



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:00 AM UTC

PDB ID : 1LNL / pdb_00001lnl
Title : Structure of deoxygenated hemocyanin from *Rapana thomasiana*
Authors : Perbandt, M.; Guthoehrlein, E.W.; Rypniewski, W.; Idakieva, K.; Stoeva, S.;
Voelter, W.; Genov, N.; Betzel, C.
Deposited on : 2002-05-03
Resolution : 3.30 Å(reported)

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

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

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

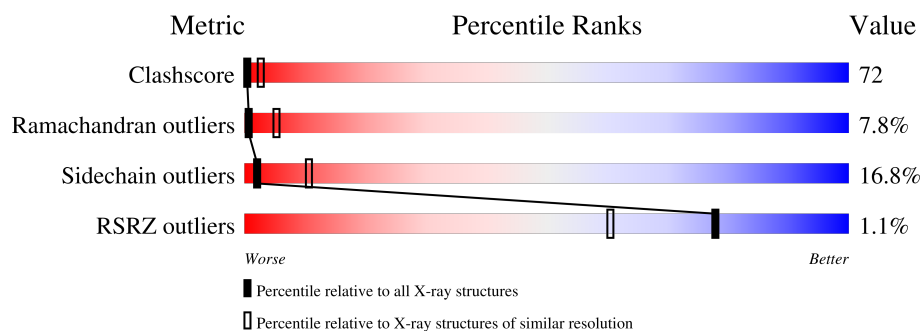
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	408	14% 49% 29% 7%
1	B	408	16% 43% 33% 8%
1	C	408	19% 40% 31% 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
3	CU	B	5503	-	-	X	-

2 Entry composition [i](#)

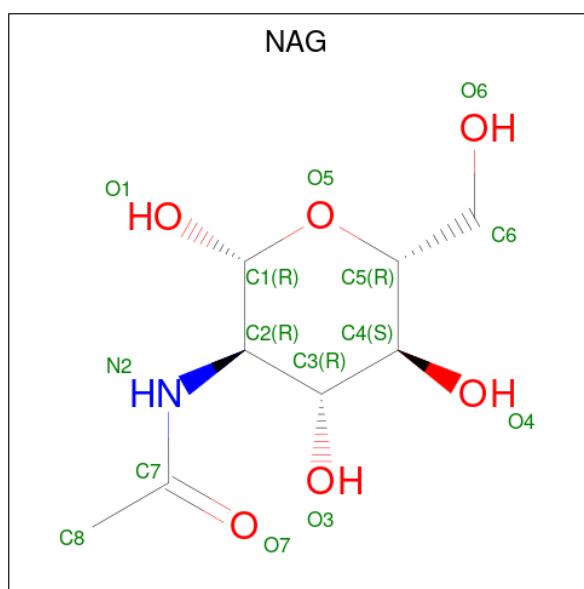
There are 3 unique types of molecules in this entry. The entry contains 9984 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3310	2115	558	625	12			
1	B	408	Total	C	N	O	S	0	0	0
			3310	2115	558	625	12			
1	C	408	Total	C	N	O	S	3	0	0
			3310	2115	558	625	12			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		

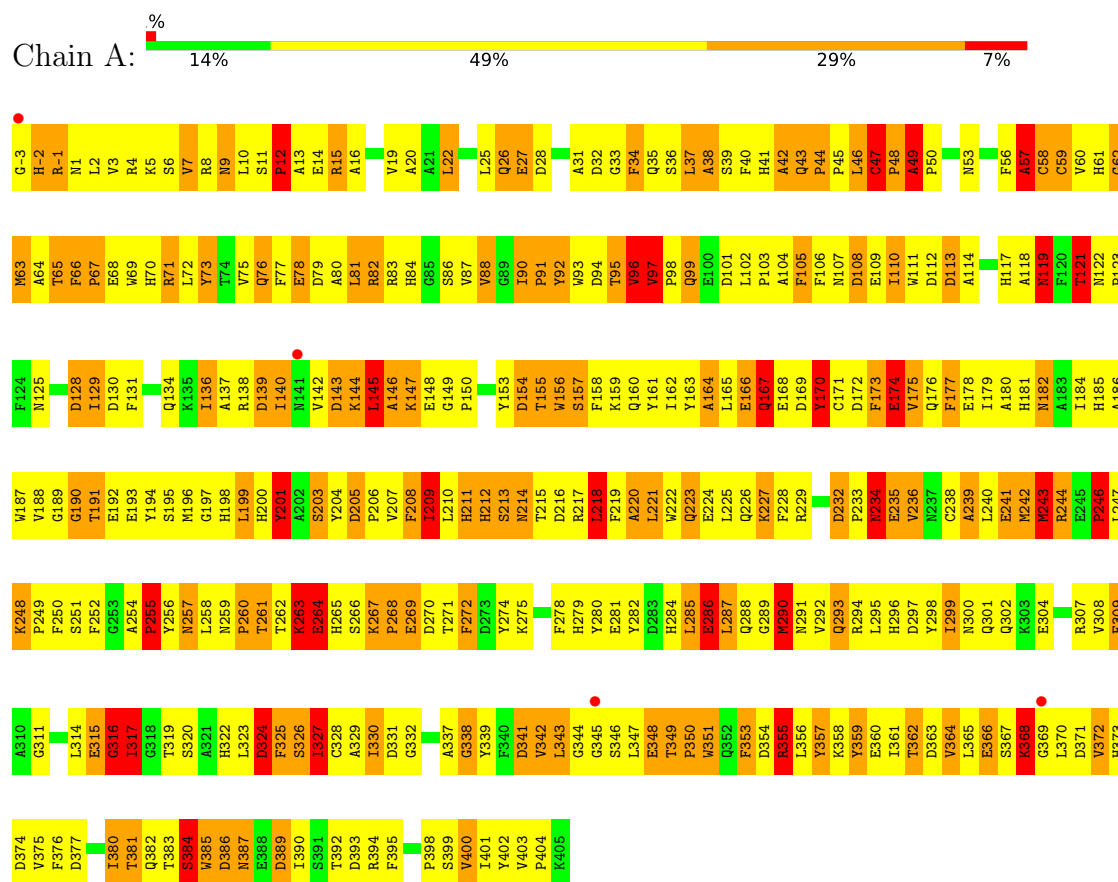
- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cu 2	0	0
3	B	4	Total 4	Cu 4	0	0
3	C	3	Total 3	Cu 3	0	0

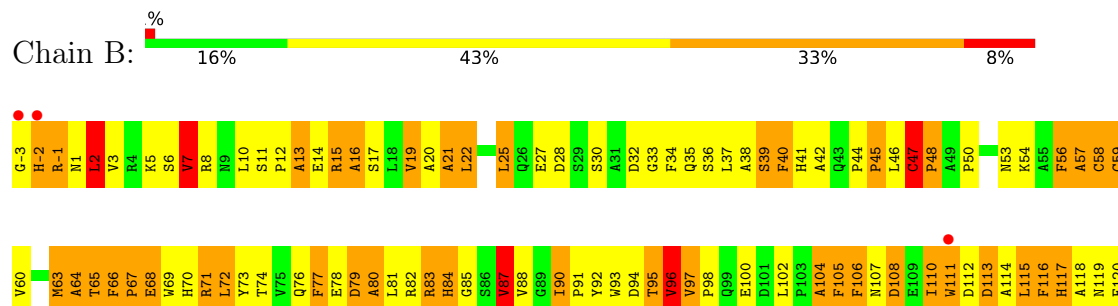
3 Residue-property plots

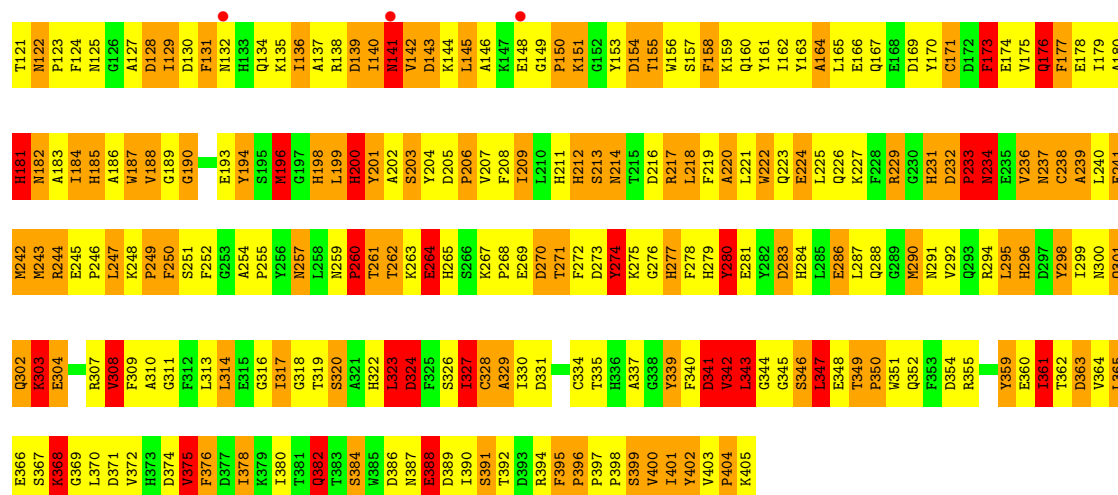
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

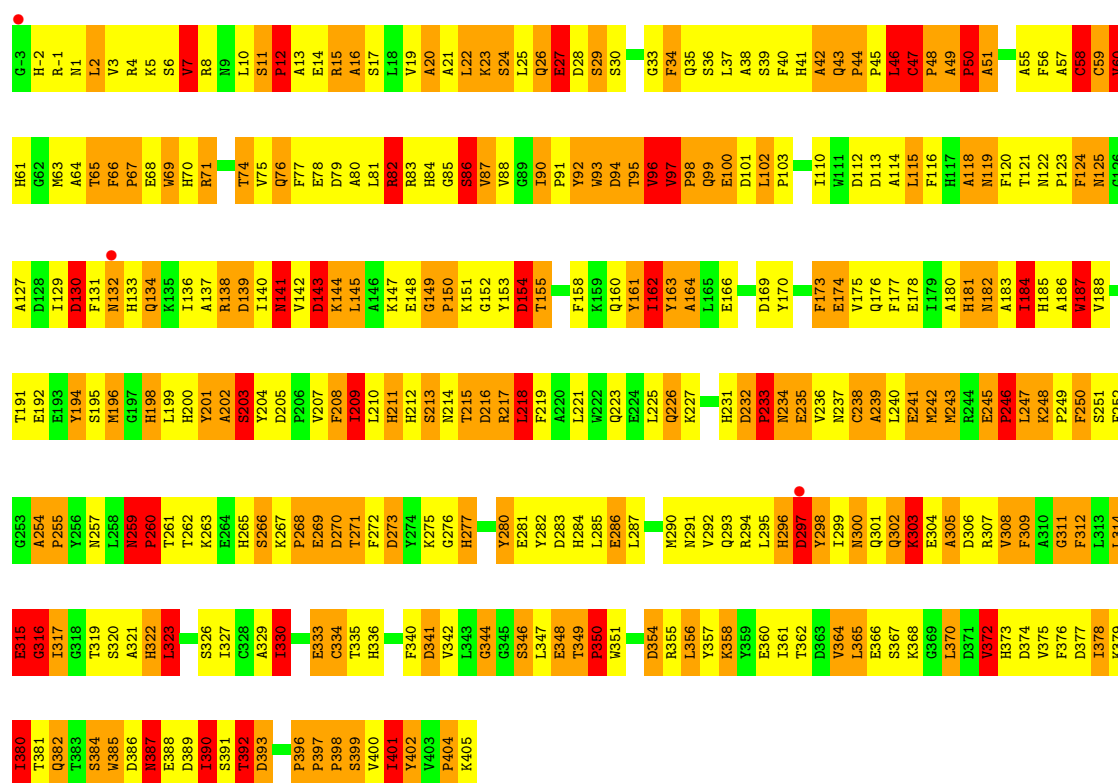
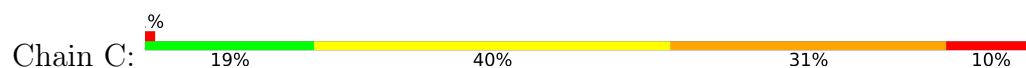


