22	1:C:307:ILE:HG22	1.54	0.72
1:A:134:VAL:O	1:A:135:TYR:C	2.32	0.71
1:C:308:LYS:HE2	1:C:308:LYS:HA	1.72	0.71
1:D:26:PRO:N	1:D:27:PRO:CD	2.52	0.71
1:D:213:TYR:HD2	1:D:213:TYR:O	1.72	0.71
1:D:225:PHE:O	1:D:226:ASN:C	2.32	0.71
1:B:239:HIS:CE1	1:B:281:ILE:HG21	2.25	0.71
1:C:285:VAL:CG1	1:C:286:GLU:H	2.04	0.71
1:C:240:ILE:HG22	1:C:241:THR:HG23	1.68	0.71
1:D:54:GLY:HA3	1:D:259:LEU:HD11	1.71	0.71
1:D:101:LEU:HA	1:D:104:LYS:HE3	1.73	0.71
1:B:263:GLU:HG2	1:B:266:LYS:NZ	2.06	0.71
1:D:138:GLN:OE1	1:D:138:GLN:CA	2.38	0.71
1:D:54:GLY:C	1:D:259:LEU:HD11	2.14	0.70
1:D:80:PHE:CE1	1:D:82:LYS:CB	2.74	0.70
1:A:91:PHE:CD1	1:A:135:TYR:HB2	2.25	0.70
1:B:283:ARG:HG2	1:B:284:LYS:N	2.06	0.70
1:A:85:LEU:CD1	1:A:89:LEU:CD1	2.70	0.70
1:B:143:GLY:CA	1:B:185:ARG:HH22	2.05	0.70
1:C:258:TYR:HB3	1:C:260:ASN:HD21	1.57	0.70
1:B:176:ARG:NH1	3:B:616:PO4:O1	2.25	0.70
1:B:160:GLN:HE22	1:B:180:CYS:H	0.77	0.70
1:D:163:ARG:O	1:D:164:VAL:C	2.29	0.70
1:D:80:PHE:O	1:D:84:VAL:HG23	1.91	0.70
1:A:68:ARG:NH2	1:A:246:GLY:HA2	2.07	0.70
1:B:177:ILE:C	1:B:178:ILE:HG13	2.16	0.70
1:A:85:LEU:CD1	1:A:89:LEU:HD11	2.22	0.69
1:A:148:ASP:OD1	1:A:150:GLU:N	2.24	0.69
1:D:261:HIS:C	1:D:264:PRO:HD2	2.18	0.69
1:D:265:LEU:HA	1:D:268:GLN:HB3	1.74	0.69
1:B:119:ASP:HA	1:B:122:GLY:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:MET:O	1:C:149:MET:HE3	1.92	0.69
1:B:274:ARG:CZ	1:B:304:HIS:HD2	2.06	0.69
1:C:93:LYS:NZ	1:C:100:GLU:HG3	2.07	0.69
1:A:279:LEU:HD12	1:A:279:LEU:C	2.15	0.69
1:B:133:PRO:HG2	1:B:190:MET:HG3	1.75	0.69
1:C:112:ASN:HD22	1:C:112:ASN:H	1.41	0.69
1:C:115:ARG:NH2	1:C:128:GLU:CA	2.54	0.69
1:D:47:LYS:O	1:D:55:THR:HG22	1.92	0.69
1:D:135:TYR:C	1:D:137:PHE:N	2.37	0.69
1:B:76:THR:C	1:B:305:PRO:HD3	2.16	0.69
1:B:282:LEU:HD11	1:B:297:GLN:HG2	1.74	0.69
1:A:76:THR:OG1	1:A:268:GLN:NE2	2.22	0.69
1:A:240:ILE:CD1	1:A:288:ILE:HA	2.20	0.69
1:A:288:ILE:HG23	1:A:289:ASP:N	2.07	0.69
1:B:277:PRO:HB3	1:B:301:TYR:CD1	2.27	0.69
1:D:164:VAL:HG13	1:D:177:ILE:CG2	2.23	0.69
1:D:166:ASP:N	1:D:166:ASP:OD2	2.16	0.69
1:D:259:LEU:O	1:D:260:ASN:C	2.35	0.69
1:A:32:GLN:NE2	1:A:64:ARG:H	1.91	0.69
1:D:91:PHE:O	1:D:136:GLY:HA2	1.93	0.69
1:C:215:ARG:HD2	1:D:175:ARG:O	1.91	0.69
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.74	0.69
1:A:97:ASN:HB3	1:A:100:GLU:H	1.59	0.68
1:C:47:LYS:O	1:C:55:THR:N	2.23	0.68
1:D:126:ARG:HD2	1:D:130:ASP:CG	2.18	0.68
1:A:115:ARG:HH22	1:A:127:GLU:HA	1.58	0.68
1:D:47:LYS:O	1:D:55:THR:CG2	2.41	0.68
1:B:105:GLY:C	1:B:106:VAL:CG2	2.66	0.68
1:B:198:LEU:HD12	1:B:198:LEU:C	2.18	0.68
1:D:160:GLN:O	1:D:161:LEU:C	2.35	0.68
1:D:279:LEU:HG	1:D:280:ARG:N	2.08	0.68
1:C:118:LEU:O	1:C:122:GLY:O	2.12	0.68
1:A:59:PHE:O	1:B:64:ARG:NH1	2.25	0.68
1:B:267:ILE:O	1:B:270:GLN:N	2.24	0.68
1:D:223:VAL:O	1:D:227:ILE:CG1	2.41	0.68
1:D:97:ASN:HB3	1:D:100:GLU:HG3	1.74	0.68
1:A:81:TRP:CD2	1:A:298:ILE:HD11	2.29	0.67
1:B:262:ILE:HG22	1:B:263:GLU:N	2.09	0.67
1:D:97:ASN:HB2	1:D:149:MET:HE1	1.76	0.67
1:D:218:ASP:C	1:D:220:GLY:H	2.02	0.67
1:B:187:LEU:H	1:B:188:PRO:HD2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:NH2	1:D:126:ARG:O	2.27	0.67
1:C:285:VAL:CG1	1:C:286:GLU:N	2.57	0.67
1:B:177:ILE:HG21	1:B:201:PHE:HB2	1.77	0.67
1:B:205:ASN:O	1:B:206:SER:HB2	1.93	0.67
1:A:171:ASN:O	1:A:174:ASP:HB2	1.95	0.67
1:A:204:VAL:HG21	1:B:45:VAL:CG2	2.24	0.67
1:D:96:THR:CG2	1:D:134:VAL:CG2	2.73	0.67
1:D:133:PRO:HG2	1:D:190:MET:HE3	1.77	0.67
1:D:165:ILE:HG22	1:D:166:ASP:N	2.10	0.67
1:A:31:LEU:HD22	1:A:273:PRO:HG2	1.77	0.66
1:A:91:PHE:CE1	1:A:135:TYR:HB2	2.30	0.66
1:D:54:GLY:CA	1:D:259:LEU:HD11	2.24	0.66
1:D:80:PHE:C	1:D:84:VAL:HG23	2.19	0.66
1:A:74:LEU:O	1:A:301:TYR:OH	2.11	0.66
1:D:281:ILE:HA	1:D:295:ASP:O	1.96	0.66
1:B:97:ASN:ND2	1:B:100:GLU:H	1.92	0.66
1:B:188:PRO:O	1:B:190:MET:N	2.28	0.66
1:A:85:LEU:HD12	1:A:89:LEU:CD1	2.25	0.66
1:D:97:ASN:ND2	1:D:99:LYS:CG	2.58	0.66
1:D:135:TYR:H	1:D:135:TYR:HD2	1.43	0.66
1:B:263:GLU:HG2	1:B:266:LYS:HZ1	1.60	0.66
1:C:88:LEU:HD22	1:C:232:LEU:HD23	1.76	0.66
1:C:98:ALA:HB2	1:C:131:LEU:HD21	1.78	0.66
1:A:130:ASP:OD2	1:A:130:ASP:C	2.37	0.66
1:C:72:PRO:HA	1:C:276:PHE:CZ	2.30	0.66
1:D:101:LEU:O	1:D:102:SER:C	2.39	0.66
1:D:274:ARG:HH11	1:D:274:ARG:CG	2.09	0.66
1:A:28:HIS:HB3	1:A:31:LEU:HD23	1.78	0.65
1:D:213:TYR:CD2	1:D:213:TYR:O	2.49	0.65
1:A:115:ARG:O	1:A:116:ASP:C	2.38	0.65
1:C:257:ILE:HD11	1:C:262:ILE:CG1	2.24	0.65
1:A:187:LEU:HD23	1:A:190:MET:CE	2.26	0.65
1:C:283:ARG:HG2	1:C:285:VAL:HG22	1.76	0.65
1:D:130:ASP:OD1	1:D:149:MET:HG2	1.97	0.65
1:D:274:ARG:HH11	1:D:274:ARG:HB2	1.61	0.65
1:C:69:ASP:OD1	1:C:69:ASP:O	2.13	0.65
1:A:140:ARG:O	1:A:141:HIS:CG	2.49	0.65
1:A:192:LEU:HD12	1:A:192:LEU:H	1.61	0.65
1:B:119:ASP:C	1:B:122:GLY:H	2.04	0.65
1:D:88:LEU:O	1:D:91:PHE:N	2.30	0.65
1:A:176:ARG:NH2	1:B:193:PRO:HG3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HA	1:A:187:LEU:HG	1.78	0.65
1:A:260:ASN:ND2	1:A:260:ASN:N	2.09	0.65
1:C:186:ASP:O	1:C:189:LEU:HB2	1.97	0.65
1:C:288:ILE:HD13	1:C:291:PHE:HD2	1.60	0.65
1:D:30:GLU:HG2	1:D:30:GLU:O	1.94	0.65
1:B:223:VAL:O	1:B:227:ILE:HG13	1.96	0.65
1:C:204:VAL:HG23	1:D:47:LYS:HD2	1.79	0.65
1:D:169:LYS:HD2	1:D:241:THR:HG22	1.78	0.65
1:A:55:THR:HG22	1:A:258:TYR:HA	1.78	0.65
1:B:172:PRO:CB	1:B:203:VAL:CG1	2.75	0.65
1:C:90:TRP:CE3	1:C:101:LEU:HD22	2.32	0.65
1:B:85:LEU:HD12	1:B:85:LEU:C	2.22	0.64
1:B:278:LYS:HB3	1:B:299:GLU:HB3	1.78	0.64
1:C:88:LEU:O	1:C:92:ILE:HG12	1.96	0.64
1:B:97:ASN:HA	1:B:129:GLY:O	1.95	0.64
1:D:30:GLU:OE1	1:D:74:LEU:HB3	1.97	0.64
1:B:88:LEU:HD21	1:B:233:LEU:HD13	1.78	0.64
1:B:100:GLU:C	1:B:103:SER:HB2	2.22	0.64
1:B:272:GLU:O	1:B:304:HIS:CE1	2.51	0.64
1:D:284:LYS:O	1:D:285:VAL:HG22	1.98	0.64
1:B:177:ILE:O	1:B:200:GLN:HA	1.98	0.64
1:A:114:SER:HB2	1:A:116:ASP:OD2	1.97	0.64
1:A:195:CYS:O	1:A:214:GLN:CA	2.43	0.64
1:B:178:ILE:HG22	1:B:179:MET:N	2.13	0.64
1:C:115:ARG:HH21	1:C:128:GLU:CA	2.07	0.64
1:D:89:LEU:HD22	1:D:291:PHE:O	1.98	0.64
1:C:292:LYS:HG3	1:C:294:GLU:OE1	1.97	0.64
1:B:40:ILE:HG21	1:B:257:ILE:HD12	1.79	0.64
1:D:101:LEU:C	1:D:103:SER:H	2.06	0.64
1:D:261:HIS:O	1:D:264:PRO:HD2	1.97	0.64
1:D:83:GLY:HA2	1:D:106:VAL:CG2	2.28	0.64
1:D:218:ASP:C	1:D:218:ASP:OD2	2.39	0.64
1:D:307:ILE:HG23	1:D:308:LYS:H	1.62	0.64
1:A:184:PRO:O	1:A:185:ARG:C	2.38	0.63
1:B:165:ILE:HG21	1:B:287:LYS:HZ1	1.63	0.63
1:C:204:VAL:CG1	1:D:45:VAL:HG21	2.27	0.63
1:B:91:PHE:HB3	1:B:139:TRP:CZ3	2.34	0.63
1:B:97:ASN:HD21	1:B:100:GLU:H	1.44	0.63
1:B:287:LYS:CD	1:B:288:ILE:N	2.45	0.63
1:B:304:HIS:CB	1:B:305:PRO:HA	2.27	0.63
1:C:76:THR:O	1:C:271:ARG:NH1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASP:C	1:C:122:GLY:CA	2.70	0.63
1:C:285:VAL:HG12	1:C:286:GLU:N	2.13	0.63
1:D:248:PHE:C	1:D:249:ILE:HG12	2.22	0.63
1:B:145:GLU:HB2	1:B:147:ARG:NH2	2.14	0.63
1:C:68:ARG:O	1:C:69:ASP:OD2	2.16	0.63
1:A:126:ARG:HD3	1:A:130:ASP:CG	2.24	0.63
1:B:220:GLY:O	1:B:221:LEU:HD12	1.98	0.63
1:B:222:GLY:O	1:B:225:PHE:HB3	1.98	0.63
1:B:174:ASP:OD1	1:B:176:ARG:HG3	1.98	0.63
1:D:282:LEU:HD11	1:D:297:GLN:HB2	1.81	0.63
1:A:207:GLU:HA	1:A:244:LYS:O	1.99	0.63
1:D:112:ASN:HB3	1:D:131:LEU:HD22	1.80	0.63
1:B:287:LYS:CG	1:B:289:ASP:OD1	2.45	0.63
1:C:85:LEU:HD11	1:C:89:LEU:HD11	1.81	0.63
1:A:32:GLN:HE21	1:A:64:ARG:H	1.45	0.63
1:B:105:GLY:O	1:B:106:VAL:HG22	1.98	0.63
1:B:135:TYR:CE1	1:B:196:HIS:HB2	2.33	0.63
1:C:88:LEU:CD2	1:C:232:LEU:HD23	2.29	0.62
1:C:184:PRO:HD2	1:D:142:PHE:CE2	2.34	0.62
1:C:277:PRO:C	1:C:278:LYS:HG2	2.23	0.62
1:C:307:ILE:HD13	1:C:307:ILE:O	1.99	0.62
1:D:148:ASP:OD2	1:D:148:ASP:C	2.43	0.62