• Molecule 1: hemocyanin





• Molecule 1: hemocyanin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.49Å 105.49Å 374.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 15.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.30) 95.8 (15.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.248 , 0.288 0.246 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9984	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: NAG, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	2.14	96/3415 (2.8%)	1.89	101/4644 (2.2%)
1	B	2.41	153/3415 (4.5%)	2.07	130/4644 (2.8%)
1	C	2.18	118/3415 (3.5%)	1.91	105/4644 (2.3%)
All	All	2.25	367/10245 (3.6%)	1.96	336/13932 (2.4%)

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

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

All (367) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	MET	SD-CE	13.87	2.14	1.79
1	B	137	ALA	CA-CB	-12.39	1.32	1.53
1	A	63	MET	SD-CE	-12.29	1.48	1.79
1	C	397	PRO	CA-C	-11.75	1.45	1.51
1	B	104	ALA	CA-CB	-11.64	1.35	1.53
1	B	257	ASN	CA-C	-11.52	1.41	1.53
1	C	58	CYS	CA-C	-11.01	1.39	1.52
1	B	16	ALA	CA-CB	-10.84	1.36	1.53
1	C	396	PRO	CA-C	-10.80	1.42	1.52
1	B	72	LEU	C-O	-10.59	1.10	1.24
1	C	164	ALA	CA-CB	-10.46	1.36	1.53
1	B	290	MET	SD-CE	10.46	2.05	1.79
1	C	378	ILE	CA-CB	-10.32	1.41	1.54
1	A	66	PHE	C-O	-10.19	1.11	1.24
1	B	66	PHE	C-O	-10.17	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	ALA	CA-CB	-9.76	1.37	1.53
1	A	175	VAL	CA-CB	-9.70	1.41	1.54
1	A	232	ASP	CA-C	-9.63	1.42	1.52
1	A	38	ALA	CA-CB	-9.42	1.37	1.54
1	B	343	LEU	CA-C	-9.42	1.42	1.53
1	B	355	ARG	CA-C	-9.25	1.40	1.52
1	B	58	CYS	CA-C	-9.24	1.36	1.52
1	A	290	MET	SD-CE	9.21	2.02	1.79
1	B	160	GLN	N-CA	-9.18	1.35	1.46
1	B	394	ARG	NE-CZ	9.15	1.43	1.33
1	B	317	ILE	CA-CB	-9.12	1.44	1.54
1	B	74	THR	C-O	-9.12	1.12	1.24
1	B	239	ALA	CA-CB	-9.07	1.40	1.53
1	B	64	ALA	CA-CB	-8.92	1.39	1.53
1	A	317	ILE	CA-CB	8.91	1.62	1.55
1	A	62	GLY	C-O	-8.86	1.14	1.24
1	B	164	ALA	CA-C	-8.77	1.40	1.52
1	C	209	ILE	CA-CB	-8.76	1.45	1.54
1	B	354	ASP	C-O	-8.76	1.12	1.24
1	B	40	PHE	C-O	-8.73	1.12	1.24
1	A	327	ILE	C-O	-8.71	1.14	1.23
1	B	188	VAL	C-O	-8.58	1.14	1.24
1	C	239	ALA	CA-CB	-8.52	1.39	1.53
1	B	13	ALA	CA-CB	-8.51	1.40	1.53
1	B	198	HIS	C-O	-8.40	1.14	1.24
1	A	400	VAL	CA-CB	-8.39	1.43	1.54
1	C	182	ASN	C-O	-8.33	1.13	1.24
1	B	45	PRO	C-O	-8.27	1.14	1.23
1	B	298	TYR	CA-C	-8.18	1.42	1.52
1	A	342	VAL	CA-CB	-8.16	1.42	1.55
1	B	45	PRO	CA-C	-8.14	1.43	1.52
1	B	173	PHE	C-O	-8.05	1.13	1.24
1	A	59	CYS	CA-C	8.03	1.62	1.52
1	B	237	ASN	CA-C	-8.02	1.43	1.53
1	B	177	PHE	C-O	-7.95	1.14	1.24
1	A	90	ILE	CA-CB	-7.93	1.44	1.54
1	A	364	VAL	CA-CB	-7.92	1.43	1.54
1	A	308	VAL	CA-CB	-7.92	1.44	1.54
1	C	397	PRO	CA-CB	-7.87	1.46	1.53
1	C	321	ALA	CA-C	-7.85	1.42	1.52
1	B	329	ALA	CA-CB	7.80	1.65	1.53
1	C	66	PHE	N-CA	7.78	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	ASP	CA-C	-7.77	1.42	1.52
1	B	20	ALA	CA-CB	7.74	1.65	1.53
1	B	243	MET	SD-CE	7.72	1.98	1.79
1	A	286	GLU	CA-C	-7.71	1.43	1.52
1	B	324	ASP	CA-C	-7.70	1.43	1.52
1	A	243	MET	SD-CE	-7.68	1.60	1.79
1	C	74	THR	CA-CB	-7.64	1.41	1.53
1	C	346	SER	CA-C	-7.61	1.46	1.53
1	B	105	PHE	CA-C	-7.57	1.42	1.52
1	B	355	ARG	C-O	-7.56	1.14	1.24
1	B	236	VAL	CA-CB	-7.56	1.44	1.54
1	C	308	VAL	C-O	-7.55	1.16	1.24
1	B	351	TRP	C-O	-7.51	1.14	1.23
1	C	396	PRO	C-O	-7.49	1.16	1.24
1	B	184	ILE	CA-CB	-7.48	1.45	1.54
1	A	354	ASP	CA-C	-7.37	1.43	1.53
1	B	194	TYR	CA-C	7.35	1.62	1.52
1	B	206	PRO	C-O	-7.30	1.15	1.24
1	A	385	TRP	CA-C	-7.29	1.42	1.52
1	B	58	CYS	C-O	-7.29	1.13	1.24
1	A	47	CYS	CA-C	-7.29	1.43	1.52
1	A	91	PRO	CA-C	7.28	1.61	1.52
1	C	342	VAL	C-O	-7.27	1.16	1.24
1	B	339	TYR	C-O	-7.27	1.16	1.23
1	A	88	VAL	CA-CB	-7.24	1.44	1.55
1	C	65	THR	CA-C	-7.24	1.43	1.52
1	A	208	PHE	N-CA	-7.23	1.37	1.46
1	B	313	LEU	C-O	-7.23	1.13	1.23
1	C	317	ILE	N-CA	-7.23	1.38	1.46
1	C	401	ILE	CA-CB	-7.20	1.46	1.54
1	B	63	MET	CA-C	7.20	1.61	1.52
1	A	272	PHE	CA-C	-7.19	1.42	1.52
1	C	344	GLY	CA-C	7.12	1.59	1.51
1	A	129	ILE	CA-CB	-7.11	1.45	1.54
1	A	351	TRP	CA-C	-7.08	1.43	1.52
1	A	45	PRO	CA-C	-7.07	1.44	1.52
1	B	141	ASN	N-CA	7.06	1.55	1.46
1	A	267	LYS	CA-C	7.05	1.61	1.52
1	B	118	ALA	CA-CB	-7.02	1.39	1.53
1	B	90	ILE	CA-CB	-7.00	1.45	1.54
1	A	351	TRP	C-O	-6.99	1.14	1.23
1	C	401	ILE	C-O	-6.98	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	401	ILE	CA-C	-6.97	1.44	1.53
1	C	2	LEU	CA-C	-6.97	1.43	1.52
1	C	213	SER	CA-C	-6.97	1.43	1.52
1	A	234	ASN	CA-C	-6.96	1.42	1.52
1	B	129	ILE	CA-CB	-6.95	1.45	1.54
1	A	221	LEU	CA-C	6.95	1.62	1.52
1	A	66	PHE	CA-C	-6.91	1.44	1.52
1	C	397	PRO	C-O	-6.91	1.19	1.25
1	B	274	TYR	CA-C	-6.87	1.44	1.52
1	B	303	LYS	CD-CE	6.83	1.73	1.52
1	B	206	PRO	C-N	-6.82	1.26	1.33
1	C	161	TYR	N-CA	6.80	1.54	1.46
1	B	346	SER	C-O	-6.80	1.16	1.24
1	C	270	ASP	CA-C	-6.79	1.43	1.53
1	B	72	LEU	CA-C	-6.78	1.43	1.52
1	B	-3	GLY	N-CA	6.77	1.56	1.45
1	B	122	ASN	CA-C	-6.74	1.44	1.52
1	B	224	GLU	CA-C	-6.74	1.44	1.53
1	C	174	GLU	C-O	-6.72	1.15	1.24
1	C	125	ASN	C-O	-6.69	1.16	1.23
1	C	315	GLU	CA-C	-6.69	1.44	1.52
1	B	131	PHE	CA-C	6.68	1.61	1.52
1	C	351	TRP	C-O	-6.65	1.15	1.23
1	A	246	PRO	C-O	-6.62	1.15	1.24
1	C	333	GLU	CD-OE1	6.62	1.38	1.25
1	C	374	ASP	CA-C	-6.62	1.44	1.52
1	B	145	LEU	CA-C	6.61	1.61	1.52
1	B	65	THR	CA-C	-6.61	1.38	1.52
1	B	327	ILE	C-O	-6.60	1.16	1.24
1	B	155	THR	CA-CB	-6.60	1.42	1.53
1	C	65	THR	C-O	-6.58	1.15	1.24
1	C	330	ILE	CA-CB	-6.57	1.45	1.54
1	C	198	HIS	CA-C	6.55	1.60	1.52
1	C	93	TRP	CA-C	-6.53	1.45	1.53
1	C	184	ILE	CG1-CD1	-6.53	1.26	1.51
1	B	97	VAL	C-O	-6.51	1.17	1.24
1	B	396	PRO	C-O	-6.46	1.17	1.24
1	C	90	ILE	CA-CB	-6.45	1.45	1.54
1	B	-2	HIS	CA-C	6.44	1.61	1.52
1	B	-2	HIS	CA-CB	6.43	1.64	1.53
1	B	19	VAL	CA-CB	-6.42	1.45	1.54
1	C	92	TYR	CA-C	6.42	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	CYS	CA-C	6.42	1.61	1.52
1	C	232	ASP	C-O	-6.42	1.16	1.24
1	B	296	HIS	N-CA	-6.40	1.38	1.46
1	A	317	ILE	CA-C	6.40	1.59	1.52
1	B	378	ILE	CA-C	-6.38	1.44	1.52
1	B	261	THR	CA-CB	-6.35	1.42	1.53
1	C	76	GLN	CG-CD	-6.34	1.36	1.52
1	C	164	ALA	CA-C	-6.34	1.44	1.52
1	A	71	ARG	CA-C	-6.33	1.44	1.52
1	B	22	LEU	CG-CD2	-6.32	1.31	1.52
1	C	51	ALA	CA-CB	6.32	1.64	1.53
1	A	381	THR	CA-C	6.31	1.59	1.52
1	B	298	TYR	N-CA	-6.31	1.38	1.46
1	C	27	GLU	CG-CD	-6.29	1.36	1.52
1	A	188	VAL	CA-C	6.29	1.60	1.52
1	B	138	ARG	C-O	-6.29	1.16	1.23
1	B	242	MET	CG-SD	6.27	1.96	1.80
1	A	7	VAL	CA-CB	-6.26	1.44	1.54
1	B	22	LEU	CA-C	-6.25	1.44	1.52
1	B	343	LEU	C-O	-6.25	1.16	1.23
1	C	298	TYR	CA-C	-6.24	1.44	1.52
1	B	382	GLN	CD-NE2	6.24	1.46	1.33
1	A	325	PHE	CA-C	-6.23	1.45	1.52
1	C	367	SER	CA-C	-6.22	1.45	1.52
1	A	20	ALA	CA-CB	6.21	1.63	1.53
1	B	188	VAL	CA-C	-6.19	1.44	1.52
1	A	353	PHE	CA-C	-6.18	1.44	1.52
1	B	314	LEU	C-O	-6.18	1.16	1.23
1	C	280	TYR	CA-C	-6.17	1.45	1.52
1	B	57	ALA	CA-CB	-6.16	1.44	1.53
1	B	176	GLN	N-CA	-6.16	1.38	1.46
1	A	236	VAL	CA-CB	-6.14	1.45	1.54
1	B	376	PHE	CA-C	-6.14	1.44	1.52
1	B	138	ARG	CA-C	-6.12	1.45	1.52
1	A	355	ARG	CB-CG	-6.12	1.34	1.52
1	B	342	VAL	CA-CB	-6.12	1.46	1.54
1	C	150	PRO	CA-C	-6.12	1.43	1.52
1	C	372	VAL	CA-C	6.11	1.61	1.52
1	C	215	THR	CA-C	-6.11	1.44	1.52
1	C	311	GLY	CA-C	-6.11	1.48	1.52
1	A	49	ALA	CA-CB	6.10	1.63	1.53
1	B	193	GLU	C-O	-6.09	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	27	GLU	CA-CB	-6.08	1.44	1.53
1	B	158	PHE	C-O	6.08	1.31	1.24
1	C	297	ASP	N-CA	-6.07	1.38	1.46
1	C	127	ALA	CA-CB	-6.07	1.44	1.53
1	C	141	ASN	CA-C	6.07	1.60	1.52
1	B	7	VAL	C-O	-6.06	1.16	1.24
1	B	121	THR	CA-CB	-6.04	1.43	1.53
1	C	227	LYS	C-O	-6.04	1.17	1.24
1	B	139	ASP	CA-C	-6.03	1.44	1.52
1	B	145	LEU	C-O	6.03	1.31	1.24
1	C	235	GLU	CA-C	-6.02	1.45	1.52
1	A	139	ASP	CA-C	-5.96	1.47	1.53
1	B	182	ASN	CA-C	-5.96	1.44	1.52
1	A	205	ASP	CA-C	-5.96	1.46	1.53
1	A	343	LEU	CA-C	-5.96	1.45	1.52
1	B	175	VAL	CA-CB	-5.94	1.47	1.54
1	C	231	HIS	CA-C	-5.91	1.45	1.52
1	B	63	MET	SD-CE	5.90	1.94	1.79
1	C	182	ASN	CA-C	-5.90	1.44	1.52
1	C	42	ALA	CA-C	5.89	1.60	1.52
1	C	187	TRP	CA-C	5.88	1.60	1.52
1	A	203	SER	C-O	-5.88	1.16	1.24
1	B	182	ASN	C-O	-5.88	1.16	1.24
1	B	275	LYS	C-O	-5.88	1.16	1.24
1	B	50	PRO	C-O	-5.87	1.16	1.24
1	A	218	LEU	CB-CG	-5.87	1.41	1.53
1	B	308	VAL	CA-C	5.87	1.59	1.52
1	C	402	TYR	C-O	5.85	1.30	1.23
1	B	56	PHE	C-O	-5.84	1.16	1.23
1	B	68	GLU	CA-C	-5.84	1.46	1.52
1	B	363	ASP	CG-OD1	5.83	1.36	1.25
1	C	60	VAL	CA-C	5.82	1.60	1.52
1	C	137	ALA	C-O	-5.82	1.17	1.24
1	A	315	GLU	C-O	-5.79	1.16	1.24
1	B	141	ASN	C-O	5.79	1.31	1.24
1	B	209	ILE	C-O	-5.78	1.17	1.24
1	B	209	ILE	CA-C	-5.77	1.45	1.52
1	C	211	HIS	CA-C	-5.77	1.47	1.53
1	B	220	ALA	CA-CB	-5.77	1.44	1.53
1	C	382	GLN	CB-CG	5.76	1.69	1.52
1	A	16	ALA	CA-CB	-5.75	1.44	1.53
1	B	19	VAL	CA-C	-5.74	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	GLU	C-O	-5.72	1.16	1.24
1	B	16	ALA	C-O	-5.71	1.17	1.24
1	B	319	THR	CA-CB	5.70	1.63	1.53
1	B	122	ASN	C-O	-5.70	1.17	1.24
1	B	361	ILE	C-O	5.69	1.30	1.24
1	A	357	TYR	CA-C	-5.69	1.45	1.53
1	C	364	VAL	CA-CB	-5.68	1.46	1.54
1	A	77	PHE	N-CA	5.67	1.53	1.46
1	C	141	ASN	C-O	5.66	1.31	1.24
1	B	21	ALA	CA-CB	-5.65	1.44	1.53
1	C	11	SER	CA-C	-5.64	1.45	1.52
1	C	49	ALA	CA-CB	5.62	1.62	1.53
1	A	215	THR	N-CA	-5.62	1.39	1.46
1	B	292	VAL	CA-CB	-5.62	1.47	1.54
1	C	292	VAL	C-O	-5.62	1.17	1.24
1	A	360	GLU	CA-C	5.62	1.60	1.52
1	C	302	GLN	N-CA	-5.61	1.39	1.46
1	C	147	LYS	N-CA	-5.59	1.42	1.46
1	C	312	PHE	CA-C	5.59	1.59	1.52
1	A	243	MET	C-O	-5.58	1.17	1.24
1	C	268	PRO	C-O	5.57	1.31	1.24
1	C	27	GLU	CA-C	-5.55	1.46	1.53
1	C	183	ALA	CA-C	-5.55	1.45	1.52
1	C	390	ILE	CA-C	5.55	1.59	1.52
1	A	136	ILE	CA-CB	-5.55	1.48	1.54
1	B	320	SER	C-O	-5.55	1.17	1.23
1	A	354	ASP	C-O	-5.54	1.16	1.23
1	B	181	HIS	CA-C	-5.53	1.45	1.52
1	B	277	HIS	CA-C	-5.53	1.47	1.53
1	B	280	TYR	C-O	-5.53	1.17	1.24
1	A	404	PRO	C-O	-5.53	1.16	1.24
1	B	359	TYR	C-O	-5.52	1.17	1.24
1	C	277	HIS	CA-C	5.51	1.60	1.52
1	C	377	ASP	CA-C	5.51	1.59	1.52
1	C	321	ALA	CA-CB	-5.50	1.44	1.53
1	C	387	ASN	CA-C	5.48	1.60	1.52
1	A	5	LYS	CG-CD	5.47	1.68	1.52
1	B	39	SER	N-CA	-5.46	1.39	1.46
1	C	69	TRP	CB-CG	-5.45	1.33	1.50
1	B	254	ALA	CA-CB	-5.44	1.45	1.53
1	A	65	THR	CA-CB	-5.44	1.44	1.53
1	C	317	ILE	CG1-CD1	5.43	1.73	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	MET	CA-C	5.41	1.59	1.52
1	C	360	GLU	C-O	-5.41	1.17	1.23
1	A	309	PHE	C-O	-5.41	1.17	1.23
1	B	105	PHE	C-O	-5.41	1.17	1.24
1	A	83	ARG	NE-CZ	5.40	1.39	1.33
1	C	216	ASP	CA-C	-5.40	1.45	1.52
1	A	209	ILE	CA-CB	-5.40	1.48	1.54
1	A	146	ALA	CA-C	-5.39	1.46	1.53
1	B	200	HIS	C-O	-5.39	1.17	1.24
1	A	377	ASP	CA-C	-5.38	1.45	1.53
1	A	356	LEU	CA-C	-5.37	1.45	1.53
1	A	324	ASP	CA-C	-5.36	1.46	1.52
1	C	154	ASP	CG-OD2	5.36	1.35	1.25
1	B	320	SER	CA-C	-5.35	1.45	1.52
1	C	94	ASP	CA-C	-5.35	1.45	1.52
1	A	73	TYR	CA-C	-5.34	1.45	1.52
1	B	177	PHE	CG-CD1	-5.34	1.27	1.38
1	B	196	MET	SD-CE	-5.34	1.66	1.79
1	A	2	LEU	CA-C	-5.33	1.45	1.52
1	C	173	PHE	CA-C	-5.33	1.46	1.52
1	A	290	MET	N-CA	5.33	1.52	1.46
1	B	108	ASP	C-O	-5.32	1.17	1.23
1	C	192	GLU	C-O	-5.32	1.17	1.23
1	C	348	GLU	C-O	-5.32	1.17	1.23
1	A	390	ILE	CA-CB	-5.31	1.48	1.54
1	C	97	VAL	CA-CB	-5.31	1.47	1.54
1	A	327	ILE	CA-C	-5.30	1.47	1.53
1	C	378	ILE	CA-C	-5.30	1.46	1.52
1	C	130	ASP	CB-CG	5.29	1.65	1.52
1	A	203	SER	CA-C	-5.29	1.45	1.52
1	C	273	ASP	CG-OD1	5.29	1.35	1.25
1	B	196	MET	CA-C	-5.28	1.45	1.52
1	A	311	GLY	CA-C	-5.28	1.48	1.52
1	B	400	VAL	CA-CB	-5.28	1.47	1.53
1	A	26	GLN	CA-C	-5.28	1.45	1.52
1	A	394	ARG	NE-CZ	5.27	1.38	1.33
1	B	323	LEU	CG-CD2	5.26	1.70	1.52
1	B	182	ASN	CG-OD1	5.25	1.33	1.23
1	B	227	LYS	CA-C	-5.25	1.46	1.52
1	B	286	GLU	CA-C	-5.24	1.45	1.52
1	B	326	SER	C-O	-5.23	1.17	1.24
1	B	388	GLU	CD-OE2	5.23	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	314	LEU	C-O	-5.23	1.17	1.24
1	A	118	ALA	CA-C	-5.23	1.47	1.53
1	C	154	ASP	CG-OD1	5.22	1.35	1.25
1	A	264	GLU	CD-OE2	5.22	1.35	1.25
1	A	42	ALA	CA-CB	-5.22	1.44	1.53
1	C	96	VAL	C-N	-5.21	1.27	1.33
1	B	92	TYR	CB-CG	5.20	1.63	1.51
1	B	83	ARG	CZ-NH1	5.20	1.40	1.32
1	A	59	CYS	C-O	5.19	1.30	1.24
1	B	232	ASP	CA-C	-5.19	1.46	1.52
1	A	211	HIS	C-O	-5.19	1.18	1.24
1	C	398	PRO	C-O	-5.18	1.17	1.23
1	A	-1	ARG	NE-CZ	5.18	1.38	1.33
1	C	243	MET	N-CA	-5.18	1.40	1.46
1	A	257	ASN	CA-C	-5.18	1.47	1.53
1	B	399	SER	CA-C	-5.17	1.46	1.52
1	B	352	GLN	CD-NE2	5.16	1.44	1.33
1	A	128	ASP	C-O	-5.16	1.17	1.23
1	C	296	HIS	CA-C	-5.16	1.46	1.52
1	B	15	ARG	N-CA	-5.15	1.40	1.46
1	C	162	ILE	N-CA	-5.15	1.40	1.46
1	A	7	VAL	CA-C	-5.14	1.44	1.52
1	B	247	LEU	CA-C	5.13	1.59	1.52
1	B	164	ALA	N-CA	-5.13	1.40	1.46
1	B	173	PHE	CA-C	-5.12	1.45	1.52
1	A	166	GLU	CA-C	-5.12	1.46	1.52
1	B	77	PHE	C-O	-5.12	1.18	1.24
1	C	183	ALA	CA-CB	-5.11	1.45	1.53
1	C	399	SER	CA-C	-5.11	1.46	1.53
1	A	111	TRP	CA-C	-5.10	1.46	1.52
1	C	317	ILE	CB-CG2	5.10	1.69	1.52
1	A	128	ASP	CA-C	-5.10	1.46	1.52
1	C	303	LYS	CG-CD	5.09	1.67	1.52
1	A	349	THR	CA-CB	-5.08	1.43	1.53
1	C	354	ASP	C-O	-5.08	1.15	1.23
1	A	201	TYR	CA-C	5.08	1.59	1.52
1	B	64	ALA	C-O	-5.08	1.18	1.24
1	C	254	ALA	CA-CB	-5.08	1.44	1.52
1	B	238	CYS	CB-SG	-5.08	1.64	1.81
1	B	346	SER	CA-C	-5.07	1.45	1.52
1	B	142	VAL	N-CA	-5.07	1.40	1.46
1	A	125	ASN	CA-C	-5.07	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	372	VAL	CA-CB	-5.07	1.47	1.54
1	B	129	ILE	CG1-CD1	-5.06	1.32	1.51
1	C	118	ALA	CA-CB	5.05	1.62	1.53
1	B	236	VAL	C-O	5.04	1.29	1.24
1	A	27	GLU	CA-CB	-5.04	1.45	1.53
1	A	381	THR	C-O	5.03	1.29	1.23
1	C	208	PHE	CA-C	-5.03	1.46	1.52
1	B	199	LEU	C-O	-5.03	1.18	1.24
1	C	366	GLU	CD-OE1	5.02	1.34	1.25
1	C	55	ALA	CA-CB	5.02	1.59	1.52
1	A	164	ALA	N-CA	-5.02	1.40	1.46
1	C	319	THR	CB-CG2	5.01	1.69	1.52
1	C	90	ILE	CA-C	-5.01	1.47	1.52
1	B	164	ALA	C-O	-5.00	1.17	1.24
1	B	401	ILE	CA-CB	-5.00	1.47	1.54
1	B	66	PHE	N-CA	5.00	1.51	1.46