1:A:81:TRP:O	1:A:82:LYS:C	2.42	0.62
1:A:262:ILE:HG22	1:A:266:LYS:HD3	1.80	0.62
1:A:85:LEU:O	1:A:89:LEU:HD12	2.00	0.62
1:A:187:LEU:C	1:A:189:LEU:N	2.56	0.62
1:A:279:LEU:O	1:A:279:LEU:HG	1.99	0.62
1:D:78:ARG:HD2	1:D:301:TYR:OH	1.99	0.62
1:D:101:LEU:HG	1:D:106:VAL:HB	1.81	0.62
1:D:263:GLU:HB2	1:D:264:PRO:HD3	1.80	0.62
1:D:133:PRO:HG2	1:D:190:MET:CE	2.30	0.62
1:B:160:GLN:NE2	1:B:180:CYS:N	2.29	0.62
1:C:97:ASN:OD1	1:C:98:ALA:N	2.32	0.62
1:C:204:VAL:HG21	1:D:47:LYS:HD2	1.80	0.62
1:C:308:LYS:HA	1:C:308:LYS:CE	2.29	0.62
1:B:29:GLY:O	1:B:32:GLN:CB	2.45	0.62
1:D:32:GLN:NE2	1:D:32:GLN:HA	2.15	0.62
1:D:50:ARG:C	1:D:52:GLY:H	2.05	0.62
1:D:85:LEU:O	1:D:89:LEU:HD12	2.00	0.62
1:D:149:MET:HG3	1:D:150:GLU:N	2.10	0.61
1:D:60:GLY:HA2	1:D:252:LEU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:THR:HG21	1:D:134:VAL:CG2	2.30	0.61
1:A:115:ARG:NH2	1:A:127:GLU:HA	2.13	0.61
1:A:283:ARG:CZ	1:A:285:VAL:CG2	2.77	0.61
1:C:218:ASP:C	1:C:218:ASP:OD1	2.41	0.61
1:D:47:LYS:CE	1:D:47:LYS:CG	2.73	0.61
1:B:301:TYR:O	1:B:303:PRO:CD	2.46	0.61
1:A:140:ARG:C	1:A:141:HIS:CG	2.79	0.61
1:B:299:GLU:C	1:B:301:TYR:N	2.58	0.61
1:C:57:SER:HB2	1:C:256:HIS:HB3	1.82	0.61
1:B:41:LEU:HD23	1:B:41:LEU:N	2.14	0.61
1:A:49:ASP:OD2	1:A:49:ASP:C	2.43	0.61
1:C:284:LYS:HA	1:C:285:VAL:HG23	1.83	0.61
1:D:85:LEU:O	1:D:89:LEU:CD1	2.48	0.61
1:A:34:LEU:HD11	1:A:76:THR:HG21	1.82	0.60
1:A:113:GLY:O	1:A:118:LEU:HD12	1.99	0.60
1:D:135:TYR:O	1:D:136:GLY:C	2.44	0.60
1:D:280:ARG:CD	1:D:299:GLU:OE2	2.44	0.60
1:A:177:ILE:C	1:A:178:ILE:HG13	2.25	0.60
1:A:268:GLN:C	1:A:270:GLN:N	2.55	0.60
1:A:298:ILE:HG22	1:A:299:GLU:N	2.11	0.60
1:B:105:GLY:C	1:B:106:VAL:HG23	2.25	0.60
1:B:177:ILE:HG21	1:B:201:PHE:H	1.62	0.60
1:D:86:GLU:C	1:D:88:LEU:N	2.54	0.60
1:D:274:ARG:CG	1:D:274:ARG:NH1	2.61	0.60
1:B:287:LYS:N	1:B:290:ASP:OD2	2.34	0.60
1:C:115:ARG:O	1:C:118:LEU:HB3	2.01	0.60
1:D:97:ASN:C	1:D:99:LYS:N	2.52	0.60
1:D:101:LEU:O	1:D:103:SER:N	2.33	0.60
1:D:259:LEU:O	1:D:262:ILE:N	2.34	0.60
1:D:274:ARG:NH1	1:D:274:ARG:HG2	2.15	0.60
1:A:85:LEU:HD11	1:A:89:LEU:CD1	2.30	0.60
1:B:279:LEU:HD12	1:B:297:GLN:O	2.01	0.60
1:C:184:PRO:HA	1:C:187:LEU:HD12	1.84	0.60
1:C:206:SER:O	1:C:244:LYS:HG2	2.02	0.60
1:C:186:ASP:HB3	1:C:189:LEU:HD13	1.84	0.60
1:D:192:LEU:HD23	1:D:193:PRO:O	2.02	0.60
1:B:263:GLU:CG	1:B:266:LYS:HZ1	2.15	0.60
1:C:143:GLY:CA	1:D:185:ARG:HH21	2.10	0.60
1:B:41:LEU:HD12	1:B:262:ILE:HD12	1.84	0.60
1:B:288:ILE:O	1:B:291:PHE:CD2	2.54	0.60
1:A:292:LYS:HA	1:A:292:LYS:CE	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:SER:OG	1:C:96:THR:N	2.34	0.59
1:C:170:THR:O	1:C:171:ASN:HB3	2.02	0.59
1:C:213:TYR:CD1	1:C:213:TYR:C	2.80	0.59
1:C:207:GLU:HA	1:C:244:LYS:O	2.03	0.59
1:C:293:ALA:O	1:C:296:PHE:HB2	2.02	0.59
1:A:152:ASP:OD1	1:A:152:ASP:C	2.46	0.59
1:A:178:ILE:HD11	1:B:215:ARG:HG3	1.83	0.59
1:B:178:ILE:HA	1:B:199:CYS:O	2.02	0.59
1:D:67:LEU:CB	1:D:245:PRO:HB2	2.31	0.59
1:B:119:ASP:OD1	1:B:122:GLY:CA	2.45	0.59
1:D:109:TRP:HB3	1:D:131:LEU:HD21	1.83	0.59
1:D:220:GLY:O	1:D:221:LEU:HD23	2.03	0.59
1:C:83:GLY:O	1:C:87:GLU:HB2	2.02	0.59
1:A:70:GLU:OE1	1:A:276:PHE:CD2	2.51	0.59
1:B:234:THR:O	1:B:237:ILE:N	2.34	0.59
1:D:67:LEU:HB3	1:D:235:TYR:CE2	2.37	0.59
1:D:96:THR:HG21	1:D:134:VAL:HG22	1.83	0.59
1:D:187:LEU:O	1:D:188:PRO:C	2.42	0.59
1:B:77:LYS:HB2	1:B:268:GLN:NE2	2.18	0.59
1:C:70:GLU:HB3	1:C:276:PHE:HB3	1.84	0.59
1:C:72:PRO:O	1:C:72:PRO:HG2	2.00	0.59
1:D:74:LEU:N	1:D:74:LEU:HD23	2.18	0.59
1:D:101:LEU:CD2	1:D:106:VAL:O	2.51	0.59
1:D:178:ILE:HG22	1:D:178:ILE:O	2.01	0.59
1:C:130:ASP:CG	1:C:149:MET:HG2	2.28	0.59
1:A:267:ILE:O	1:A:270:GLN:HB2	2.03	0.58
1:C:178:ILE:HG23	1:C:200:GLN:HA	1.85	0.58
1:D:92:ILE:HG23	1:D:161:LEU:CD2	2.33	0.58
1:A:98:ALA:HB2	1:A:131:LEU:HD21	1.85	0.58
1:A:268:GLN:C	1:A:270:GLN:H	2.08	0.58
1:B:175:ARG:HG2	3:B:616:PO4:O4	2.02	0.58
1:B:304:HIS:HB2	1:B:305:PRO:CA	2.31	0.58
1:D:86:GLU:O	1:D:88:LEU:N	2.35	0.58
1:A:219:MET:HA	1:A:223:VAL:HB	1.84	0.58
1:A:292:LYS:CA	1:A:292:LYS:CE	2.80	0.58
1:B:299:GLU:HG3	1:B:300:GLY:H	1.67	0.58
1:C:123:PHE:HA	1:C:124:SER:OG	2.02	0.58
1:D:102:SER:HB3	1:D:110:ASP:OD2	2.02	0.58
1:D:265:LEU:O	1:D:269:LEU:N	2.35	0.58
1:A:50:ARG:HD2	1:B:176:ARG:NH1	2.17	0.58
1:A:114:SER:OG	1:A:117:PHE:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD21	1:B:233:LEU:HA	1.85	0.58
1:B:208:LEU:HD12	1:B:209:SER:N	2.18	0.58
1:C:213:TYR:CD2	1:D:213:TYR:HD1	2.18	0.58
1:D:177:ILE:CD1	1:D:177:ILE:N	2.67	0.58
1:C:115:ARG:CZ	1:C:118:LEU:HD22	2.34	0.58
1:C:307:ILE:O	1:C:307:ILE:CG1	2.52	0.58
1:A:114:SER:OG	1:A:114:SER:O	2.20	0.58
1:C:151:SER:HB3	1:C:153:TYR:CE1	2.38	0.58
1:D:43:CYS:SG	1:D:43:CYS:CA	2.90	0.58
1:A:69:ASP:HA	1:A:235:TYR:OH	2.04	0.58
1:C:107:LYS:C	1:C:109:TRP:N	2.54	0.58
1:B:102:SER:O	1:B:103:SER:C	2.46	0.57
1:C:97:ASN:OD1	1:C:97:ASN:C	2.44	0.57
1:C:237:ILE:O	1:C:241:THR:HG23	2.03	0.57
1:D:90:TRP:NE1	1:D:101:LEU:HB3	2.18	0.57
1:A:204:VAL:CG2	1:B:45:VAL:HG21	2.34	0.57
1:B:227:ILE:HG23	1:B:248:PHE:CE2	2.38	0.57
1:C:175:ARG:HG3	1:D:254:ASP:OD1	2.04	0.57
1:D:80:PHE:CE1	1:D:82:LYS:HB3	2.37	0.57
1:D:179:MET:HE2	1:D:199:CYS:SG	2.44	0.57
1:D:274:ARG:HH11	1:D:274:ARG:CB	2.17	0.57
1:A:62:GLN:HG3	1:A:251:THR:OG1	2.02	0.57
1:A:271:ARG:NH2	1:A:307:ILE:HB	2.19	0.57
1:B:88:LEU:O	1:B:89:LEU:C	2.46	0.57
1:B:160:GLN:NE2	1:B:179:MET:HA	2.18	0.57
1:B:244:LYS:CD	1:B:244:LYS:CB	2.80	0.57
1:B:68:ARG:O	1:B:69:ASP:HB2	2.03	0.57
1:B:123:PHE:HB3	1:B:126:ARG:HD2	1.87	0.57
1:B:124:SER:C	1:B:126:ARG:H	2.11	0.57
1:D:101:LEU:HD21	1:D:106:VAL:O	2.05	0.57
1:A:50:ARG:NH1	1:B:176:ARG:HH21	2.00	0.57
1:B:223:VAL:HB	1:B:224:PRO:HD3	1.86	0.57
1:C:288:ILE:HD13	1:C:291:PHE:CD2	2.39	0.57
1:C:178:ILE:HG23	1:C:200:GLN:CB	2.33	0.57
1:D:204:VAL:O	1:D:207:GLU:CB	2.42	0.57
1:A:33:TYR:HA	1:A:36:GLN:HG3	1.87	0.57
1:C:277:PRO:O	1:C:278:LYS:HG2	2.05	0.57
1:C:68:ARG:O	1:C:69:ASP:CG	2.48	0.57
1:D:263:GLU:N	1:D:264:PRO:CD	2.67	0.57
1:A:202:TYR:O	1:A:202:TYR:CD2	2.58	0.57
1:B:239:HIS:C	1:B:239:HIS:CD2	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HA	1:A:276:PHE:CD1	2.40	0.56
1:D:203:VAL:CG2	1:D:208:LEU:CD1	2.82	0.56
1:A:56:LEU:HD13	1:A:259:LEU:CD2	2.35	0.56
1:A:68:ARG:NH2	1:A:246:GLY:CA	2.66	0.56
1:A:154:SER:C	1:A:156:GLN:H	2.13	0.56
1:A:187:LEU:CA	1:A:190:MET:HE3	2.29	0.56
1:A:294:GLU:CD	1:A:294:GLU:H	2.12	0.56
1:B:290:ASP:O	1:B:292:LYS:HE3	2.05	0.56
1:A:183:ASN:O	1:A:187:LEU:HG	2.05	0.56
1:A:185:ARG:HB3	1:A:185:ARG:HH21	1.67	0.56
1:B:40:ILE:HD13	1:B:58:VAL:HB	1.87	0.56
1:C:190:MET:O	1:C:191:ALA:C	2.49	0.56
1:D:183:ASN:ND2	1:D:186:ASP:OD1	2.38	0.56
1:A:79:VAL:HG12	1:A:80:PHE:N	2.11	0.56
1:B:94:GLY:HA2	1:B:136:GLY:O	2.05	0.56
1:C:239:HIS:CE1	1:C:284:LYS:HB2	2.41	0.56
1:D:178:ILE:HG13	1:D:200:GLN:HG3	1.86	0.56
1:D:222:GLY:O	1:D:226:ASN:OD1	2.24	0.56
1:B:110:ASP:C	1:B:112:ASN:N	2.64	0.56
1:B:238:ALA:HB1	1:B:243:LEU:O	2.06	0.56
1:C:115:ARG:HH22	1:C:127:GLU:C	2.12	0.56
1:A:232:LEU:HD12	1:A:232:LEU:C	2.23	0.56
1:B:205:ASN:O	1:B:206:SER:CB	2.48	0.56
1:D:135:TYR:CD2	1:D:135:TYR:N	2.73	0.56
1:D:176:ARG:NH1	3:D:616:PO4:O1	2.39	0.56
1:D:263:GLU:N	1:D:264:PRO:HD2	2.21	0.56
1:B:118:LEU:O	1:B:123:PHE:HB2	2.05	0.56
1:A:130:ASP:CB	1:A:149:MET:HG2	2.35	0.56
1:B:58:VAL:O	1:B:255:ALA:N	2.38	0.56
1:A:187:LEU:N	1:A:188:PRO:HD3	2.21	0.55
1:A:202:TYR:CE1	1:B:47:LYS:HE3	2.41	0.55
1:C:280:ARG:HA	1:C:280:ARG:HD3	1.86	0.55
1:D:92:ILE:HG22	1:D:92:ILE:O	2.06	0.55
1:C:79:VAL:HG12	1:C:80:PHE:N	2.21	0.55
1:C:294:GLU:C	1:C:296:PHE:H	2.13	0.55
1:B:265:LEU:O	1:B:269:LEU:HB2	2.07	0.55