All (336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ASP	N-CA-C	-13.80	96.77	113.19
1	B	47	CYS	CA-CB-SG	-12.83	84.89	114.40
1	C	143	ASP	N-CA-C	-11.48	97.11	112.26
1	C	115	LEU	N-CA-C	-11.25	86.83	110.80
1	B	317	ILE	N-CA-C	10.73	120.51	110.42
1	A	215	THR	N-CA-C	-10.69	99.59	111.14
1	B	201	TYR	N-CA-C	10.38	123.86	111.82
1	C	397	PRO	O-C-N	10.22	126.01	121.31
1	B	48	PRO	N-CA-C	-9.96	97.64	113.78
1	B	213	SER	N-CA-C	-9.70	101.55	113.97
1	C	82	ARG	N-CA-C	-9.67	101.48	113.18
1	A	385	TRP	N-CA-C	-9.48	101.47	113.23
1	C	145	LEU	N-CA-C	-9.48	101.03	112.59
1	A	220	ALA	N-CA-C	-9.42	101.10	111.36
1	C	147	LYS	N-CA-C	9.39	116.48	108.78
1	B	237	ASN	N-CA-C	-9.38	97.37	111.81
1	B	347	LEU	N-CA-C	9.32	123.93	113.21
1	B	222	TRP	N-CA-C	-9.04	101.39	111.07
1	A	263	LYS	N-CA-C	-9.00	101.42	111.14
1	C	385	TRP	N-CA-C	-8.93	102.52	113.15
1	B	354	ASP	N-CA-C	-8.89	102.42	113.18
1	A	48	PRO	N-CA-C	-8.87	100.53	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	HIS	N-CA-C	-8.80	101.65	111.07
1	B	39	SER	N-CA-C	-8.74	100.94	111.69
1	A	275	LYS	N-CA-C	-8.73	96.76	109.59
1	C	323	LEU	N-CA-C	8.67	123.53	109.40
1	C	27	GLU	CB-CG-CD	-8.56	98.06	112.60
1	C	315	GLU	N-CA-C	-8.54	102.62	113.72
1	A	233	PRO	N-CD-CG	-8.51	90.44	103.20
1	A	47	CYS	N-CA-C	8.50	128.60	109.81
1	C	48	PRO	N-CA-C	-8.48	101.51	113.81
1	C	44	PRO	N-CD-CG	-8.38	93.75	103.80
1	A	113	ASP	N-CA-C	8.34	128.56	110.80
1	B	317	ILE	CB-CA-C	-8.30	101.17	111.87
1	C	47	CYS	CA-CB-SG	-8.24	95.44	114.40
1	B	47	CYS	N-CA-C	8.21	127.97	109.81
1	A	348	GLU	CA-C-N	-8.17	109.72	120.67
1	A	348	GLU	C-N-CA	-8.17	109.72	120.67
1	C	397	PRO	N-CD-CG	-8.14	90.98	103.20
1	A	44	PRO	CA-C-N	8.13	128.19	119.90
1	A	44	PRO	C-N-CA	8.13	128.19	119.90
1	C	311	GLY	CA-C-N	-8.08	111.85	123.00
1	C	311	GLY	C-N-CA	-8.08	111.85	123.00
1	A	9	ASN	N-CA-C	-8.08	100.43	113.19
1	A	121	THR	N-CA-C	8.04	121.57	110.24
1	C	344	GLY	N-CA-C	8.00	122.42	110.75
1	C	83	ARG	N-CA-C	-7.92	103.51	113.01
1	A	223	GLN	N-CA-C	-7.88	101.65	111.11
1	C	147	LYS	CA-C-O	7.86	122.50	117.94
1	A	143	ASP	N-CA-C	-7.83	101.87	113.61
1	B	396	PRO	N-CA-C	-7.70	101.30	110.70
1	B	375	VAL	N-CA-C	7.70	119.61	107.98
1	B	96	VAL	CA-C-N	-7.63	115.04	123.43
1	B	96	VAL	C-N-CA	-7.63	115.04	123.43
1	A	48	PRO	N-CD-CG	-7.56	91.85	103.20
1	B	298	TYR	N-CA-C	-7.51	103.17	111.36
1	A	308	VAL	CB-CA-C	-7.48	99.94	110.12
1	B	65	THR	N-CA-CB	7.48	121.41	110.57
1	B	302	GLN	N-CA-C	-7.43	102.12	112.45
1	A	315	GLU	N-CA-C	-7.43	104.19	113.18
1	C	49	ALA	N-CA-C	-7.38	93.49	109.81
1	B	171	CYS	N-CA-C	7.37	119.10	111.14
1	B	76	GLN	N-CA-C	-7.34	103.36	111.36
1	C	217	ARG	N-CA-C	-7.32	103.00	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	LEU	CB-CG-CD2	-7.30	88.79	110.70
1	A	83	ARG	N-CA-C	-7.30	104.11	112.87
1	A	136	ILE	N-CA-C	7.21	118.35	110.21
1	B	238	CYS	N-CA-C	7.20	120.13	108.76
1	C	50	PRO	N-CA-C	-7.17	106.38	114.92
1	B	355	ARG	CA-C-O	-7.16	113.45	121.40
1	A	255	PRO	N-CD-CG	-7.10	95.28	103.80
1	B	143	ASP	CB-CG-OD2	7.02	134.54	118.40
1	B	328	CYS	N-CA-C	7.01	120.13	110.24
1	A	76	GLN	N-CA-C	-6.91	103.83	111.36
1	B	2	LEU	N-CA-C	-6.90	98.15	108.99
1	C	243	MET	N-CA-C	-6.86	103.73	111.07
1	B	238	CYS	CA-CB-SG	-6.84	98.67	114.40
1	B	255	PRO	CA-C-N	-6.82	111.92	122.49
1	B	255	PRO	C-N-CA	-6.82	111.92	122.49
1	B	238	CYS	O-C-N	-6.81	115.85	123.48
1	B	310	ALA	N-CA-C	-6.81	99.87	110.42
1	A	311	GLY	CA-C-O	-6.80	114.73	120.92
1	B	212	HIS	CA-C-N	-6.79	110.97	122.11
1	B	212	HIS	C-N-CA	-6.79	110.97	122.11
1	B	231	HIS	N-CA-C	6.76	120.61	110.14
1	B	350	PRO	N-CD-CG	-6.75	93.08	103.20
1	A	214	ASN	N-CA-C	-6.74	103.74	112.23
1	C	301	GLN	N-CA-C	-6.74	105.09	113.38
1	B	212	HIS	N-CA-C	-6.71	104.12	113.37
1	C	58	CYS	CB-CA-C	-6.70	97.64	109.71
1	A	27	GLU	CB-CA-C	-6.70	99.39	110.72
1	C	208	PHE	N-CA-C	-6.70	103.67	110.97
1	C	158	PHE	N-CA-C	-6.68	103.93	111.14
1	A	182	ASN	N-CA-C	6.66	121.00	112.34
1	A	95	THR	N-CA-C	-6.60	104.45	113.30
1	A	148	GLU	N-CA-C	-6.56	99.48	109.85
1	C	316	GLY	CA-C-N	-6.55	114.78	122.11
1	C	316	GLY	C-N-CA	-6.55	114.78	122.11
1	B	45	PRO	N-CD-CG	-6.54	93.38	103.20
1	B	244	ARG	NE-CZ-NH1	-6.54	114.96	121.50
1	B	349	THR	CA-C-N	6.52	126.55	119.90
1	B	349	THR	C-N-CA	6.52	126.55	119.90
1	C	233	PRO	CA-C-N	-6.52	112.33	122.37
1	C	233	PRO	C-N-CA	-6.52	112.33	122.37
1	A	346	SER	N-CA-C	-6.49	102.66	111.55
1	B	351	TRP	CA-C-O	-6.47	114.34	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	397	PRO	CA-C-N	6.47	126.39	119.85
1	C	397	PRO	C-N-CA	6.47	126.39	119.85
1	A	359	TYR	CA-CB-CG	6.47	125.55	113.90
1	A	144	LYS	N-CA-C	-6.42	105.43	113.20
1	A	244	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	C	163	TYR	N-CA-C	-6.40	104.23	111.07
1	B	48	PRO	N-CD-CG	-6.39	93.62	103.20
1	B	292	VAL	N-CA-C	-6.38	104.30	110.42
1	C	321	ALA	CA-C-O	-6.35	114.47	121.33
1	A	236	VAL	CB-CA-C	-6.34	103.18	110.73
1	A	45	PRO	CB-CA-C	-6.33	103.52	111.56
1	B	403	VAL	CB-CA-C	-6.33	103.90	111.18
1	A	314	LEU	N-CA-C	6.32	119.10	108.23
1	C	2	LEU	CA-C-N	-6.32	115.36	123.19
1	C	2	LEU	C-N-CA	-6.32	115.36	123.19
1	B	22	LEU	CD1-CG-CD2	-6.31	96.92	110.80
1	A	145	LEU	N-CA-C	-6.29	105.32	112.87
1	C	259	ASN	N-CA-C	-6.28	102.23	110.39
1	A	349	THR	OG1-CB-CG2	-6.26	96.79	109.30
1	B	349	THR	OG1-CB-CG2	-6.26	96.79	109.30
1	B	403	VAL	O-C-N	6.25	126.67	120.92
1	A	328	CYS	N-CA-C	6.22	118.87	108.73
1	A	82	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	B	257	ASN	CB-CA-C	-6.19	103.32	111.42
1	B	283	ASP	N-CA-C	-6.18	103.85	111.33
1	B	20	ALA	N-CA-C	-6.18	104.81	112.90
1	B	314	LEU	CA-C-O	-6.18	114.83	121.56
1	A	71	ARG	N-CA-C	-6.17	103.88	112.45
1	A	236	VAL	CA-C-O	-6.16	114.28	120.31
1	B	27	GLU	CB-CA-C	-6.16	101.11	111.02
1	C	98	PRO	CA-C-O	-6.14	114.83	121.27
1	B	316	GLY	CA-C-N	6.13	128.20	120.72
1	B	316	GLY	C-N-CA	6.13	128.20	120.72
1	A	67	PRO	N-CD-CG	-6.12	94.02	103.20
1	B	45	PRO	CA-C-O	-6.11	114.06	121.03
1	B	39	SER	CA-C-N	-6.11	109.87	121.54
1	B	39	SER	C-N-CA	-6.11	109.87	121.54
1	A	146	ALA	CA-C-O	-6.11	115.02	122.41
1	A	12	PRO	N-CA-C	-6.10	104.96	113.81
1	B	128	ASP	N-CA-C	-6.10	100.95	110.17
1	C	124	PHE	N-CA-C	-6.10	104.91	113.20
1	C	334	CYS	N-CA-C	6.09	119.54	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	THR	N-CA-C	-6.07	99.01	109.15
1	B	84	HIS	CA-C-N	-6.07	113.61	122.46
1	B	84	HIS	C-N-CA	-6.07	113.61	122.46
1	B	106	PHE	CA-C-N	-6.04	111.28	122.09
1	B	106	PHE	C-N-CA	-6.04	111.28	122.09
1	B	214	ASN	N-CA-C	-6.03	105.75	113.23
1	C	219	PHE	N-CA-C	-6.03	104.62	111.07
1	B	80	ALA	N-CA-C	-6.02	105.02	112.90
1	A	201	TYR	CA-C-O	6.01	126.80	119.11
1	B	187	TRP	CA-C-N	-6.00	114.51	121.71
1	B	187	TRP	C-N-CA	-6.00	114.51	121.71
1	C	26	GLN	CA-C-N	-5.99	114.24	123.17
1	C	26	GLN	C-N-CA	-5.99	114.24	123.17
1	C	7	VAL	CB-CA-C	-5.99	101.47	111.29
1	A	242	MET	CA-C-O	5.98	125.37	118.97
1	A	316	GLY	N-CA-C	5.96	127.31	113.18
1	A	99	GLN	N-CA-C	5.96	117.91	108.67
1	C	67	PRO	N-CD-CG	-5.92	94.31	103.20
1	C	218	LEU	CB-CG-CD2	-5.89	93.02	110.70
1	B	384	SER	CB-CA-C	-5.88	97.63	109.68
1	A	235	GLU	CA-C-N	-5.87	115.00	123.11
1	A	235	GLU	C-N-CA	-5.87	115.00	123.11
1	B	53	ASN	N-CA-C	5.87	118.18	111.02
1	A	174	GLU	CA-C-N	-5.85	111.44	121.97
1	A	174	GLU	C-N-CA	-5.85	111.44	121.97
1	C	143	ASP	CA-C-N	-5.85	112.20	122.62
1	C	143	ASP	C-N-CA	-5.85	112.20	122.62
1	B	91	PRO	N-CD-CG	-5.85	94.43	103.20
1	C	238	CYS	N-CA-CB	-5.84	100.69	110.80
1	C	202	ALA	N-CA-C	-5.84	104.82	111.07
1	B	227	LYS	N-CA-C	-5.84	105.00	111.36
1	C	86	SER	CA-CB-OG	5.83	122.75	111.10
1	C	396	PRO	CA-C-N	5.80	123.90	119.66
1	C	396	PRO	C-N-CA	5.80	123.90	119.66
1	B	67	PRO	CA-C-N	-5.80	111.70	122.60
1	B	67	PRO	C-N-CA	-5.80	111.70	122.60
1	A	47	CYS	CA-CB-SG	-5.80	101.07	114.40
1	C	298	TYR	N-CA-C	-5.79	105.71	112.89
1	C	74	THR	CB-CA-C	-5.79	101.80	110.88
1	A	78	GLU	N-CA-C	-5.75	105.01	111.28
1	B	260	PRO	CA-C-N	-5.75	111.57	120.31
1	B	260	PRO	C-N-CA	-5.75	111.57	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ASP	CA-C-N	-5.74	115.70	122.93
1	A	389	ASP	C-N-CA	-5.74	115.70	122.93
1	B	400	VAL	N-CA-CB	-5.74	104.67	111.90
1	B	5	LYS	N-CA-C	5.72	118.89	110.59
1	B	287	LEU	N-CA-C	-5.70	99.94	109.24
1	C	321	ALA	CA-C-N	-5.70	113.86	122.81
1	C	321	ALA	C-N-CA	-5.70	113.86	122.81
1	A	384	SER	CB-CA-C	-5.70	99.08	110.42
1	B	150	PRO	N-CA-C	-5.69	106.64	113.98
1	A	272	PHE	N-CA-CB	5.69	119.06	110.30
1	B	63	MET	CG-SD-CE	5.68	113.40	100.90
1	B	203	SER	N-CA-C	-5.68	105.53	113.37
1	B	25	LEU	N-CA-C	-5.65	105.02	111.07
1	B	87	VAL	CA-C-N	-5.65	114.66	122.69
1	B	87	VAL	C-N-CA	-5.65	114.66	122.69
1	C	397	PRO	N-CA-CB	-5.65	100.03	103.19
1	B	97	VAL	CB-CA-C	-5.65	104.33	110.37
1	B	308	VAL	O-C-N	-5.61	117.80	123.19
1	A	395	PHE	N-CA-C	-5.60	102.72	109.72
1	C	378	ILE	CB-CA-C	-5.60	103.08	110.98
1	B	59	CYS	N-CA-C	5.57	119.00	110.20
1	A	398	PRO	N-CD-CG	-5.57	94.85	103.20
1	A	244	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	79	ASP	CA-C-O	5.56	126.17	119.61
1	A	57	ALA	CA-C-N	-5.55	110.93	121.54
1	A	57	ALA	C-N-CA	-5.55	110.93	121.54
1	C	198	HIS	N-CA-C	5.55	117.40	107.80
1	A	327	ILE	CB-CA-C	-5.55	105.24	111.23
1	B	276	GLY	N-CA-C	-5.53	100.06	113.18
1	B	277	HIS	N-CA-C	-5.53	104.17	111.96
1	B	341	ASP	N-CA-C	5.52	118.18	108.75
1	A	360	GLU	N-CA-C	5.51	118.23	109.96
1	B	308	VAL	CA-C-N	-5.51	113.94	122.59
1	B	308	VAL	C-N-CA	-5.51	113.94	122.59
1	C	317	ILE	O-C-N	5.51	128.40	122.67
1	B	213	SER	CA-C-O	5.50	124.86	118.97
1	C	181	HIS	N-CA-C	-5.50	99.08	110.80
1	B	394	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	C	356	LEU	CB-CG-CD1	5.48	127.14	110.70
1	B	401	ILE	N-CA-C	5.48	120.73	109.34
1	C	65	THR	OG1-CB-CG2	-5.47	98.36	109.30
1	C	2	LEU	N-CA-C	-5.47	100.78	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	VAL	CB-CA-C	-5.46	104.05	111.15
1	B	159	LYS	N-CA-C	-5.45	104.73	111.33
1	B	395	PHE	N-CA-C	-5.45	97.77	109.81
1	A	317	ILE	N-CA-C	5.44	114.33	107.70
1	C	234	ASN	N-CA-C	-5.42	105.30	112.94
1	C	266	SER	N-CA-CB	-5.42	102.56	110.47
1	C	201	TYR	N-CA-C	5.41	122.87	114.64
1	B	206	PRO	N-CD-CG	-5.41	95.08	103.20
1	B	403	VAL	CA-C-N	5.40	126.59	119.84
1	B	403	VAL	C-N-CA	5.40	126.59	119.84
1	C	12	PRO	N-CA-C	-5.40	105.98	113.81
1	B	217	ARG	N-CA-C	-5.39	105.32	111.14
1	B	317	ILE	N-CA-CB	-5.38	104.56	110.65
1	C	226	GLN	N-CA-C	-5.38	105.33	111.14
1	B	206	PRO	O-C-N	-5.38	115.01	122.27
1	C	27	GLU	OE1-CD-OE2	5.38	135.80	122.90
1	A	326	SER	N-CA-C	5.37	118.15	109.40
1	B	50	PRO	N-CD-CG	-5.36	95.16	103.20
1	B	218	LEU	CA-C-O	-5.36	114.87	120.55
1	C	375	VAL	N-CA-CB	-5.36	105.55	111.66
1	B	238	CYS	CA-C-N	-5.36	114.25	122.61
1	B	238	CYS	C-N-CA	-5.36	114.25	122.61
1	B	350	PRO	CA-C-O	-5.35	115.31	121.36
1	A	154	ASP	N-CA-CB	-5.34	104.37	110.35
1	A	317	ILE	CA-C-O	5.33	124.23	120.66
1	A	261	THR	CA-C-N	-5.32	113.39	122.11
1	A	261	THR	C-N-CA	-5.32	113.39	122.11
1	B	15	ARG	N-CA-CB	-5.31	102.02	109.94
1	A	170	TYR	CA-C-N	-5.31	112.63	120.38
1	A	170	TYR	C-N-CA	-5.31	112.63	120.38
1	A	286	GLU	CA-C-O	-5.31	115.63	121.31
1	C	16	ALA	CA-C-N	-5.30	113.55	120.44
1	C	16	ALA	C-N-CA	-5.30	113.55	120.44
1	C	358	LYS	CD-CE-NZ	5.29	128.84	111.90
1	C	392	THR	N-CA-C	-5.27	105.55	112.72
1	A	232	ASP	N-CA-C	-5.27	101.62	109.42
1	A	338	GLY	CA-C-O	-5.27	116.41	121.41
1	A	174	GLU	N-CA-C	-5.26	106.00	112.90
1	C	245	GLU	CA-C-N	5.26	126.42	119.84
1	C	245	GLU	C-N-CA	5.26	126.42	119.84
1	A	284	HIS	CA-C-O	-5.26	115.56	121.40
1	C	351	TRP	N-CA-C	5.26	117.07	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	C	373	HIS	CA-C-N	-5.23	113.99	122.36
1	C	373	HIS	C-N-CA	-5.23	113.99	122.36
1	B	174	GLU	CA-C-N	-5.23	113.29	120.46
1	B	174	GLU	C-N-CA	-5.23	113.29	120.46
1	C	203	SER	CA-CB-OG	-5.23	100.64	111.10
1	C	370	LEU	CA-CB-CG	-5.23	98.00	116.30
1	A	59	CYS	CA-C-O	5.22	126.07	120.38
1	A	20	ALA	N-CA-C	-5.21	106.77	113.23
1	C	47	CYS	N-CA-C	5.21	121.31	109.81
1	B	330	ILE	N-CA-C	-5.20	104.40	111.89
1	C	305	ALA	N-CA-C	5.20	116.75	108.79
1	C	192	GLU	N-CA-C	5.19	118.46	110.42
1	A	338	GLY	N-CA-C	-5.18	103.68	111.19
1	B	271	THR	CB-CA-C	-5.17	101.14	110.35
1	C	139	ASP	CB-CA-C	-5.17	104.25	111.85
1	A	368	LYS	N-CA-C	-5.17	99.80	110.80
1	C	236	VAL	CA-C-N	-5.16	114.89	122.83
1	C	236	VAL	C-N-CA	-5.16	114.89	122.83
1	B	206	PRO	CA-C-N	-5.15	113.09	121.54
1	B	206	PRO	C-N-CA	-5.15	113.09	121.54
1	A	67	PRO	CA-C-N	-5.15	112.86	120.28
1	A	67	PRO	C-N-CA	-5.15	112.86	120.28
1	A	113	ASP	CA-C-N	5.15	131.38	121.54
1	A	113	ASP	C-N-CA	5.15	131.38	121.54
1	C	380	ILE	CA-C-N	5.15	128.93	121.26
1	C	380	ILE	C-N-CA	5.15	128.93	121.26
1	B	186	ALA	N-CA-C	5.15	116.97	111.36
1	B	391	SER	CA-C-N	-5.14	114.45	122.73
1	B	391	SER	C-N-CA	-5.14	114.45	122.73
1	C	144	LYS	N-CA-C	-5.13	104.52	111.55
1	B	295	LEU	N-CA-C	-5.13	105.34	111.03
1	C	147	LYS	CB-CA-C	-5.12	109.70	117.07
1	A	125	ASN	N-CA-C	-5.11	105.40	113.02
1	A	97	VAL	N-CA-C	5.11	114.58	108.96
1	C	271	THR	CA-C-O	5.11	124.14	118.52
1	C	213	SER	N-CA-C	-5.11	106.31	112.54
1	A	48	PRO	CA-N-CD	5.09	119.12	112.00
1	B	131	PHE	CA-C-O	5.08	126.12	120.63
1	C	65	THR	CA-CB-OG1	5.08	117.22	109.60
1	B	234	ASN	N-CA-C	5.08	121.62	110.80
1	B	264	GLU	CA-C-N	-5.07	114.68	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	GLU	C-N-CA	-5.07	114.68	123.25
1	C	143	ASP	OD1-CG-OD2	-5.07	110.74	122.90
1	C	20	ALA	N-CA-C	-5.06	105.95	111.82
1	B	342	VAL	CA-CB-CG1	-5.06	101.79	110.40
1	C	302	GLN	N-CA-C	-5.06	105.85	112.23
1	A	147	LYS	N-CA-C	5.06	121.58	110.80
1	A	46	LEU	N-CA-C	-5.06	105.41	112.03
1	A	167	GLN	CA-C-N	-5.05	114.71	122.60
1	A	167	GLN	C-N-CA	-5.05	114.71	122.60
1	C	90	ILE	CA-C-N	5.05	125.33	119.92
1	C	90	ILE	C-N-CA	5.05	125.33	119.92
1	A	227	LYS	N-CA-C	-5.05	105.66	111.07
1	B	65	THR	CB-CA-C	-5.02	101.83	110.72
1	A	81	LEU	CB-CG-CD1	-5.02	95.65	110.70
1	A	213	SER	N-CA-C	-5.02	107.71	113.88
1	C	97	VAL	CB-CA-C	-5.02	102.23	111.36
1	C	184	ILE	CG1-CB-CG2	-5.01	95.66	110.70
1	B	56	PHE	N-CA-C	5.01	117.03	109.41
1	A	47	CYS	CA-C-N	-5.00	113.62	119.32
1	A	47	CYS	C-N-CA	-5.00	113.62	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	82	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3310	0	3075	479	2
1	B	3310	0	3074	430	0
1	C	3310	0	3074	474	0
2	A	15	0	15	3	0
2	C	30	0	30	1	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	2
3	C	3	0	0	0	0
All	All	9984	0	9268	1381	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 72.