1:C:93:LYS:HZ3	1:C:100:GLU:HG3	1.69	0.55
1:C:112:ASN:H	1:C:112:ASN:ND2	2.03	0.55
1:A:116:ASP:OD1	1:A:116:ASP:N	2.38	0.55
1:B:287:LYS:CD	1:B:288:ILE:CG2	2.72	0.55
1:C:97:ASN:CB	1:C:149:MET:SD	2.91	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:PRO:HA	1:C:187:LEU:CG	2.37	0.55
1:D:86:GLU:HB2	1:D:106:VAL:HG21	1.89	0.55
1:A:81:TRP:O	1:A:83:GLY:N	2.40	0.55
1:A:263:GLU:O	1:A:266:LYS:HB2	2.07	0.55
1:B:82:LYS:HD3	1:B:106:VAL:HG22	1.89	0.55
1:B:145:GLU:HB2	1:B:147:ARG:HH21	1.72	0.55
1:C:186:ASP:O	1:C:190:MET:CG	2.52	0.55
1:D:97:ASN:OD1	1:D:129:GLY:C	2.50	0.55
1:D:115:ARG:HH21	1:D:127:GLU:CA	2.05	0.55
1:D:140:ARG:O	1:D:141:HIS:CG	2.60	0.55
1:D:266:LYS:CB	1:D:266:LYS:CD	2.80	0.55
1:A:187:LEU:HA	1:A:190:MET:HE2	1.86	0.55
1:C:115:ARG:NE	1:C:128:GLU:HB3	2.21	0.55
1:B:118:LEU:O	1:B:123:PHE:N	2.38	0.55
1:C:107:LYS:CA	1:C:110:ASP:OD1	2.42	0.55
1:C:130:ASP:HB2	1:C:149:MET:CG	2.33	0.55
1:D:87:GLU:HG2	1:D:87:GLU:O	2.06	0.55
1:A:103:SER:OG	1:A:104:LYS:NZ	2.40	0.55
1:A:183:ASN:HD21	1:A:185:ARG:NH2	2.05	0.55
1:D:203:VAL:HG23	1:D:208:LEU:HD13	1.86	0.55
1:A:175:ARG:NH2	1:B:55:THR:HG21	2.21	0.54
1:B:75:THR:O	1:B:304:HIS:O	2.26	0.54
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.43	0.54
1:B:34:LEU:HD11	1:B:76:THR:HG21	1.88	0.54
1:D:198:LEU:HD13	1:D:199:CYS:N	2.22	0.54
1:D:218:ASP:C	1:D:220:GLY:N	2.58	0.54
1:A:296:PHE:N	1:A:296:PHE:CD1	2.74	0.54
1:A:307:ILE:CD1	1:A:308:LYS:H	2.17	0.54
1:C:170:THR:O	1:C:171:ASN:CB	2.51	0.54
1:D:97:ASN:O	1:D:100:GLU:N	2.30	0.54
1:A:187:LEU:N	1:A:188:PRO:CD	2.70	0.54
1:A:221:LEU:CD2	1:A:221:LEU:CD1	2.80	0.54
1:B:76:THR:OG1	1:B:268:GLN:NE2	2.35	0.54
1:D:264:PRO:O	1:D:267:ILE:HB	2.07	0.54
1:D:92:ILE:C	1:D:94:GLY:N	2.60	0.54
1:D:218:ASP:O	1:D:220:GLY:N	2.40	0.54
1:A:288:ILE:CG2	1:A:289:ASP:N	2.71	0.54
1:A:164:VAL:O	1:A:168:ILE:HG12	2.07	0.54
1:C:100:GLU:OE1	1:C:100:GLU:HA	2.08	0.54
1:D:92:ILE:O	1:D:140:ARG:HD3	2.08	0.54
1:D:153:TYR:O	1:D:156:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:GLN:OE1	1:D:250:HIS:NE2	2.39	0.54
1:B:171:ASN:O	1:B:171:ASN:ND2	2.41	0.54
1:B:177:ILE:HG21	1:B:201:PHE:CB	2.37	0.54
1:D:274:ARG:HD3	1:D:274:ARG:N	2.23	0.54
1:A:101:LEU:O	1:A:101:LEU:HD12	2.08	0.54
1:B:240:ILE:CG2	1:B:240:ILE:O	2.52	0.54
1:C:91:PHE:O	1:C:136:GLY:HA2	2.08	0.54
1:C:92:ILE:C	1:C:94:GLY:N	2.66	0.54
1:C:283:ARG:NH1	1:C:290:ASP:OD2	2.41	0.54
1:D:101:LEU:HD23	1:D:101:LEU:C	2.32	0.54
1:A:50:ARG:HD2	1:B:176:ARG:CZ	2.37	0.53
1:A:135:TYR:CZ	1:A:194:PRO:HB3	2.43	0.53
1:A:195:CYS:HA	1:A:215:ARG:HG2	1.89	0.53
1:C:223:VAL:O	1:C:227:ILE:HG13	2.09	0.53
1:D:155:GLY:C	1:D:156:GLN:HG2	2.33	0.53
1:D:30:GLU:HG3	1:D:74:LEU:HD13	1.88	0.53
1:A:261:HIS:O	1:A:262:ILE:C	2.50	0.53
1:B:274:ARG:CZ	1:B:304:HIS:CD2	2.88	0.53
1:D:113:GLY:HA3	1:D:129:GLY:HA2	1.89	0.53
1:D:232:LEU:O	1:D:233:LEU:C	2.51	0.53
1:B:273:PRO:HA	1:B:304:HIS:HE1	1.71	0.53
1:C:118:LEU:O	1:C:122:GLY:HA2	2.09	0.53
1:C:131:LEU:HD12	1:C:134:VAL:HG21	1.91	0.53
1:D:148:ASP:OD2	1:D:148:ASP:O	2.26	0.53
1:A:210:CYS:HB3	1:A:248:PHE:HD1	1.73	0.53
1:B:135:TYR:OH	1:B:195:CYS:N	2.31	0.53
1:C:85:LEU:CD1	1:C:89:LEU:HD11	2.38	0.53
1:C:94:GLY:HA2	1:C:136:GLY:HA3	1.91	0.53
1:C:178:ILE:CG2	1:C:200:GLN:HB2	2.38	0.53
1:C:307:ILE:O	1:C:307:ILE:CD1	2.56	0.53
1:D:301:TYR:CZ	1:D:303:PRO:CG	2.89	0.53
1:D:73:LEU:CD1	1:D:228:ALA:CB	2.86	0.53
1:D:88:LEU:HD23	1:D:232:LEU:HD23	1.89	0.53
1:D:271:ARG:HB3	1:D:304:HIS:CE1	2.44	0.53
1:D:137:PHE:C	1:D:137:PHE:CD2	2.87	0.53
1:C:228:ALA:O	1:C:229:SER:C	2.49	0.53
1:C:283:ARG:CG	1:C:285:VAL:CG2	2.86	0.53
1:A:91:PHE:O	1:A:92:ILE:C	2.51	0.53
1:C:88:LEU:CD2	1:C:232:LEU:CD2	2.87	0.53
1:C:92:ILE:O	1:C:93:LYS:C	2.52	0.53
1:D:60:GLY:O	1:D:61:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:O	1:A:156:GLN:N	2.42	0.52
1:A:299:GLU:O	1:A:299:GLU:HG2	2.09	0.52
1:A:196:HIS:N	1:A:196:HIS:CD2	2.75	0.52
1:B:211:GLN:HA	1:B:249:ILE:O	2.09	0.52
1:B:305:PRO:HB2	1:B:306:THR:HG22	1.91	0.52
1:C:88:LEU:HD23	1:C:232:LEU:CD2	2.39	0.52
1:D:37:ILE:HG22	1:D:269:LEU:HD21	1.86	0.52
1:A:257:ILE:HD11	1:A:262:ILE:CG1	2.23	0.52
1:B:92:ILE:O	1:B:140:ARG:HD3	2.09	0.52
1:D:142:PHE:CD2	1:D:143:GLY:N	2.78	0.52
1:A:102:SER:CB	1:A:110:ASP:OD2	2.53	0.52
1:C:93:LYS:HZ1	1:C:100:GLU:HG3	1.74	0.52
1:D:177:ILE:N	1:D:177:ILE:HD12	2.24	0.52
1:A:184:PRO:CA	1:A:187:LEU:HG	2.39	0.52
1:C:81:TRP:O	1:C:84:VAL:N	2.43	0.52
1:A:283:ARG:NH1	1:A:285:VAL:CG2	2.73	0.52
1:B:75:THR:C	1:B:77:LYS:H	2.16	0.52
1:B:301:TYR:O	1:B:301:TYR:CG	2.61	0.52
1:D:233:LEU:HD11	1:D:237:ILE:HD11	1.91	0.52
1:A:222:GLY:O	1:A:223:VAL:C	2.51	0.52
1:B:159:ASP:O	1:B:160:GLN:C	2.52	0.52
1:D:149:MET:HG3	1:D:150:GLU:OE1	2.10	0.52
1:A:149:MET:HE2	1:A:150:GLU:HG3	1.90	0.52
1:A:204:VAL:CG2	1:B:45:VAL:CG2	2.88	0.52
1:B:30:GLU:OE1	1:B:76:THR:HG23	2.10	0.52
1:B:182:TRP:CZ3	1:B:194:PRO:HD2	2.44	0.52
1:B:288:ILE:HD12	1:B:291:PHE:CE2	2.45	0.52
1:C:261:HIS:O	1:C:265:LEU:HB2	2.10	0.52
1:C:285:VAL:HG12	1:C:286:GLU:H	1.70	0.52
1:D:65:TYR:N	1:D:248:PHE:O	2.40	0.52
1:A:283:ARG:CZ	1:A:285:VAL:HG22	2.40	0.52
1:B:76:THR:HA	1:B:304:HIS:ND1	2.25	0.52
1:B:277:PRO:HB3	1:B:301:TYR:HD1	1.71	0.52
1:D:87:GLU:OE1	1:D:91:PHE:HE2	1.93	0.52
1:D:272:GLU:OE2	1:D:273:PRO:HD2	2.10	0.52
1:B:88:LEU:HD11	1:B:233:LEU:HD13	1.92	0.52
1:C:132:GLY:O	1:C:134:VAL:N	2.43	0.52
1:C:221:LEU:CD1	1:C:221:LEU:CB	2.79	0.52
1:A:215:ARG:NH1	1:B:175:ARG:O	2.43	0.51
1:B:178:ILE:CG2	1:B:179:MET:N	2.73	0.51
1:D:87:GLU:O	1:D:90:TRP:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:HG2	1:D:128:GLU:CD	2.35	0.51
1:D:261:HIS:HA	1:D:264:PRO:HG2	1.92	0.51
1:B:47:LYS:O	1:B:55:THR:CG2	2.58	0.51
1:B:97:ASN:HD21	1:B:100:GLU:N	2.09	0.51
1:C:96:THR:CG2	1:C:137:PHE:HB2	2.41	0.51
1:C:172:PRO:O	1:C:203:VAL:HB	2.10	0.51
1:C:178:ILE:HD12	1:C:178:ILE:H	1.75	0.51
1:D:177:ILE:CD1	1:D:177:ILE:H	2.22	0.51
1:B:94:GLY:HA3	1:B:140:ARG:HG3	1.93	0.51
1:B:97:ASN:ND2	1:B:97:ASN:O	2.43	0.51
1:C:134:VAL:O	1:C:138:GLN:CG	2.58	0.51
1:B:274:ARG:NE	1:B:304:HIS:CD2	2.79	0.51
1:C:76:THR:CB	1:C:268:GLN:NE2	2.66	0.51
1:C:99:LYS:C	1:C:101:LEU:N	2.66	0.51
1:C:292:LYS:CG	1:C:294:GLU:OE1	2.58	0.51
1:D:35:GLY:O	1:D:38:GLN:HB3	2.10	0.51
1:C:184:PRO:HA	1:C:187:LEU:HG	1.93	0.51
1:B:88:LEU:HD21	1:B:233:LEU:CD1	2.39	0.51
1:B:88:LEU:HD12	1:B:92:ILE:HG12	1.92	0.51
1:D:162:GLN:O	1:D:166:ASP:OD2	2.28	0.51
1:B:145:GLU:CB	1:B:147:ARG:NH2	2.73	0.51
1:C:114:SER:O	1:C:114:SER:OG	2.18	0.51
1:C:162:GLN:C	1:C:164:VAL:N	2.61	0.51
1:C:307:ILE:O	1:C:308:LYS:HE2	2.11	0.51
1:C:307:ILE:O	1:C:307:ILE:HG12	2.10	0.51
1:D:268:GLN:C	1:D:270:GLN:N	2.66	0.51
1:A:97:ASN:ND2	1:A:99:LYS:HB2	2.25	0.51
1:A:195:CYS:O	1:A:214:GLN:HG3	2.10	0.51
1:C:159:ASP:C	1:C:159:ASP:OD1	2.54	0.51
1:C:190:MET:SD	1:C:194:PRO:HD2	2.50	0.51
1:C:205:ASN:O	1:C:206:SER:OG	2.21	0.51
1:A:130:ASP:OD1	1:A:149:MET:HG2	2.11	0.51
1:A:190:MET:HB2	1:A:192:LEU:O	2.11	0.51
1:C:59:PHE:HA	1:C:253:GLY:O	2.11	0.51
1:C:165:ILE:HG21	1:C:240:ILE:HG21	1.91	0.51
1:D:86:GLU:CD	1:D:104:LYS:NZ	2.69	0.51
1:D:284:LYS:O	1:D:285:VAL:CG2	2.58	0.51
1:A:292:LYS:O	1:A:293:ALA:C	2.52	0.50
1:B:90:TRP:HA	1:B:93:LYS:HE3	1.93	0.50
1:D:67:LEU:HB3	1:D:235:TYR:HE2	1.76	0.50
1:B:160:GLN:HE22	1:B:179:MET:C	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ASP:OD1	1:C:153:TYR:N	2.44	0.50
1:D:171:ASN:O	1:D:172:PRO:C	2.52	0.50
1:A:37:ILE:O	1:A:38:GLN:C	2.51	0.50
1:A:99:LYS:O	1:A:101:LEU:N	2.45	0.50
1:C:142:PHE:CD2	1:D:184:PRO:HG2	2.47	0.50
1:C:236:MET:HE2	1:C:288:ILE:HD11	1.94	0.50
1:D:80:PHE:CZ	1:D:82:LYS:HD3	2.45	0.50