All (1381) 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:290:MET:SD	1:A:290:MET:CE	2.02	1.47
1:B:290:MET:SD	1:B:290:MET:CE	2.05	1.44
1:C:59:CYS:SG	1:C:61:HIS:CE1	2.18	1.36
1:C:242:MET:CE	1:C:242:MET:SD	2.14	1.36
1:C:-2:HIS:CD2	1:C:-1:ARG:HE	1.57	1.22
1:B:200:HIS:CE1	1:B:347:LEU:HB2	1.76	1.20
1:C:71:ARG:HH22	1:C:223:GLN:NE2	1.39	1.20
1:B:372:VAL:HG11	1:B:402:TYR:CD1	1.80	1.16
1:A:316:GLY:O	1:A:317:ILE:HG23	1.44	1.14
1:A:59:CYS:SG	1:A:61:HIS:CE1	2.43	1.11
1:B:226:GLN:NE2	1:B:229:ARG:HH12	1.47	1.11
1:A:59:CYS:SG	1:A:61:HIS:NE2	2.24	1.10
1:A:290:MET:HB2	1:A:294:ARG:HB2	1.20	1.09
1:A:355:ARG:HH11	1:A:355:ARG:HB3	1.19	1.05
1:C:139:ASP:OD1	1:C:141:ASN:HB2	1.56	1.05
1:B:132:ASN:ND2	1:B:134:GLN:HG3	1.73	1.03
1:B:-1:ARG:HH11	1:B:-1:ARG:HG2	1.14	1.03
1:A:69:TRP:HD1	1:A:247:LEU:HD22	1.24	1.02
1:A:69:TRP:CD1	1:A:247:LEU:HD22	1.96	1.01
1:B:328:CYS:HA	1:B:334:CYS:HA	1.41	1.01
1:C:97:VAL:HG12	1:C:98:PRO:HD2	1.40	1.01
1:C:113:ASP:HB3	1:C:118:ALA:HB3	1.40	1.01
1:C:316:GLY:O	1:C:317:ILE:CG1	2.08	1.01
1:A:96:VAL:HG11	1:A:287:LEU:HD11	1.41	1.01
1:C:78:GLU:C	1:C:80:ALA:H	1.69	1.01
1:B:-2:HIS:CE1	1:B:-1:ARG:NH1	2.30	0.99
1:B:200:HIS:HE1	1:B:347:LEU:HB2	0.84	0.99
1:B:342:VAL:HG12	1:B:343:LEU:H	1.23	0.99
1:B:402:TYR:HE2	1:B:404:PRO:HG3	1.26	0.98
1:C:149:GLY:O	1:C:152:GLY:N	1.96	0.98
1:A:290:MET:HB2	1:A:294:ARG:CB	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:CYS:HB3	1:A:355:ARG:HH21	1.29	0.98
1:B:110:ILE:HD12	1:B:110:ILE:H	1.27	0.98
1:C:7:VAL:HG11	1:C:210:LEU:HD23	1.46	0.98
1:A:365:LEU:O	1:A:370:LEU:HB2	1.63	0.97
1:B:142:VAL:HG13	1:B:144:LYS:HB2	1.42	0.97
1:C:316:GLY:O	1:C:317:ILE:HG13	1.63	0.96
1:A:66:PHE:HB3	1:A:67:PRO:HD3	1.45	0.95
1:C:129:ILE:HG13	1:C:136:ILE:HD11	1.46	0.95
1:B:234:ASN:HD21	1:B:273:ASP:CB	1.80	0.95
1:A:182:ASN:HD22	1:A:342:VAL:HA	1.28	0.94
1:A:386:ASP:O	1:A:387:ASN:CG	2.10	0.94
1:C:259:ASN:HD21	1:C:261:THR:N	1.64	0.94
1:B:22:LEU:HD12	1:B:25:LEU:HD23	1.47	0.94
1:B:161:TYR:CD2	1:B:218:LEU:HD13	2.03	0.94
1:C:121:THR:O	1:C:123:PRO:HD3	1.67	0.94
1:A:56:PHE:HD1	1:A:349:THR:HG22	1.32	0.93
1:B:401:ILE:HG22	1:B:402:TYR:N	1.83	0.93
1:B:196:MET:CE	1:B:207:VAL:HG13	1.99	0.93
1:C:65:THR:HG22	1:C:243:MET:HE2	1.50	0.92
1:B:196:MET:HE2	1:B:207:VAL:HG13	1.51	0.92
1:B:372:VAL:HG11	1:B:402:TYR:HD1	1.35	0.92
1:A:39:SER:HB3	1:A:44:PRO:HD2	1.48	0.91
1:C:78:GLU:O	1:C:80:ALA:N	2.03	0.91
1:B:259:ASN:CG	1:B:262:THR:HB	1.94	0.91
1:C:-2:HIS:CD2	1:C:-1:ARG:NE	2.34	0.91
1:C:210:LEU:HD12	1:C:210:LEU:H	1.34	0.91
1:B:145:LEU:HD12	1:B:146:ALA:N	1.84	0.91
1:C:71:ARG:NH2	1:C:223:GLN:HE22	1.67	0.91
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.36	0.90
1:C:260:PRO:HG2	1:C:261:THR:N	1.86	0.90
1:C:198:HIS:CE1	1:C:200:HIS:HB2	2.05	0.90
1:C:-1:ARG:HB2	1:C:1:ASN:N	1.86	0.90
1:C:136:ILE:HD12	1:C:136:ILE:H	1.35	0.90
1:C:175:VAL:HG23	1:C:176:GLN:H	1.36	0.90
1:C:71:ARG:HH22	1:C:223:GLN:HE22	0.91	0.90
1:C:113:ASP:CB	1:C:118:ALA:HB3	2.02	0.89
1:C:380:ILE:HD11	1:C:392:THR:HB	1.54	0.89
1:C:22:LEU:HD23	1:C:26:GLN:HG3	1.52	0.89
1:B:402:TYR:CE2	1:B:404:PRO:HG3	2.07	0.89
1:A:136:ILE:HD11	1:A:204:TYR:CB	2.02	0.89
1:C:247:LEU:HD22	1:C:268:PRO:HG3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:SER:O	1:C:88:VAL:N	2.06	0.88
1:B:151:LYS:HE2	1:B:151:LYS:HA	1.56	0.88
1:B:148:GLU:HG2	1:B:155:THR:HB	1.53	0.88
1:A:372:VAL:HG11	1:A:402:TYR:HE1	1.39	0.88
1:A:97:VAL:HG12	1:A:288:GLN:HG3	1.56	0.87
1:B:71:ARG:HD3	1:B:216:ASP:OD2	1.74	0.87
1:A:140:ILE:HG22	1:A:142:VAL:O	1.74	0.87
1:C:131:PHE:HE2	1:C:204:TYR:HH	1.23	0.87
1:C:265:HIS:CD2	1:C:277:HIS:HB3	2.10	0.87
1:B:132:ASN:ND2	1:B:134:GLN:CG	2.36	0.87
1:C:161:TYR:CD2	1:C:218:LEU:HD22	2.10	0.86
1:A:198:HIS:O	1:A:200:HIS:N	2.08	0.86
1:A:60:VAL:HG11	1:A:65:THR:OG1	1.75	0.86
1:A:-1:ARG:O	1:A:279:HIS:ND1	2.09	0.86
1:B:181:HIS:O	1:B:181:HIS:CG	2.27	0.86
1:B:382:GLN:HB3	1:B:390:ILE:HB	1.58	0.85
1:C:-1:ARG:HB2	1:C:1:ASN:H2	1.40	0.85
1:C:33:GLY:O	1:C:34:PHE:O	1.94	0.85
1:B:132:ASN:HD21	1:B:134:GLN:HG3	1.37	0.84
1:C:4:ARG:HD2	1:C:282:TYR:CE1	2.12	0.84
1:C:33:GLY:O	1:C:34:PHE:C	2.17	0.84
1:C:81:LEU:HB3	1:C:86:SER:HB3	1.58	0.84
1:C:59:CYS:HG	1:C:61:HIS:CE1	1.90	0.84
1:A:198:HIS:O	1:A:199:LEU:C	2.21	0.84
1:C:316:GLY:C	1:C:317:ILE:HG13	2.03	0.84
1:A:65:THR:HG23	1:A:242:MET:HG3	1.59	0.84
1:A:220:ALA:HA	1:A:223:GLN:HE21	1.41	0.84
1:B:148:GLU:HG2	1:B:155:THR:CB	2.06	0.83
1:B:226:GLN:NE2	1:B:229:ARG:NH1	2.26	0.83
1:A:330:ILE:HD12	1:A:330:ILE:H	1.43	0.83
1:C:149:GLY:C	1:C:152:GLY:H	1.87	0.83
1:C:346:SER:HB2	1:C:347:LEU:HD22	1.59	0.83
1:A:94:ASP:HA	1:A:214:ASN:ND2	1.94	0.82
1:A:292:VAL:O	1:A:295:LEU:HB2	1.79	0.82
1:A:140:ILE:CG2	1:A:142:VAL:O	2.27	0.82
1:A:47:CYS:HB2	1:A:57:ALA:O	1.79	0.82
1:B:-1:ARG:HG2	1:B:-1:ARG:NH1	1.94	0.82
1:C:238:CYS:O	1:C:239:ALA:HB3	1.79	0.82
1:C:145:LEU:HD23	1:C:145:LEU:H	1.44	0.82
1:A:316:GLY:O	1:A:317:ILE:CG2	2.28	0.82
1:A:153:TYR:HB2	1:A:288:GLN:OE1	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:CYS:O	1:C:59:CYS:HB3	1.78	0.82
1:A:140:ILE:HD12	1:A:140:ILE:H	1.44	0.82
1:B:200:HIS:HE1	1:B:347:LEU:CB	1.81	0.81
1:A:136:ILE:HD11	1:A:204:TYR:C	2.04	0.81
1:B:141:ASN:ND2	1:B:142:VAL:H	1.78	0.81
1:C:76:GLN:O	1:C:76:GLN:HG3	1.80	0.81
1:A:15:ARG:O	1:A:19:VAL:HG23	1.80	0.81
1:A:244:ARG:HG2	1:A:244:ARG:NH1	1.94	0.81
1:B:165:LEU:HD23	1:B:222:TRP:HD1	1.44	0.81
1:C:140:ILE:O	1:C:142:VAL:N	2.14	0.81
1:A:56:PHE:CD1	1:A:349:THR:HG22	2.16	0.81
1:B:345:GLY:O	1:B:348:GLU:HG2	1.81	0.80
1:B:11:SER:O	1:B:14:GLU:N	2.13	0.80
1:A:96:VAL:HG11	1:A:287:LEU:CD1	2.12	0.80
1:A:-3:GLY:HA2	1:A:1:ASN:N	1.97	0.80
1:A:207:VAL:HA	1:A:210:LEU:HD12	1.61	0.80
1:B:236:VAL:HG12	1:B:238:CYS:N	1.97	0.80
1:A:290:MET:CB	1:A:294:ARG:HB2	2.09	0.80
1:B:39:SER:O	1:B:40:PHE:C	2.18	0.80
1:B:303:LYS:HE2	1:B:405:LYS:HG2	1.63	0.80
1:C:150:PRO:HD2	1:C:154:ASP:HB3	1.61	0.80
1:C:78:GLU:C	1:C:80:ALA:N	2.36	0.80
1:B:142:VAL:C	1:B:144:LYS:H	1.90	0.80
1:A:98:PRO:HB3	1:A:147:LYS:HA	1.64	0.79
1:C:-2:HIS:O	1:C:-1:ARG:NE	2.15	0.79
1:C:259:ASN:ND2	1:C:261:THR:N	2.29	0.79
1:B:45:PRO:HG2	1:B:45:PRO:O	1.82	0.79
1:B:327:ILE:HG23	1:B:327:ILE:O	1.81	0.79
1:B:110:ILE:HD12	1:B:110:ILE:N	1.98	0.79
1:C:93:TRP:HE1	1:C:99:GLN:HE22	1.28	0.78
1:B:-2:HIS:CE1	1:B:-1:ARG:HH12	2.01	0.78
1:B:249:PRO:O	1:B:250:PHE:C	2.25	0.78
1:C:136:ILE:HG21	1:C:205:ASP:HB2	1.64	0.78
1:C:247:LEU:HB2	1:C:266:SER:O	1.82	0.78
1:C:112:ASP:C	1:C:114:ALA:H	1.90	0.78
1:C:246:PRO:HG3	1:C:267:LYS:HE3	1.64	0.78
1:C:260:PRO:HG2	1:C:261:THR:H	1.46	0.78
1:C:234:ASN:OD1	1:C:273:ASP:HB2	1.83	0.78
1:C:245:GLU:O	1:C:246:PRO:O	2.01	0.78
1:A:8:ARG:HE	1:A:103:PRO:HG3	1.47	0.78
1:A:110:ILE:HD12	1:A:110:ILE:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:HD22	1:C:347:LEU:N	1.99	0.77
1:C:320:SER:HB3	1:C:344:GLY:H	1.48	0.77
1:A:236:VAL:HG21	1:A:272:PHE:CZ	2.20	0.77
1:B:372:VAL:CG1	1:B:402:TYR:CD1	2.67	0.77
1:C:113:ASP:HB3	1:C:118:ALA:CB	2.14	0.77
1:C:175:VAL:HG23	1:C:176:GLN:N	1.96	0.77
1:C:268:PRO:O	1:C:270:ASP:N	2.17	0.77
1:C:402:TYR:CE2	1:C:404:PRO:HG3	2.20	0.77
1:A:1:ASN:HB3	1:A:279:HIS:HB3	1.65	0.77
1:B:342:VAL:HG12	1:B:343:LEU:N	1.98	0.77
1:C:207:VAL:HA	1:C:210:LEU:HD13	1.66	0.77
1:B:262:THR:HG22	1:B:263:LYS:N	1.98	0.77
1:C:401:ILE:HG22	1:C:402:TYR:N	2.00	0.77
1:C:320:SER:HB3	1:C:344:GLY:N	2.00	0.76
1:B:236:VAL:HG12	1:B:237:ASN:N	1.95	0.76
1:B:244:ARG:O	1:B:244:ARG:HG2	1.86	0.76
1:C:198:HIS:O	1:C:199:LEU:C	2.28	0.76
1:A:108:ASP:HB2	1:A:110:ILE:HD12	1.67	0.76
1:C:150:PRO:HD2	1:C:154:ASP:O	1.85	0.76
1:C:335:THR:HG21	1:C:368:LYS:HE3	1.66	0.76
1:B:41:HIS:O	1:B:59:CYS:HB3	1.84	0.76
1:A:171:CYS:CB	1:A:355:ARG:HH21	1.98	0.76
1:A:264:GLU:HG3	1:A:265:HIS:CE1	2.20	0.76
1:C:39:SER:OG	1:C:44:PRO:HD2	1.86	0.75
1:A:-1:ARG:O	1:A:279:HIS:CG	2.39	0.75
1:B:132:ASN:HD22	1:B:134:GLN:CG	1.98	0.75
1:B:236:VAL:HG12	1:B:238:CYS:H	1.52	0.75
1:C:316:GLY:O	1:C:317:ILE:HG12	1.85	0.75
1:C:354:ASP:O	1:C:355:ARG:HB3	1.84	0.75
1:C:386:ASP:O	1:C:388:GLU:N	2.19	0.75
1:A:68:GLU:HB3	1:A:271:THR:OG1	1.86	0.75
1:A:136:ILE:CG2	1:A:137:ALA:N	2.49	0.75
1:B:161:TYR:CE2	1:B:218:LEU:HD13	2.21	0.75
1:C:202:ALA:O	1:C:203:SER:C	2.29	0.75
1:C:237:ASN:HA	1:C:240:LEU:HD21	1.69	0.75
1:C:174:GLU:OE1	1:C:178:GLU:OE2	2.05	0.75
1:B:257:ASN:HD21	1:B:262:THR:HG22	1.52	0.74
1:A:325:PHE:O	1:A:337:ALA:HB3	1.87	0.74
1:B:166:GLU:OE1	1:B:307:ARG:NH2	2.20	0.74
1:C:71:ARG:NH2	1:C:223:GLN:NE2	2.25	0.74
1:A:69:TRP:HD1	1:A:247:LEU:CD2	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ASN:ND2	1:C:262:THR:H	1.85	0.74
1:A:218:LEU:O	1:A:221:LEU:HB3	1.86	0.74
1:B:32:ASP:HA	1:B:37:LEU:HD21	1.70	0.74
1:A:291:ASN:O	1:A:295:LEU:HD12	1.87	0.74
1:A:380:ILE:HD12	1:A:380:ILE:O	1.88	0.74
1:C:8:ARG:HH12	1:C:103:PRO:HA	1.50	0.74
1:B:-1:ARG:HH11	1:B:-1:ARG:CG	1.95	0.74
1:A:136:ILE:CD1	1:A:204:TYR:C	2.61	0.73
1:C:284:HIS:O	1:C:286:GLU:N	2.21	0.73
1:A:47:CYS:SG	1:A:248:LYS:HG3	2.29	0.73
1:C:7:VAL:O	1:C:10:LEU:HG	1.87	0.73
1:C:205:ASP:OD1	1:C:207:VAL:HG22	1.88	0.73
1:A:384:SER:OG	1:A:386:ASP:N	2.21	0.73
1:C:77:PHE:O	1:C:80:ALA:HB3	1.88	0.73
1:A:355:ARG:HB3	1:A:355:ARG:NH1	2.00	0.73
1:B:317:ILE:N	1:B:317:ILE:HD13	2.04	0.73
1:B:148:GLU:CG	1:B:155:THR:HA	2.19	0.72
1:C:41:HIS:CE1	1:C:61:HIS:HE1	2.06	0.72
1:A:57:ALA:O	1:A:58:CYS:HB2	1.88	0.72
1:A:184:ILE:O	1:A:185:HIS:C	2.30	0.72
1:B:47:CYS:HB2	1:B:56:PHE:O	1.88	0.72
1:C:132:ASN:HB3	1:C:134:GLN:HE22	1.55	0.72
1:B:372:VAL:CG1	1:B:402:TYR:HD1	2.01	0.72
1:C:175:VAL:HG23	1:C:176:GLN:HG2	1.71	0.72
1:C:217:ARG:HA	1:C:282:TYR:CE2	2.24	0.72
1:C:265:HIS:NE2	1:C:277:HIS:HB3	2.04	0.72
1:B:142:VAL:C	1:B:144:LYS:N	2.41	0.72
1:A:171:CYS:HB3	1:A:355:ARG:NH2	2.05	0.71
1:B:234:ASN:HD21	1:B:273:ASP:HB3	1.52	0.71
1:C:81:LEU:HB3	1:C:86:SER:CB	2.21	0.71
1:A:91:PRO:HG2	1:A:210:LEU:CD2	2.21	0.71
1:B:257:ASN:ND2	1:B:262:THR:HG22	2.05	0.71
1:A:173:PHE:CE1	1:A:177:PHE:HB2	2.25	0.71
1:B:28:ASP:O	1:B:33:GLY:HA3	1.91	0.71
1:A:31:ALA:HB3	1:A:258:LEU:CD1	2.21	0.71
1:C:22:LEU:HA	1:C:25:LEU:HB3	1.72	0.71
1:A:47:CYS:O	1:A:48:PRO:C	2.31	0.70
1:B:166:GLU:HB3	1:B:167:GLN:HE21	1.56	0.70
1:B:236:VAL:CG1	1:B:237:ASN:N	2.52	0.70
1:B:265:HIS:CE1	1:B:277:HIS:HD2	2.08	0.70
1:B:371:ASP:N	1:B:371:ASP:OD1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ILE:HG22	1:C:402:TYR:H	1.55	0.70
1:A:224:GLU:O	1:A:227:LYS:HB3	1.90	0.70
1:B:184:ILE:CD1	1:B:184:ILE:N	2.54	0.70
1:C:68:GLU:HG2	1:C:268:PRO:HB3	1.73	0.70
1:A:7:VAL:HA	1:A:10:LEU:CD1	2.22	0.70
1:B:142:VAL:HA	1:B:144:LYS:HG2	1.74	0.70
1:C:58:CYS:O	1:C:59:CYS:CB	2.40	0.70
1:C:300:ASN:O	1:C:303:LYS:HG3	1.92	0.70
1:B:148:GLU:HG2	1:B:155:THR:CA	2.22	0.70
1:C:7:VAL:CG1	1:C:210:LEU:HD23	2.20	0.70
1:C:129:ILE:HG13	1:C:136:ILE:CD1	2.21	0.70
1:B:71:ARG:HH22	1:B:223:GLN:HE22	1.39	0.69
1:B:234:ASN:HD21	1:B:273:ASP:HB2	1.56	0.69
1:A:136:ILE:HD13	1:A:205:ASP:CA	2.23	0.69
1:A:136:ILE:HD11	1:A:204:TYR:HB2	1.74	0.69
1:B:198:HIS:HD2	1:B:200:HIS:H	1.38	0.69
1:C:74:THR:OG1	1:C:75:VAL:N	2.20	0.69
1:B:263:LYS:O	1:B:265:HIS:N	2.26	0.69
1:B:196:MET:HA	1:B:202:ALA:HB2	1.75	0.69
1:B:249:PRO:O	1:B:251:SER:N	2.26	0.69
1:C:200:HIS:CE1	1:C:346:SER:H	2.11	0.69
1:B:238:CYS:SG	1:B:239:ALA:N	2.66	0.68
1:C:322:HIS:HB2	1:C:341:ASP:HB3	1.75	0.68
1:C:4:ARG:CD	1:C:282:TYR:HE1	2.07	0.68
1:C:259:ASN:ND2	1:C:262:THR:N	2.41	0.68
1:A:95:THR:HG21	1:A:184:ILE:HG12	1.75	0.68
1:A:220:ALA:HA	1:A:223:GLN:NE2	2.08	0.68
1:A:319:THR:HA	1:A:344:GLY:O	1.93	0.68
1:A:-3:GLY:O	1:A:-1:ARG:N	2.27	0.68
1:A:161:TYR:O	1:A:165:LEU:HG	1.93	0.68
1:A:372:VAL:HG11	1:A:402:TYR:CE1	2.25	0.68
1:B:150:PRO:O	1:B:151:LYS:HD2	1.93	0.68
1:A:169:ASP:O	1:A:171:CYS:N	2.27	0.68
1:B:136:ILE:O	1:B:136:ILE:HD12	1.94	0.68
1:C:11:SER:H	1:C:14:GLU:HB2	1.59	0.68
1:A:323:LEU:HA	1:A:381:THR:O	1.94	0.68
1:B:3:VAL:O	1:B:3:VAL:HG13	1.94	0.68
1:B:234:ASN:ND2	1:B:273:ASP:HB2	2.09	0.68
1:B:401:ILE:CG2	1:B:402:TYR:N	2.54	0.67
1:A:36:SER:C	1:A:38:ALA:H	2.02	0.67