1:D:101:LEU:HD23	1:D:102:SER:H	1.72	0.50
1:D:192:LEU:HD23	1:D:194:PRO:HA	1.93	0.50
1:A:108:ILE:HG13	1:A:109:TRP:N	2.25	0.50
1:A:186:ASP:C	1:A:190:MET:HE2	2.37	0.50
1:C:97:ASN:OD1	1:C:129:GLY:HA3	2.11	0.50
1:D:165:ILE:O	1:D:168:ILE:N	2.44	0.50
1:A:38:GLN:HG2	1:A:269:LEU:HD21	1.92	0.50
1:A:118:LEU:HD22	1:A:126:ARG:O	2.11	0.50
1:B:84:VAL:HG22	1:B:225:PHE:CE1	2.47	0.50
1:B:97:ASN:ND2	1:B:97:ASN:C	2.70	0.50
1:C:276:PHE:HD1	1:C:277:PRO:HD2	1.76	0.50
1:D:86:GLU:C	1:D:88:LEU:H	2.17	0.50
1:D:135:TYR:HD2	1:D:135:TYR:N	2.09	0.50
1:A:119:ASP:O	1:A:120:SER:C	2.55	0.50
1:B:77:LYS:HB2	1:B:268:GLN:HE22	1.76	0.50
1:B:287:LYS:HD3	1:B:288:ILE:CA	2.41	0.50
1:B:293:ALA:C	1:B:295:ASP:H	2.19	0.50
1:C:130:ASP:N	1:C:149:MET:SD	2.85	0.50
1:D:28:HIS:ND1	1:D:28:HIS:C	2.69	0.50
1:D:240:ILE:HD11	1:D:291:PHE:CE2	2.46	0.50
1:A:46:ARG:HA	1:A:55:THR:O	2.12	0.50
1:C:29:GLY:O	1:C:30:GLU:C	2.53	0.50
1:D:50:ARG:C	1:D:52:GLY:N	2.68	0.50
1:D:140:ARG:C	1:D:141:HIS:CG	2.89	0.50
1:D:203:VAL:HG23	1:D:208:LEU:CD1	2.42	0.50
1:D:232:LEU:O	1:D:236:MET:N	2.34	0.50
1:C:142:PHE:CZ	1:D:184:PRO:HD2	2.47	0.50
1:C:292:LYS:O	1:C:293:ALA:C	2.51	0.50
1:D:251:THR:HG22	1:D:252:LEU:N	2.25	0.50
1:B:230:TYR:O	1:B:233:LEU:HB3	2.12	0.50
1:B:266:LYS:O	1:B:269:LEU:HB3	2.12	0.50
1:C:192:LEU:CD1	1:C:192:LEU:N	2.74	0.50
1:D:81:TRP:N	1:D:84:VAL:HG23	2.26	0.50
1:A:50:ARG:CD	3:B:616:PO4:O3	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:OE2	1:B:273:PRO:HB2	2.12	0.49
1:D:47:LYS:O	1:D:55:THR:HG23	2.10	0.49
1:D:79:VAL:HG11	1:D:225:PHE:CA	2.41	0.49
1:A:102:SER:C	1:A:104:LYS:N	2.68	0.49
1:B:101:LEU:O	1:B:102:SER:C	2.56	0.49
1:B:170:THR:HB	1:B:171:ASN:HB3	1.94	0.49
1:B:76:THR:OG1	1:B:268:GLN:HG3	2.12	0.49
1:C:99:LYS:C	1:C:101:LEU:H	2.19	0.49
1:A:102:SER:HB2	1:A:110:ASP:CG	2.37	0.49
1:B:160:GLN:O	1:B:164:VAL:HG23	2.12	0.49
1:C:225:PHE:O	1:C:226:ASN:C	2.52	0.49
1:D:234:THR:O	1:D:235:TYR:C	2.56	0.49
1:B:231:ALA:O	1:B:232:LEU:C	2.56	0.49
1:B:283:ARG:CG	1:B:284:LYS:N	2.57	0.49
1:D:298:ILE:CG2	1:D:301:TYR:HB2	2.42	0.49
1:B:119:ASP:HA	1:B:122:GLY:H	1.76	0.49
1:D:135:TYR:O	1:D:139:TRP:HB2	2.12	0.49
1:A:186:ASP:O	1:A:189:LEU:HB3	2.12	0.49
1:B:36:GLN:O	1:B:39:HIS:HB3	2.13	0.49
1:C:173:ASP:O	1:C:174:ASP:C	2.52	0.49
1:C:237:ILE:N	1:C:237:ILE:HD13	2.28	0.49
1:A:140:ARG:C	1:A:141:HIS:CD2	2.90	0.49
1:A:142:PHE:O	1:A:142:PHE:CD2	2.66	0.49
1:A:227:ILE:O	1:A:228:ALA:C	2.56	0.49
1:B:176:ARG:NH1	3:B:616:PO4:O4	2.44	0.49
1:C:143:GLY:O	1:D:185:ARG:NH2	2.46	0.49
1:D:84:VAL:HG22	1:D:225:PHE:CE1	2.47	0.49
1:D:204:VAL:O	1:D:204:VAL:CG1	2.59	0.49
1:C:211:GLN:HG3	1:C:212:LEU:N	2.28	0.49
1:C:288:ILE:C	1:C:290:ASP:H	2.20	0.49
1:D:32:GLN:HA	1:D:32:GLN:HE21	1.77	0.49
1:B:292:LYS:O	1:B:295:ASP:OD1	2.30	0.49
1:D:111:ALA:O	1:D:112:ASN:C	2.51	0.49
1:D:211:GLN:HG3	1:D:249:ILE:O	2.12	0.49
1:D:259:LEU:O	1:D:261:HIS:N	2.46	0.49
1:C:143:GLY:C	1:D:185:ARG:NH2	2.71	0.48
1:D:77:LYS:CG	1:D:78:ARG:H	2.26	0.48
1:D:261:HIS:O	1:D:262:ILE:C	2.54	0.48
1:A:139:TRP:O	1:A:140:ARG:CB	2.58	0.48
1:C:72:PRO:HA	1:C:276:PHE:CD1	2.44	0.48
1:D:36:GLN:O	1:D:37:ILE:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLU:O	1:D:90:TRP:HB2	2.14	0.48
1:A:147:ARG:HB2	1:A:151:SER:OG	2.13	0.48
1:C:34:LEU:O	1:C:38:GLN:N	2.42	0.48
1:C:96:THR:O	1:C:131:LEU:HG	2.13	0.48
1:C:98:ALA:CB	1:C:131:LEU:HD21	2.42	0.48
1:C:184:PRO:CA	1:C:187:LEU:HD12	2.42	0.48
1:C:201:PHE:N	1:C:201:PHE:CD2	2.81	0.48
1:D:86:GLU:O	1:D:87:GLU:C	2.56	0.48
1:D:92:ILE:HG23	1:D:161:LEU:HD22	1.95	0.48
1:D:115:ARG:NH1	1:D:119:ASP:OD2	2.46	0.48
1:D:251:THR:CG2	1:D:252:LEU:N	2.76	0.48
1:B:233:LEU:HA	1:B:233:LEU:HD12	1.31	0.48
1:C:212:LEU:HD12	1:C:213:TYR:H	1.79	0.48
1:D:268:GLN:O	1:D:270:GLN:N	2.47	0.48
1:A:173:ASP:O	1:A:174:ASP:C	2.53	0.48
1:B:135:TYR:CZ	1:B:194:PRO:HA	2.49	0.48
1:C:116:ASP:O	1:C:119:ASP:N	2.46	0.48
1:C:257:ILE:CD1	1:C:258:TYR:O	2.62	0.48
1:D:74:LEU:HD23	1:D:74:LEU:H	1.78	0.48
1:D:126:ARG:HB3	1:D:130:ASP:HB3	1.95	0.48
1:A:135:TYR:O	1:A:139:TRP:N	2.46	0.48
1:C:83:GLY:HA2	1:C:106:VAL:HG21	1.94	0.48
1:C:139:TRP:H	1:C:139:TRP:CD1	2.32	0.48
1:C:257:ILE:HD12	1:C:258:TYR:O	2.13	0.48
1:D:172:PRO:O	1:D:174:ASP:N	2.46	0.48
1:C:162:GLN:HG3	1:C:166:ASP:OD1	2.13	0.48
1:D:187:LEU:N	1:D:187:LEU:HD23	2.28	0.48
1:D:265:LEU:HA	1:D:268:GLN:CB	2.43	0.48
1:A:62:GLN:HA	1:A:250:HIS:O	2.14	0.48
1:B:172:PRO:O	1:B:203:VAL:HG12	2.14	0.48
1:D:148:ASP:OD2	1:D:151:SER:OG	2.23	0.48
1:D:285:VAL:HG13	1:D:290:ASP:HB2	1.96	0.48
1:A:142:PHE:CD2	1:A:142:PHE:C	2.92	0.48
1:B:40:ILE:CG2	1:B:257:ILE:HD12	2.42	0.48
1:B:299:GLU:CG	1:B:300:GLY:H	2.26	0.48
1:C:31:LEU:O	1:C:32:GLN:C	2.55	0.48
1:C:161:LEU:O	1:C:164:VAL:HB	2.14	0.48
1:D:105:GLY:HA2	1:D:107:LYS:NZ	2.29	0.48
1:D:118:LEU:O	1:D:119:ASP:C	2.57	0.48
1:D:198:LEU:C	1:D:198:LEU:HD13	2.35	0.48
1:A:183:ASN:O	1:A:187:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:MET:HG2	1:A:291:PHE:CE2	2.48	0.48
1:B:164:VAL:O	1:B:168:ILE:HG12	2.13	0.48
1:B:200:GLN:O	1:B:210:CYS:HA	2.14	0.48
1:B:304:HIS:C	1:B:305:PRO:O	2.56	0.48
1:D:45:VAL:HG23	1:D:46:ARG:O	2.13	0.48
1:D:54:GLY:HA3	1:D:259:LEU:CD1	2.42	0.48
1:D:259:LEU:HA	1:D:262:ILE:HD12	1.95	0.48
1:C:90:TRP:NE1	1:C:95:SER:HB3	2.30	0.47
1:C:138:GLN:O	1:C:160:GLN:NE2	2.47	0.47
1:C:178:ILE:HD13	1:D:182:TRP:CZ2	2.48	0.47
1:C:231:ALA:O	1:C:232:LEU:C	2.57	0.47
1:D:284:LYS:C	1:D:285:VAL:CG2	2.87	0.47
1:B:41:LEU:HD23	1:B:41:LEU:H	1.79	0.47
1:C:86:GLU:O	1:C:87:GLU:C	2.56	0.47
1:C:135:TYR:O	1:C:136:GLY:C	2.55	0.47
1:B:119:ASP:OD2	1:B:124:SER:HB3	2.14	0.47
1:B:159:ASP:C	1:B:161:LEU:N	2.72	0.47
1:C:145:GLU:OE1	1:C:145:GLU:HA	2.14	0.47
1:D:105:GLY:HA2	1:D:107:LYS:HZ1	1.79	0.47
1:D:142:PHE:C	1:D:144:ALA:H	2.22	0.47
1:D:142:PHE:N	1:D:158:VAL:O	2.34	0.47
1:A:240:ILE:HG22	1:A:241:THR:N	2.24	0.47
1:A:268:GLN:O	1:A:270:GLN:N	2.47	0.47
1:A:147:ARG:N	1:A:153:TYR:OH	2.43	0.47
1:B:228:ALA:O	1:B:231:ALA:HB3	2.13	0.47
1:D:198:LEU:CD1	1:D:199:CYS:N	2.78	0.47
1:A:148:ASP:OD1	1:A:148:ASP:C	2.58	0.47
1:B:91:PHE:O	1:B:92:ILE:C	2.56	0.47
1:D:64:ARG:O	1:D:64:ARG:CG	2.60	0.47
1:B:99:LYS:HZ3	1:B:99:LYS:HB2	1.80	0.47
1:B:105:GLY:O	1:B:106:VAL:CG2	2.62	0.47
1:B:140:ARG:HH21	1:B:159:ASP:CG	2.16	0.47
1:B:223:VAL:HG12	1:B:227:ILE:HD11	1.95	0.47
1:B:273:PRO:HA	1:B:304:HIS:NE2	2.29	0.47
1:C:97:ASN:OD1	1:C:129:GLY:CA	2.62	0.47
1:C:177:ILE:O	1:C:201:PHE:N	2.39	0.47
1:D:177:ILE:H	1:D:177:ILE:HD13	1.79	0.47
1:B:41:LEU:N	1:B:41:LEU:CD2	2.77	0.47
1:C:184:PRO:O	1:C:186:ASP:N	2.48	0.47
1:D:114:SER:O	1:D:118:LEU:HB2	2.15	0.47
1:A:72:PRO:HA	1:A:276:PHE:CZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:GLN:NE2	1:C:64:ARG:O	2.48	0.47
1:D:89:LEU:O	1:D:90:TRP:C	2.57	0.47
1:D:133:PRO:O	1:D:190:MET:HE1	2.10	0.47
1:D:265:LEU:O	1:D:268:GLN:N	2.48	0.47
1:A:162:GLN:O	1:A:163:ARG:C	2.57	0.47
1:C:78:ARG:CZ	1:C:303:PRO:HG3	2.45	0.47
1:C:115:ARG:NH2	1:C:118:LEU:HD22	2.30	0.47
1:D:96:THR:HG23	1:D:134:VAL:HG23	1.97	0.47
1:D:268:GLN:C	1:D:270:GLN:H	2.22	0.47
1:A:93:LYS:HZ1	1:A:100:GLU:HG3	1.80	0.46
1:A:183:ASN:ND2	1:A:185:ARG:HH22	2.13	0.46
1:A:187:LEU:CD2	1:A:190:MET:HE3	2.37	0.46
1:B:299:GLU:CG	1:B:300:GLY:N	2.77	0.46
1:D:33:TYR:OH	1:D:219:MET:O	2.32	0.46
1:D:111:ALA:O	1:D:113:GLY:N	2.47	0.46
1:D:117:PHE:O	1:D:118:LEU:C	2.58	0.46
1:B:165:ILE:HG21	1:B:287:LYS:HZ2	1.79	0.46
1:B:177:ILE:CG2	1:B:201:PHE:HD2	2.28	0.46
1:C:269:LEU:HA	1:C:269:LEU:HD12	1.27	0.46
1:D:32:GLN:O	1:D:33:TYR:C	2.58	0.46
1:D:225:PHE:O	1:D:228:ALA:N	2.48	0.46
1:A:271:ARG:HB3	1:A:304:HIS:CE1	2.50	0.46
1:B:60:GLY:HA2	1:B:252:LEU:O	2.16	0.46
1:D:66:SER:O	1:D:67:LEU:HD23	2.15	0.46
1:A:152:ASP:OD1	1:A:154:SER:OG	2.31	0.46
1:A:183:ASN:HD21	1:A:185:ARG:HH22	1.63	0.46
1:C:198:LEU:HD12	1:C:199:CYS:N	2.30	0.46
1:D:81:TRP:CA	1:D:84:VAL:HG23	2.46	0.46
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.59	0.46
1:B:34:LEU:N	1:B:34:LEU:HD23	2.19	0.46
1:C:134:VAL:O	1:C:138:GLN:HG2	2.16	0.46
1:D:134:VAL:O	1:D:137:PHE:HB3	2.16	0.46
1:A:167:THR:O	1:A:168:ILE:C	2.57	0.46
1:A:201:PHE:N	1:A:201:PHE:CD2	2.82	0.46
1:B:64:ARG:HG3	1:B:249:ILE:CD1	2.46	0.46
1:B:96:THR:CG2	1:B:137:PHE:HB2	2.45	0.46
1:C:148:ASP:OD1	1:C:150:GLU:HB3	2.15	0.46
1:C:203:VAL:C	1:C:204:VAL:HG23	2.35	0.46
1:A:81:TRP:CE3	1:A:298:ILE:HD11	2.51	0.46
1:A:127:GLU:O	1:A:128:GLU:C	2.58	0.46
1:A:244:LYS:HA	1:A:245:PRO:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:VAL:HG13	1:C:286:GLU:H	1.79	0.46
1:D:280:ARG:O	1:D:296:PHE:HA	2.16	0.46
1:A:102:SER:O	1:A:103:SER:C	2.54	0.46
1:C:85:LEU:O	1:C:85:LEU:HD12	2.15	0.46
1:A:202:TYR:CD1	1:B:59:PHE:CD2	3.04	0.46
1:B:119:ASP:C	1:B:121:LEU:N	2.74	0.46
1:B:173:ASP:O	1:B:174:ASP:C	2.59	0.46
1:B:223:VAL:O	1:B:224:PRO:C	2.58	0.46
1:C:50:ARG:NE	1:C:50:ARG:CA	2.53	0.46
1:C:304:HIS:O	1:C:305:PRO:C	2.59	0.46
1:D:142:PHE:C	1:D:144:ALA:N	2.72	0.46
1:A:260:ASN:H	1:A:260:ASN:HD22	0.58	0.46
1:A:298:ILE:CG2	1:A:299:GLU:N	2.76	0.46
1:C:193:PRO:HA	1:C:194:PRO:HD2	1.55	0.46
1:D:207:GLU:HA	1:D:207:GLU:OE1	2.15	0.46
1:A:211:GLN:HB2	1:A:249:ILE:HB	1.98	0.45
1:D:234:THR:C	1:D:236:MET:N	2.70	0.45
1:A:175:ARG:HH11	1:A:175:ARG:HB2	1.81	0.45
1:B:140:ARG:HE	1:B:140:ARG:HB3	1.42	0.45
1:B:288:ILE:HD12	1:B:291:PHE:HE2	1.81	0.45
1:C:174:ASP:CG	1:C:175:ARG:H	2.24	0.45
1:C:223:VAL:N	1:C:224:PRO:CD	2.79	0.45
1:C:243:LEU:HD23	1:C:243:LEU:HA	1.71	0.45
1:D:61:MET:HB2	1:D:252:LEU:HB2	1.98	0.45
1:D:92:ILE:CG2	1:D:161:LEU:CD2	2.94	0.45
1:A:133:PRO:HD3	1:A:146:TYR:CD2	2.51	0.45
1:A:138:GLN:O	1:A:160:GLN:NE2	2.44	0.45
1:A:202:TYR:CD2	1:A:202:TYR:C	2.94	0.45
1:A:214:GLN:HB3	1:A:252:LEU:HD23	1.98	0.45
1:B:182:TRP:CZ3	1:B:215:ARG:CD	3.00	0.45
1:B:233:LEU:HD12	1:B:233:LEU:O	2.15	0.45
1:C:72:PRO:CA	1:C:276:PHE:CE1	2.86	0.45
1:D:97:ASN:HD22	1:D:99:LYS:CB	2.02	0.45
1:B:49:ASP:HB2	1:B:50:ARG:H	1.60	0.45
1:B:274:ARG:NE	1:B:304:HIS:HD2	2.13	0.45
1:C:68:ARG:HH22	1:C:247:ASP:CG	2.24	0.45
1:C:88:LEU:O	1:C:92:ILE:CG1	2.64	0.45
1:D:112:ASN:HD22	1:D:191:ALA:HB3	1.75	0.45
1:B:30:GLU:CD	1:B:76:THR:HG23	2.42	0.45
1:B:81:TRP:C	1:B:83:GLY:N	2.67	0.45
1:B:232:LEU:O	1:B:233:LEU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:TRP:CD1	1:C:139:TRP:N	2.84	0.45
1:D:54:GLY:C	1:D:259:LEU:CD1	2.88	0.45
1:A:45:VAL:HG21	1:B:204:VAL:HG21	1.98	0.45
1:B:274:ARG:HD2	1:B:304:HIS:CD2	2.51	0.45
1:D:79:VAL:HG12	1:D:225:PHE:HD1	1.82	0.45
1:D:87:GLU:OE1	1:D:91:PHE:CE2	2.70	0.45
1:D:169:LYS:CD	1:D:241:THR:HG22	2.45	0.45
1:B:225:PHE:C	1:B:225:PHE:CD2	2.95	0.45
1:C:222:GLY:O	1:C:226:ASN:N	2.30	0.45
1:A:182:TRP:CZ3	1:A:194:PRO:HD2	2.51	0.45
1:C:264:PRO:O	1:C:267:ILE:HB	2.17	0.45
1:D:85:LEU:O	1:D:89:LEU:HD11	2.16	0.45
1:A:113:GLY:O	1:A:118:LEU:CD1	2.65	0.45
1:B:102:SER:O	1:B:104:LYS:N	2.49	0.45
1:C:81:TRP:O	1:C:82:LYS:C	2.57	0.45
1:C:305:PRO:O	1:C:306:THR:HG22	2.16	0.45
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.64	0.45
1:C:57:SER:HA	1:C:255:ALA:O	2.17	0.45
1:C:95:SER:OG	1:C:97:ASN:N	2.43	0.45
1:C:239:HIS:CE1	1:C:284:LYS:CG	2.93	0.45
1:C:257:ILE:HD13	1:C:265:LEU:HD12	1.99	0.45
1:C:280:ARG:CD	1:C:280:ARG:HA	2.47	0.45
1:D:229:SER:HB3	1:D:230:TYR:HD2	1.82	0.45
1:B:55:THR:HA	1:B:257:ILE:O	2.17	0.44
1:B:80:PHE:CE1	1:B:82:LYS:HB3	2.52	0.44
1:D:78:ARG:CZ	1:D:303:PRO:HG2	2.44	0.44
1:D:135:TYR:HA	1:D:138:GLN:HB2	2.00	0.44
1:D:219:MET:O	1:D:220:GLY:C	2.55	0.44
1:B:171:ASN:HA	1:B:172:PRO:HD3	1.43	0.44
1:D:88:LEU:O	1:D:89:LEU:C	2.59	0.44
1:D:96:THR:HG22	1:D:96:THR:O	2.17	0.44
1:D:301:TYR:OH	1:D:303:PRO:HG3	2.15	0.44
1:A:68:ARG:NE	1:A:207:GLU:OE2	2.50	0.44
1:C:37:ILE:HD12	1:C:37:ILE:HG23	1.57	0.44
1:C:178:ILE:HG23	1:C:200:GLN:CA	2.46	0.44
1:C:238:ALA:O	1:C:243:LEU:N	2.50	0.44
1:D:244:LYS:HB2	1:D:244:LYS:HE2	1.68	0.44
1:A:175:ARG:HB2	1:A:175:ARG:NH1	2.33	0.44
1:B:98:ALA:N	1:B:129:GLY:O	2.42	0.44
1:B:142:PHE:HB3	1:B:158:VAL:HB	2.00	0.44
1:C:69:ASP:HA	1:C:235:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TYR:O	1:C:154:SER:C	2.60	0.44
1:D:115:ARG:CG	1:D:128:GLU:OE1	2.60	0.44
1:D:141:HIS:HB3	1:D:144:ALA:HB3	1.99	0.44
1:D:238:ALA:O	1:D:240:ILE:N	2.50	0.44
1:B:192:LEU:HG	1:B:193:PRO:HD2	1.99	0.44
1:B:223:VAL:N	1:B:224:PRO:HD2	2.32	0.44
1:D:26:PRO:O	1:D:27:PRO:C	2.60	0.44
1:A:182:TRP:HD1	1:A:184:PRO:HD3	1.82	0.44
1:A:225:PHE:O	1:A:228:ALA:HB3	2.17	0.44
1:A:232:LEU:HD12	1:A:232:LEU:O	2.18	0.44
1:A:257:ILE:O	1:A:257:ILE:CG1	2.46	0.44
1:D:206:SER:HA	1:D:243:LEU:HD21	1.99	0.44
1:A:99:LYS:O	1:A:100:GLU:C	2.61	0.44
1:A:287:LYS:HE3	1:A:287:LYS:HB2	1.21	0.44
1:B:82:LYS:O	1:B:82:LYS:HG2	2.16	0.44
1:B:297:GLN:HA	1:B:297:GLN:OE1	2.18	0.44
1:C:89:LEU:O	1:C:90:TRP:C	2.55	0.44
1:C:186:ASP:HA	1:C:189:LEU:HD12	2.00	0.44
1:C:212:LEU:HD12	1:C:213:TYR:N	2.32	0.44
1:D:276:PHE:O	1:D:277:PRO:C	2.56	0.44
1:A:93:LYS:NZ	1:A:100:GLU:HG3	2.33	0.44
1:A:97:ASN:HB2	1:A:149:MET:HE3	1.99	0.44
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.60	0.44
1:B:66:SER:O	1:B:67:LEU:HD23	2.18	0.44
1:B:213:TYR:CD2	1:B:213:TYR:C	2.96	0.44
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.27	0.44
1:D:164:VAL:CG1	1:D:177:ILE:CG2	2.94	0.44
1:D:298:ILE:O	1:D:298:ILE:HG22	2.17	0.44
1:A:202:TYR:O	1:A:202:TYR:HD2	2.00	0.44
1:A:216:SER:OG	1:A:256:HIS:HE1	2.01	0.44
1:B:215:ARG:NH1	1:B:215:ARG:CG	2.64	0.44
1:B:272:GLU:OE2	1:B:273:PRO:HD2	2.18	0.44
1:B:304:HIS:CB	1:B:305:PRO:CA	2.95	0.44
1:C:279:LEU:HD13	1:C:298:ILE:HD13	2.00	0.44
1:D:79:VAL:HG12	1:D:225:PHE:CD1	2.52	0.44
1:D:126:ARG:NH1	1:D:132:GLY:N	2.65	0.44
1:A:207:GLU:HG3	1:A:244:LYS:HG3	2.00	0.43
1:B:99:LYS:HZ2	1:B:99:LYS:HG3	1.58	0.43
1:C:184:PRO:CA	1:C:187:LEU:CD1	2.91	0.43
1:D:238:ALA:C	1:D:240:ILE:N	2.74	0.43
1:A:45:VAL:CG2	1:B:204:VAL:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:HIS:NE2	1:A:226:ASN:ND2	2.66	0.43
1:A:274:ARG:O	1:A:275:PRO:C	2.55	0.43
1:B:158:VAL:C	1:B:160:GLN:H	2.25	0.43
1:D:155:GLY:C	1:D:156:GLN:CG	2.91	0.43
1:A:47:LYS:HD2	1:B:204:VAL:HG23	2.01	0.43
1:A:190:MET:HB2	1:A:192:LEU:C	2.43	0.43
1:A:203:VAL:HG13	1:A:243:LEU:HD13	1.99	0.43
1:B:87:GLU:O	1:B:90:TRP:HB3	2.16	0.43
1:B:164:VAL:O	1:B:165:ILE:C	2.56	0.43
1:D:220:GLY:C	1:D:221:LEU:CG	2.86	0.43
1:B:177:ILE:HG21	1:B:201:PHE:N	2.25	0.43
1:A:97:ASN:O	1:A:100:GLU:N	2.52	0.43
1:A:194:PRO:O	1:A:215:ARG:NE	2.43	0.43
1:B:75:THR:C	1:B:77:LYS:N	2.76	0.43
1:B:177:ILE:O	1:B:178:ILE:HG13	2.18	0.43
1:C:165:ILE:HG23	1:C:241:THR:CG2	2.49	0.43
1:C:305:PRO:O	1:C:306:THR:CG2	2.66	0.43
1:D:71:PHE:HA	1:D:72:PRO:HD2	1.68	0.43
1:D:101:LEU:HA	1:D:104:LYS:CE	2.45	0.43
1:D:292:LYS:O	1:D:293:ALA:C	2.61	0.43
1:A:79:VAL:CG1	1:A:80:PHE:N	2.73	0.43
1:B:62:GLN:HA	1:B:250:HIS:O	2.18	0.43
1:B:124:SER:C	1:B:126:ARG:N	2.77	0.43
1:B:177:ILE:HG23	1:B:201:PHE:HD2	1.84	0.43
1:B:199:CYS:HB2	1:B:211:GLN:O	2.18	0.43
1:C:161:LEU:C	1:C:164:VAL:H	2.27	0.43
1:D:126:ARG:HH12	1:D:132:GLY:N	2.17	0.43
1:D:236:MET:HG2	1:D:291:PHE:CE2	2.54	0.43
1:D:240:ILE:O	1:D:240:ILE:CG2	2.66	0.43
1:A:148:ASP:C	1:A:150:GLU:H	2.27	0.43
1:A:218:ASP:C	1:A:218:ASP:OD1	2.60	0.43
1:B:174:ASP:OD1	1:B:176:ARG:CG	2.67	0.43
1:B:203:VAL:HA	1:B:207:GLU:O	2.18	0.43
1:A:142:PHE:CD2	1:B:184:PRO:HG2	2.54	0.43
1:A:268:GLN:O	1:A:269:LEU:C	2.59	0.43
1:B:140:ARG:NH2	1:B:159:ASP:OD2	2.25	0.43
1:C:73:LEU:HD21	1:C:81:TRP:HB2	2.00	0.43
1:C:148:ASP:OD1	1:C:150:GLU:CB	2.66	0.43
1:D:97:ASN:C	1:D:99:LYS:H	2.23	0.43
1:A:294:GLU:O	1:A:295:ASP:C	2.59	0.43
1:B:35:GLY:O	1:B:36:GLN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:HB3	1:B:244:LYS:O	2.18	0.43
1:C:99:LYS:O	1:C:101:LEU:N	2.52	0.43
1:D:85:LEU:O	1:D:85:LEU:HD12	2.19	0.43
1:D:287:LYS:O	1:D:289:ASP:N	2.52	0.43
1:A:113:GLY:C	1:A:118:LEU:HD12	2.44	0.42
1:A:304:HIS:HB3	1:A:305:PRO:CD	2.49	0.42
1:B:293:ALA:C	1:B:295:ASP:N	2.76	0.42
1:C:184:PRO:C	1:C:186:ASP:N	2.76	0.42
1:D:233:LEU:CD1	1:D:237:ILE:HD11	2.49	0.42
1:A:81:TRP:CE2	1:A:298:ILE:HD11	2.54	0.42
1:B:201:PHE:HA	1:B:209:SER:O	2.19	0.42
1:B:298:ILE:HG23	1:B:301:TYR:HB2	2.00	0.42
1:C:96:THR:HG22	1:C:137:PHE:HB2	2.00	0.42
1:D:67:LEU:HG	1:D:246:GLY:O	2.19	0.42
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.56	0.42
1:A:283:ARG:NH1	1:A:285:VAL:HG21	2.35	0.42
1:B:172:PRO:HB2	1:B:203:VAL:HG11	1.81	0.42
1:B:227:ILE:O	1:B:228:ALA:C	2.62	0.42
1:C:175:ARG:CG	1:D:254:ASP:OD1	2.66	0.42
1:D:227:ILE:HD13	1:D:227:ILE:HG23	1.75	0.42
1:A:88:LEU:O	1:A:89:LEU:C	2.61	0.42
1:A:225:PHE:CD2	1:A:225:PHE:C	2.97	0.42
1:C:92:ILE:HD13	1:C:92:ILE:HG23	1.73	0.42
1:C:112:ASN:ND2	1:C:112:ASN:N	2.66	0.42
1:C:139:TRP:O	1:C:140:ARG:HD2	2.19	0.42
1:A:91:PHE:CD1	1:A:135:TYR:CB	3.00	0.42
1:A:291:PHE:HA	1:A:295:ASP:OD1	2.19	0.42
1:B:88:LEU:O	1:B:92:ILE:N	2.49	0.42
1:C:115:ARG:HH21	1:C:128:GLU:HB2	1.69	0.42
1:C:192:LEU:HD13	1:C:192:LEU:N	2.34	0.42
1:D:86:GLU:OE2	1:D:86:GLU:CA	2.67	0.42
1:D:162:GLN:O	1:D:163:ARG:C	2.59	0.42
1:D:218:ASP:O	1:D:219:MET:C	2.58	0.42
1:A:257:ILE:HG13	1:A:258:TYR:O	2.20	0.42
1:C:161:LEU:O	1:C:164:VAL:N	2.52	0.42
1:D:86:GLU:OE2	1:D:86:GLU:HA	2.19	0.42
1:D:183:ASN:CG	1:D:186:ASP:HB2	2.45	0.42
1:A:90:TRP:CD2	1:A:101:LEU:HD22	2.54	0.42
1:A:140:ARG:HA	1:A:159:ASP:HA	2.02	0.42
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.83	0.42
1:A:288:ILE:O	1:A:288:ILE:CG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:HIS:HD2	1:C:61:MET:HE3	1.83	0.42
1:C:55:THR:HB	1:C:257:ILE:O	2.20	0.42
1:D:32:GLN:NE2	1:D:32:GLN:CA	2.80	0.42
1:D:71:PHE:O	1:D:277:PRO:HG2	2.19	0.42
1:B:161:LEU:C	1:B:161:LEU:HD12	2.45	0.42
1:B:171:ASN:ND2	1:B:171:ASN:C	2.78	0.42
1:B:218:ASP:O	1:B:219:MET:C	2.63	0.42
1:D:107:LYS:O	1:D:110:ASP:HB2	2.20	0.42
1:A:164:VAL:HG12	1:A:165:ILE:N	2.34	0.42
1:A:202:TYR:CZ	1:B:59:PHE:HB2	2.54	0.42
1:B:162:GLN:O	1:B:165:ILE:N	2.53	0.42
1:B:298:ILE:O	1:B:298:ILE:HG22	2.20	0.42
1:C:204:VAL:HG21	1:D:47:LYS:CD	2.49	0.42
1:C:258:TYR:HB2	1:C:261:HIS:CD2	2.55	0.42
1:A:71:PHE:CZ	1:A:231:ALA:HB3	2.55	0.42
1:A:102:SER:OG	1:A:107:LYS:HD3	2.20	0.42
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.74	0.42
1:B:77:LYS:HA	1:B:305:PRO:HD2	2.01	0.42
1:B:119:ASP:CA	1:B:122:GLY:H	2.33	0.42
1:B:140:ARG:O	1:B:141:HIS:CG	2.73	0.42
1:D:79:VAL:C	1:D:81:TRP:H	2.28	0.42
1:A:130:ASP:C	1:A:132:GLY:H	2.28	0.41
1:A:176:ARG:HH11	1:A:176:ARG:HD2	1.56	0.41
1:A:176:ARG:HH22	1:B:193:PRO:HG3	1.83	0.41
1:A:284:LYS:CD	1:A:284:LYS:CB	2.90	0.41
1:B:37:ILE:C	1:B:39:HIS:N	2.77	0.41
1:B:48:ASP:OD2	1:B:54:GLY:HA2	2.20	0.41
1:C:135:TYR:OH	1:C:195:CYS:N	2.51	0.41
1:A:203:VAL:O	1:A:204:VAL:HB	2.19	0.41
1:A:299:GLU:O	1:A:299:GLU:CG	2.67	0.41
1:A:306:THR:O	1:A:306:THR:CG2	2.67	0.41
1:D:263:GLU:O	1:D:264:PRO:C	2.63	0.41
1:A:32:GLN:O	1:A:36:GLN:HG3	2.21	0.41
1:A:183:ASN:C	1:A:187:LEU:HG	2.44	0.41
1:B:84:VAL:HG22	1:B:225:PHE:CZ	2.55	0.41
1:B:118:LEU:HB3	1:B:123:PHE:O	2.20	0.41
1:B:160:GLN:NE2	1:B:179:MET:CA	2.83	0.41
1:C:143:GLY:CA	1:D:185:ARG:CZ	2.98	0.41
1:C:182:TRP:CE2	1:D:178:ILE:HG21	2.55	0.41
1:D:30:GLU:OE2	1:D:273:PRO:HB3	2.20	0.41
1:A:33:TYR:O	1:A:34:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:C	1:A:101:LEU:H	2.28	0.41
1:A:153:TYR:O	1:A:154:SER:C	2.63	0.41
1:A:238:ALA:O	1:A:242:GLY:N	2.53	0.41
1:B:41:LEU:H	1:B:41:LEU:CD2	2.33	0.41
1:B:298:ILE:HG23	1:B:299:GLU:N	2.29	0.41
1:C:178:ILE:HD12	1:C:178:ILE:N	2.34	0.41
1:D:161:LEU:HA	1:D:161:LEU:HD12	1.65	0.41
1:D:237:ILE:H	1:D:237:ILE:HG13	1.53	0.41
1:D:257:ILE:HD13	1:D:265:LEU:CD1	2.50	0.41
1:A:142:PHE:O	1:A:142:PHE:HD2	2.02	0.41
1:D:142:PHE:CG	1:D:143:GLY:N	2.89	0.41
1:A:171:ASN:HA	1:A:172:PRO:HD3	1.17	0.41
1:B:71:PHE:CD1	1:B:71:PHE:C	2.98	0.41
1:B:178:ILE:HG23	1:B:199:CYS:O	2.21	0.41
1:C:108:ILE:HG13	1:C:109:TRP:N	2.27	0.41
1:A:97:ASN:CG	1:A:99:LYS:HB2	2.45	0.41
1:B:141:HIS:CD2	1:B:153:TYR:HB3	2.55	0.41
1:B:175:ARG:C	1:B:176:ARG:HG2	2.45	0.41
1:D:118:LEU:O	1:D:119:ASP:O	2.38	0.41
1:A:234:THR:O	1:A:237:ILE:N	2.54	0.41
1:B:33:TYR:O	1:B:34:LEU:C	2.62	0.41
1:B:88:LEU:O	1:B:91:PHE:HB2	2.20	0.41
1:B:123:PHE:HD1	1:B:123:PHE:HA	1.60	0.41
1:B:231:ALA:HB3	1:B:232:LEU:H	1.60	0.41
1:C:60:GLY:O	1:D:64:ARG:NH1	2.54	0.41
1:C:107:LYS:O	1:C:108:ILE:C	2.62	0.41
1:C:134:VAL:O	1:C:138:GLN:HG3	2.21	0.41
1:C:177:ILE:HD13	1:C:177:ILE:HG21	1.77	0.41
1:A:71:PHE:O	1:A:277:PRO:HD2	2.20	0.41
1:A:90:TRP:CD1	1:A:95:SER:HB3	2.55	0.41
1:A:114:SER:CB	1:A:116:ASP:OD2	2.66	0.41
1:A:167:THR:HG21	1:A:174:ASP:OD1	2.21	0.41
1:A:175:ARG:HH21	1:B:55:THR:HG21	1.83	0.41
1:A:176:ARG:NH2	1:B:50:ARG:NH1	2.68	0.41
1:B:97:ASN:O	1:B:100:GLU:HB2	2.21	0.41
1:B:233:LEU:HD12	1:B:233:LEU:C	2.33	0.41
1:B:263:GLU:HG2	1:B:266:LYS:HZ2	1.84	0.41
1:C:88:LEU:HD23	1:C:232:LEU:HG	2.03	0.41
1:C:265:LEU:HD23	1:C:265:LEU:HA	1.61	0.41
1:D:55:THR:OG1	1:D:56:LEU:N	2.54	0.41
1:D:85:LEU:HD11	1:D:296:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:SER:O	1:D:115:ARG:C	2.63	0.41
1:A:99:LYS:C	1:A:101:LEU:N	2.78	0.41
1:B:161:LEU:HD13	1:B:179:MET:HE1	2.03	0.41
1:A:58:VAL:CG1	1:A:59:PHE:N	2.80	0.40
1:A:109:TRP:O	1:A:111:ALA:N	2.54	0.40
1:A:177:ILE:HG21	1:A:177:ILE:HD13	1.62	0.40
1:A:182:TRP:CD1	1:A:184:PRO:HD3	2.56	0.40
1:D:66:SER:C	1:D:67:LEU:HD23	2.46	0.40
1:D:79:VAL:O	1:D:81:TRP:N	2.46	0.40
1:D:97:ASN:HB2	1:D:149:MET:CE	2.48	0.40
1:B:31:LEU:CD2	1:B:31:LEU:N	2.84	0.40
1:B:208:LEU:O	1:B:246:GLY:N	2.51	0.40
1:C:275:PRO:O	1:C:276:PHE:C	2.64	0.40
1:D:101:LEU:HD23	1:D:106:VAL:O	2.21	0.40
1:D:113:GLY:CA	1:D:129:GLY:HA2	2.50	0.40
1:D:208:LEU:HA	1:D:208:LEU:HD12	1.61	0.40
1:D:240:ILE:HD11	1:D:291:PHE:CZ	2.57	0.40
1:B:56:LEU:HD12	1:B:56:LEU:HA	1.88	0.40
1:B:81:TRP:O	1:B:85:LEU:N	2.46	0.40
1:B:135:TYR:OH	1:B:194:PRO:HA	2.21	0.40
1:C:119:ASP:HA	1:C:122:GLY:C	2.44	0.40
1:C:181:ALA:HB3	1:C:196:HIS:O	2.21	0.40
1:C:298:ILE:HD13	1:C:298:ILE:HA	1.76	0.40
1:D:225:PHE:O	1:D:227:ILE:N	2.53	0.40
1:D:236:MET:O	1:D:237:ILE:C	2.64	0.40
1:D:236:MET:O	1:D:238:ALA:N	2.54	0.40
1:D:307:ILE:CG2	1:D:308:LYS:H	2.32	0.40
1:A:226:ASN:O	1:A:227:ILE:C	2.63	0.40
1:B:292:LYS:O	1:B:295:ASP:CG	2.64	0.40
1:C:32:GLN:NE2	1:C:64:ARG:N	2.62	0.40
1:D:73:LEU:CD1	1:D:228:ALA:HB1	2.51	0.40
1:D:99:LYS:O	1:D:103:SER:OG	2.39	0.40
1:D:261:HIS:O	1:D:264:PRO:CD	2.67	0.40
1:D:301:TYR:CE2	1:D:303:PRO:CG	3.04	0.40
1:D:307:ILE:CD1	1:D:307:ILE:CB	2.88	0.40
1:A:88:LEU:C	1:A:90:TRP:N	2.75	0.40
1:A:130:ASP:HB2	1:A:149:MET:HG2	2.02	0.40
1:A:139:TRP:C	1:A:140:ARG:HG2	2.46	0.40
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.72	0.40
1:B:183:ASN:HB3	1:B:186:ASP:HB2	2.04	0.40
1:B:236:MET:HE2	1:B:288:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ARG:HB3	1:B:275:PRO:HD2	2.04	0.40
1:C:125:THR:O	1:C:126:ARG:C	2.64	0.40
1:D:235:TYR:O	1:D:238:ALA:CB	2.51	0.40
1:D:260:ASN:OD1	1:D:260:ASN:N	2.54	0.40
1:D:274:ARG:NH1	1:D:302:ASN:O	2.53	0.40

There are no symmetry-related clashes.

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	281/313 (90%)	225 (80%)	37 (13%)	19 (7%)	1	2
1	B	279/313 (89%)	205 (74%)	57 (20%)	17 (6%)	1	3
1	C	281/313 (90%)	228 (81%)	41 (15%)	12 (4%)	2	6
1	D	281/313 (90%)	193 (69%)	55 (20%)	33 (12%)	0	0
All	All	1122/1252 (90%)	851 (76%)	190 (17%)	81 (7%)	1	2

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	116	ASP
1	A	305	PRO
1	B	38	GLN
1	B	76	THR
1	B	186	ASP
1	D	27	PRO
1	D	81	TRP
1	D	238	ALA
1	D	264	PRO

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Mol	Chain	Res	Type
1	D	265	LEU
1	D	271	ARG
1	D	307	ILE
1	A	68	ARG
1	A	119	ASP
1	A	142	PHE
1	A	291	PHE
1	B	32	GLN
1	B	52	GLY
1	B	103	SER
1	B	115	ARG
1	B	189	LEU
1	B	228	ALA
1	B	231	ALA
1	B	300	GLY
1	C	127	GLU
1	C	157	GLY
1	C	172	PRO
1	C	277	PRO
1	D	85	LEU
1	D	87	GLU
1	D	102	SER
1	D	173	ASP
1	D	227	ILE
1	D	236	MET
1	D	260	ASN
1	D	294	GLU
1	A	27	PRO
1	A	81	TRP
1	A	115	ARG
1	A	118	LEU
1	A	155	GLY
1	A	189	LEU
1	B	72	PRO
1	B	160	GLN
1	B	305	PRO
1	C	111	ALA
1	C	306	THR
1	D	80	PHE
1	D	119	ASP
1	D	226	ASN
1	D	237	ILE

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Mol	Chain	Res	Type
1	D	269	LEU
1	D	288	ILE
1	A	140	ARG
1	A	204	VAL
1	B	187	LEU
1	C	93	LYS
1	C	134	VAL
1	D	84	VAL
1	D	135	TYR
1	D	151	SER
1	D	293	ALA
1	A	233	LEU
1	C	123	PHE
1	C	305	PRO
1	D	72	PRO
1	D	90	TRP
1	D	158	VAL
1	A	222	GLY
1	B	158	VAL
1	C	124	SER
1	C	149	MET
1	D	175	ARG
1	A	157	GLY
1	D	184	PRO
1	D	303	PRO
1	D	246	GLY
1	D	94	GLY
1	A	263	GLU
1	B	277	PRO

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	247/271 (91%)	177 (72%)	70 (28%)	0	1
1	B	245/271 (90%)	178 (73%)	67 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	247/271 (91%)	179 (72%)	68 (28%)	0	1
1	D	247/271 (91%)	172 (70%)	75 (30%)	0	1
All	All	986/1084 (91%)	706 (72%)	280 (28%)	0	1

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	38	GLN
1	A	40	ILE
1	A	51	THR
1	A	58	VAL
1	A	68	ARG
1	A	85	LEU
1	A	86	GLU
1	A	89	LEU
1	A	103	SER
1	A	104	LYS
1	A	106	VAL
1	A	107	LYS
1	A	108	ILE
1	A	115	ARG
1	A	116	ASP
1	A	118	LEU
1	A	127	GLU
1	A	128	GLU
1	A	140	ARG
1	A	149	MET
1	A	152	ASP
1	A	154	SER
1	A	160	GLN
1	A	162	GLN
1	A	164	VAL
1	A	170	THR
1	A	175	ARG
1	A	179	MET
1	A	185	ARG
1	A	189	LEU
1	A	190	MET
1	A	192	LEU
1	A	195	CYS

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Mol	Chain	Res	Type
1	A	198	LEU
1	A	200	GLN
1	A	202	TYR
1	A	204	VAL
1	A	207	GLU
1	A	211	GLN
1	A	221	LEU
1	A	233	LEU
1	A	236	MET
1	A	240	ILE
1	A	244	LYS
1	A	249	ILE
1	A	251	THR
1	A	257	ILE
1	A	259	LEU
1	A	260	ASN
1	A	269	LEU
1	A	270	GLN
1	A	271	ARG
1	A	272	GLU
1	A	275	PRO
1	A	279	LEU
1	A	280	ARG
1	A	281	ILE
1	A	285	VAL
1	A	286	GLU
1	A	287	LYS
1	A	288	ILE
1	A	289	ASP
1	A	292	LYS
1	A	294	GLU
1	A	297	GLN
1	A	299	GLU
1	A	306	THR
1	A	307	ILE
1	A	308	LYS
1	B	26	PRO
1	B	31	LEU
1	B	32	GLN
1	B	40	ILE
1	B	41	LEU
1	B	42	ARG

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Mol	Chain	Res	Type
1	B	43	CYS
1	B	45	VAL
1	B	47	LYS
1	B	55	THR
1	B	56	LEU
1	B	76	THR
1	B	77	LYS
1	B	85	LEU
1	B	88	LEU
1	B	89	LEU
1	B	93	LYS
1	B	96	THR
1	B	97	ASN
1	B	99	LYS
1	B	103	SER
1	B	106	VAL
1	B	108	ILE
1	B	114	SER
1	B	116	ASP
1	B	119	ASP
1	B	128	GLU
1	B	140	ARG
1	B	148	ASP
1	B	149	MET
1	B	150	GLU
1	B	151	SER
1	B	152	ASP
1	B	154	SER
1	B	156	GLN
1	B	167	THR
1	B	168	ILE
1	B	170	THR
1	B	171	ASN
1	B	177	ILE
1	B	179	MET
1	B	192	LEU
1	B	198	LEU
1	B	202	TYR
1	B	206	SER
1	B	207	GLU
1	B	208	LEU
1	B	212	LEU

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Mol	Chain	Res	Type
1	B	215	ARG
1	B	216	SER
1	B	221	LEU
1	B	224	PRO
1	B	226	ASN
1	B	240	ILE
1	B	260	ASN
1	B	262	ILE
1	B	266	LYS
1	B	268	GLN
1	B	269	LEU
1	B	272	GLU
1	B	278	LYS
1	B	280	ARG
1	B	284	LYS
1	B	289	ASP
1	B	290	ASP
1	B	292	LYS
1	B	298	ILE
1	C	38	GLN
1	C	40	ILE
1	C	48	ASP
1	C	50	ARG
1	C	56	LEU
1	C	57	SER
1	C	58	VAL
1	C	67	LEU
1	C	72	PRO
1	C	74	LEU
1	C	76	THR
1	C	80	PHE
1	C	82	LYS
1	C	85	LEU
1	C	86	GLU
1	C	87	GLU
1	C	88	LEU
1	C	91	PHE
1	C	93	LYS
1	C	95	SER
1	C	99	LYS
1	C	102	SER
1	C	103	SER

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Mol	Chain	Res	Type
1	C	107	LYS
1	C	108	ILE
1	C	110	ASP
1	C	112	ASN
1	C	115	ARG
1	C	120	SER
1	C	123	PHE
1	C	127	GLU
1	C	131	LEU
1	C	140	ARG
1	C	145	GLU
1	C	151	SER
1	C	158	VAL
1	C	163	ARG
1	C	167	THR
1	C	170	THR
1	C	171	ASN
1	C	178	ILE
1	C	180	CYS
1	C	189	LEU
1	C	190	MET
1	C	192	LEU
1	C	204	VAL
1	C	218	ASP
1	C	221	LEU
1	C	240	ILE
1	C	249	ILE
1	C	251	THR
1	C	257	ILE
1	C	260	ASN
1	C	263	GLU
1	C	268	GLN
1	C	276	PHE
1	C	278	LYS
1	C	280	ARG
1	C	283	ARG
1	C	284	LYS
1	C	286	GLU
1	C	288	ILE
1	C	292	LYS
1	C	297	GLN
1	C	298	ILE

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Mol	Chain	Res	Type
1	C	302	ASN
1	C	307	ILE
1	C	308	LYS
1	D	31	LEU
1	D	40	ILE
1	D	42	ARG
1	D	50	ARG
1	D	51	THR
1	D	56	LEU
1	D	64	ARG
1	D	69	ASP
1	D	73	LEU
1	D	74	LEU
1	D	79	VAL
1	D	84	VAL
1	D	90	TRP
1	D	92	ILE
1	D	93	LYS
1	D	95	SER
1	D	96	THR
1	D	101	LEU
1	D	104	LYS
1	D	108	ILE
1	D	112	ASN
1	D	115	ARG
1	D	117	PHE
1	D	118	LEU
1	D	127	GLU
1	D	128	GLU
1	D	133	PRO
1	D	135	TYR
1	D	140	ARG
1	D	150	GLU
1	D	151	SER
1	D	152	ASP
1	D	156	GLN
1	D	158	VAL
1	D	165	ILE
1	D	169	LYS
1	D	170	THR
1	D	177	ILE
1	D	178	ILE

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Mol	Chain	Res	Type
1	D	192	LEU
1	D	198	LEU
1	D	204	VAL
1	D	209	SER
1	D	215	ARG
1	D	219	MET
1	D	221	LEU
1	D	223	VAL
1	D	227	ILE
1	D	229	SER
1	D	233	LEU
1	D	236	MET
1	D	240	ILE
1	D	243	LEU
1	D	244	LYS
1	D	249	ILE
1	D	257	ILE
1	D	259	LEU
1	D	266	LYS
1	D	267	ILE
1	D	270	GLN
1	D	272	GLU
1	D	274	ARG
1	D	276	PHE
1	D	278	LYS
1	D	279	LEU
1	D	280	ARG
1	D	281	ILE
1	D	286	GLU
1	D	287	LYS
1	D	288	ILE
1	D	292	LYS
1	D	294	GLU
1	D	306	THR
1	D	307	ILE
1	D	308	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	36	GLN

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Mol	Chain	Res	Type
1	A	183	ASN
1	A	226	ASN
1	A	256	HIS
1	A	260	ASN
1	A	268	GLN
1	A	270	GLN
1	A	304	HIS
1	B	32	GLN
1	B	39	HIS
1	B	97	ASN
1	B	138	GLN
1	B	160	GLN
1	B	171	ASN
1	B	205	ASN
1	B	304	HIS
1	C	32	GLN
1	C	39	HIS
1	C	112	ASN
1	C	183	ASN
1	C	226	ASN
1	C	239	HIS
1	C	260	ASN
1	C	268	GLN
1	D	32	GLN
1	D	39	HIS
1	D	97	ASN
1	D	112	ASN
1	D	160	GLN
1	D	211	GLN
1	D	226	ASN
1	D	256	HIS
1	D	297	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	616	-	4,4,4	1.37	0	6,6,6	3.28	4 (66%)
2	SO4	C	616	-	4,4,4	0.46	0	6,6,6	0.93	0
3	PO4	B	616	-	4,4,4	1.74	2 (50%)	6,6,6	3.92	4 (66%)
3	PO4	D	616	-	4,4,4	0.46	0	6,6,6	2.38	2 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	616	PO4	P-O2	2.09	1.60	1.54
3	B	616	PO4	P-O1	-2.09	1.45	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	616	PO4	O3-P-O1	-5.62	91.07	110.95
3	B	616	PO4	O3-P-O2	5.39	124.69	107.91
2	A	616	SO4	O4-S-O1	-4.98	83.52	109.56
2	A	616	SO4	O3-S-O1	4.62	133.71	109.56
3	D	616	PO4	O3-P-O1	-4.31	95.71	110.95
3	B	616	PO4	O4-P-O3	-4.23	94.74	107.91
2	A	616	SO4	O3-S-O2	-3.49	91.33	109.56
3	D	616	PO4	O4-P-O3	3.19	117.85	107.91
3	B	616	PO4	O4-P-O2	3.08	117.48	107.91
2	A	616	SO4	O2-S-O1	2.27	125.06	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	616	PO4	7	0
3	D	616	PO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	283/313 (90%)	0.15	4 (1%) 73 67	26, 53, 94, 116	0
1	B	281/313 (89%)	0.50	16 (5%) 29 24	30, 67, 111, 149	0
1	C	283/313 (90%)	0.31	13 (4%) 37 31	25, 58, 109, 144	0
1	D	283/313 (90%)	0.59	20 (7%) 22 17	29, 71, 115, 130	0
All	All	1130/1252 (90%)	0.38	53 (4%) 36 31	25, 63, 109, 149	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	5.8
1	D	92	ILE	5.7
1	D	95	SER	5.3
1	C	113	GLY	5.3
1	B	304	HIS	4.7
1	D	96	THR	4.5
1	B	301	TYR	4.4
1	B	305	PRO	4.3
1	A	182	TRP	4.1
1	C	135	TYR	4.0
1	B	306	THR	3.7
1	B	120	SER	3.6
1	B	303	PRO	3.1
1	B	109	TRP	3.1
1	C	275	PRO	3.1
1	C	111	ALA	3.1
1	C	283	ARG	3.0
1	D	123	PHE	3.0
1	D	298	ILE	2.7
1	D	88	LEU	2.7
1	D	192	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	298	ILE	2.7
1	D	185	ARG	2.7
1	B	302	ASN	2.7
1	D	109	TRP	2.6
1	D	288	ILE	2.6
1	C	128	GLU	2.6
1	B	26	PRO	2.6
1	D	121	LEU	2.6
1	C	136	GLY	2.5
1	C	134	VAL	2.5
1	D	187	LEU	2.5
1	D	161	LEU	2.5
1	D	136	GLY	2.4
1	D	108	ILE	2.4
1	B	300	GLY	2.3
1	A	185	ARG	2.3
1	B	189	LEU	2.3
1	D	143	GLY	2.3
1	D	94	GLY	2.3
1	B	108	ILE	2.2
1	C	115	ARG	2.2
1	B	95	SER	2.2
1	B	296	PHE	2.1
1	D	91	PHE	2.1
1	A	305	PRO	2.1
1	D	112	ASN	2.1
1	C	178	ILE	2.1
1	D	117	PHE	2.1
1	C	189	LEU	2.0
1	B	135	TYR	2.0
1	C	123	PHE	2.0
1	C	120	SER	2.0

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($\text{\AA}^2$)	Q<0.9
2	SO4	C	616	5/5	0.92	0.10	68,69,70,71	0
2	SO4	A	616	5/5	0.93	0.09	61,62,66,67	0
3	PO4	D	616	5/5	0.93	0.07	58,58,63,63	0
3	PO4	B	616	5/5	0.95	0.10	54,58,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.