1:A:60:VAL:C	1:A:61:HIS:HD2	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HG2	1:A:210:LEU:HD22	1.77	0.67
1:B:47:CYS:O	1:B:48:PRO:C	2.36	0.67
1:C:150:PRO:CD	1:C:154:ASP:HB3	2.23	0.67
1:A:266:SER:O	1:A:268:PRO:HD3	1.94	0.67
1:B:182:ASN:HD22	1:B:342:VAL:HA	1.59	0.67
1:C:122:ASN:HD22	1:C:122:ASN:C	1.99	0.67
1:C:8:ARG:HG2	1:C:8:ARG:HH11	1.58	0.67
1:A:205:ASP:C	1:A:205:ASP:OD1	2.37	0.67
1:B:145:LEU:HD12	1:B:145:LEU:C	2.18	0.67
1:C:66:PHE:HB3	1:C:67:PRO:HD3	1.77	0.67
1:C:132:ASN:O	1:C:134:GLN:NE2	2.27	0.67
1:C:210:LEU:H	1:C:210:LEU:CD1	2.08	0.67
1:A:286:GLU:HG2	1:A:290:MET:O	1.94	0.67
1:A:299:ILE:O	1:A:302:GLN:N	2.28	0.67
1:B:112:ASP:O	1:B:113:ASP:C	2.37	0.67
1:C:249:PRO:O	1:C:250:PHE:C	2.35	0.67
1:A:108:ASP:HB2	1:A:110:ILE:CD1	2.23	0.67
1:C:71:ARG:HD3	1:C:216:ASP:OD1	1.94	0.67
1:B:97:VAL:HG13	1:B:98:PRO:HD2	1.77	0.67
1:B:307:ARG:O	1:B:308:VAL:HG23	1.95	0.67
1:C:330:ILE:H	1:C:330:ILE:CD1	2.07	0.67
1:B:15:ARG:O	1:B:19:VAL:HG23	1.96	0.66
1:C:186:ALA:O	1:C:188:VAL:N	2.27	0.66
1:A:119:ASN:OD1	1:A:119:ASN:O	2.14	0.66
1:A:214:ASN:O	1:A:217:ARG:HB3	1.95	0.66
1:B:226:GLN:HE21	1:B:229:ARG:HH12	1.41	0.66
1:C:131:PHE:CG	1:C:132:ASN:N	2.63	0.66
1:A:136:ILE:HD13	1:A:205:ASP:HA	1.75	0.66
1:A:169:ASP:O	1:A:172:ASP:N	2.19	0.66
1:B:231:HIS:O	1:B:233:PRO:HD3	1.96	0.66
1:C:60:VAL:HG11	1:C:65:THR:C	2.20	0.66
1:A:36:SER:O	1:A:38:ALA:N	2.27	0.66
1:B:320:SER:HA	1:B:344:GLY:H	1.61	0.66
1:A:66:PHE:CB	1:A:67:PRO:HD3	2.24	0.66
1:A:330:ILE:H	1:A:330:ILE:CD1	2.03	0.66
1:B:141:ASN:HD21	1:B:187:TRP:HA	1.60	0.66
1:A:110:ILE:HD12	1:A:110:ILE:N	2.11	0.66
1:C:8:ARG:HH12	1:C:103:PRO:CA	2.08	0.66
1:A:98:PRO:HB3	1:A:147:LYS:CA	2.26	0.66
1:A:286:GLU:CD	1:A:289:GLY:C	2.63	0.66
1:B:111:TRP:C	1:B:111:TRP:CD1	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASN:ND2	1:B:273:ASP:CB	2.57	0.66
1:C:28:ASP:O	1:C:33:GLY:HA3	1.96	0.66
1:C:249:PRO:O	1:C:251:SER:N	2.29	0.66
1:A:325:PHE:CD2	1:A:337:ALA:HB3	2.30	0.66
1:A:66:PHE:HB3	1:A:67:PRO:CD	2.23	0.65
1:A:372:VAL:HG21	1:A:402:TYR:CE1	2.31	0.65
1:B:112:ASP:O	1:B:114:ALA:N	2.29	0.65
1:B:240:LEU:HD12	1:B:240:LEU:H	1.61	0.65
1:B:257:ASN:OD1	1:B:259:ASN:HB3	1.96	0.65
1:C:92:TYR:HB2	1:C:214:ASN:HB2	1.79	0.65
1:B:161:TYR:CE2	1:B:218:LEU:CD1	2.79	0.65
1:A:232:ASP:OD2	1:A:234:ASN:N	2.27	0.65
1:C:136:ILE:HD12	1:C:136:ILE:N	2.08	0.65
1:C:260:PRO:CG	1:C:261:THR:N	2.60	0.65
1:C:22:LEU:HG	1:C:25:LEU:HD23	1.78	0.65
1:C:161:TYR:CD2	1:C:218:LEU:CD2	2.80	0.65
1:A:169:ASP:O	1:A:170:TYR:C	2.40	0.65
1:A:192:GLU:HB2	1:A:195:SER:OG	1.97	0.65
1:C:59:CYS:SG	1:C:61:HIS:HE1	2.11	0.64
1:A:145:LEU:O	1:A:145:LEU:HD12	1.98	0.64
1:B:104:ALA:O	1:B:107:ASN:N	2.30	0.64
1:B:328:CYS:CA	1:B:334:CYS:HA	2.25	0.64
1:A:82:ARG:C	1:A:84:HIS:H	2.05	0.64
1:B:141:ASN:HD22	1:B:142:VAL:HG23	1.62	0.64
1:B:225:LEU:O	1:B:229:ARG:HB2	1.98	0.64
1:C:330:ILE:H	1:C:330:ILE:HD12	1.62	0.64
1:A:162:ILE:HD12	1:A:165:LEU:HD12	1.79	0.64
1:A:376:PHE:CD1	1:A:376:PHE:C	2.76	0.64
1:C:131:PHE:HE2	1:C:204:TYR:OH	1.80	0.64
1:A:236:VAL:HG12	1:A:238:CYS:H	1.62	0.64
1:B:90:ILE:HG21	1:B:209:ILE:HG22	1.80	0.64
1:A:222:TRP:O	1:A:223:GLN:C	2.41	0.64
1:A:281:GLU:HG2	1:A:282:TYR:N	2.10	0.64
1:C:129:ILE:CD1	1:C:136:ILE:HD12	2.28	0.64
1:A:192:GLU:C	1:A:194:TYR:N	2.54	0.64
1:B:-1:ARG:O	1:B:1:ASN:N	2.31	0.64
1:B:180:ALA:C	1:B:182:ASN:H	2.06	0.64
1:A:86:SER:OG	1:A:87:VAL:N	2.30	0.63
1:B:201:TYR:O	1:B:202:ALA:C	2.38	0.63
1:C:145:LEU:H	1:C:145:LEU:CD2	2.11	0.63
1:C:198:HIS:CE1	1:C:200:HIS:CB	2.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASP:OD1	1:A:207:VAL:HG22	1.98	0.63
1:B:155:THR:O	1:B:158:PHE:N	2.31	0.63
1:B:-2:HIS:NE2	1:B:-1:ARG:HG2	2.13	0.63
1:C:11:SER:HB3	1:C:14:GLU:H	1.63	0.63
1:B:-2:HIS:CE1	1:B:-1:ARG:HH11	2.13	0.63
1:B:372:VAL:HG11	1:B:402:TYR:CE1	2.30	0.63
1:A:156:TRP:O	1:A:157:SER:C	2.41	0.63
1:A:158:PHE:O	1:A:162:ILE:HG22	1.98	0.63
1:A:242:MET:C	1:A:244:ARG:H	2.07	0.63
1:A:292:VAL:HA	1:A:295:LEU:HD12	1.80	0.63
1:C:41:HIS:CE1	1:C:61:HIS:CE1	2.86	0.63
1:C:143:ASP:HA	1:C:145:LEU:HD22	1.81	0.63
1:C:376:PHE:O	1:C:376:PHE:CD1	2.51	0.63
1:C:199:LEU:CD2	1:C:348:GLU:HB3	2.29	0.63
1:A:316:GLY:HA3	1:A:351:TRP:CZ2	2.33	0.63
1:C:4:ARG:CD	1:C:282:TYR:CE1	2.81	0.63
1:C:4:ARG:HB2	1:C:282:TYR:CD1	2.32	0.63
1:C:93:TRP:HE1	1:C:99:GLN:NE2	1.97	0.63
1:C:113:ASP:CG	1:C:118:ALA:HB3	2.24	0.63
1:C:327:ILE:HD11	1:C:361:ILE:CD1	2.29	0.63
1:A:82:ARG:C	1:A:84:HIS:N	2.54	0.62
1:A:181:HIS:CE1	1:A:185:HIS:CD2	2.86	0.62
1:A:109:GLU:N	1:A:109:GLU:OE2	2.32	0.62
1:B:196:MET:HA	1:B:202:ALA:CB	2.28	0.62
1:B:401:ILE:HG22	1:B:402:TYR:H	1.65	0.62
1:A:163:TYR:O	1:A:166:GLU:N	2.33	0.62
1:B:222:TRP:O	1:B:223:GLN:C	2.41	0.62
1:B:257:ASN:ND2	1:B:262:THR:CG2	2.62	0.62
1:C:388:GLU:O	1:C:389:ASP:C	2.41	0.62
1:B:166:GLU:CD	1:B:307:ARG:HH22	2.07	0.62
1:A:291:ASN:O	1:A:295:LEU:CD1	2.47	0.62
1:A:291:ASN:CG	1:A:292:VAL:H	2.08	0.62
1:B:184:ILE:HB	1:B:211:HIS:CE1	2.34	0.62
1:B:189:GLY:O	1:B:190:GLY:C	2.42	0.62
1:B:283:ASP:OD2	1:B:284:HIS:N	2.32	0.62
1:A:121:THR:O	1:A:123:PRO:HD3	2.00	0.62
1:B:37:LEU:O	1:B:73:TYR:OH	2.10	0.62
1:C:299:ILE:O	1:C:302:GLN:HB2	1.99	0.62
1:B:54:LYS:HD3	1:B:56:PHE:CZ	2.34	0.62
1:C:86:SER:O	1:C:87:VAL:C	2.42	0.62
1:A:228:PHE:HE2	1:A:296:HIS:HD2	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:HG2	1:B:155:THR:HA	1.82	0.61
1:C:221:LEU:HD21	1:C:295:LEU:CD1	2.30	0.61
1:A:25:LEU:HG	1:A:34:PHE:HB2	1.82	0.61
1:A:322:HIS:O	1:A:382:GLN:HA	2.00	0.61
1:A:324:ASP:N	1:A:324:ASP:OD1	2.33	0.61
1:A:192:GLU:C	1:A:194:TYR:H	2.07	0.61
1:B:94:ASP:OD2	1:B:95:THR:N	2.33	0.61
1:A:351:TRP:CG	1:A:351:TRP:O	2.52	0.61
1:B:265:HIS:CE1	1:B:277:HIS:CD2	2.88	0.61
1:C:-2:HIS:HB3	1:C:1:ASN:HB2	1.82	0.61
1:A:211:HIS:C	1:A:213:SER:H	2.09	0.61
1:B:47:CYS:HB3	1:B:48:PRO:HD3	1.81	0.61
1:B:184:ILE:N	1:B:184:ILE:HD12	2.14	0.61
1:A:61:HIS:O	1:A:63:MET:HG3	2.01	0.61
1:A:136:ILE:HD11	1:A:204:TYR:HB3	1.82	0.61
1:B:346:SER:OG	1:B:347:LEU:HD13	2.00	0.61
1:C:121:THR:O	1:C:123:PRO:CD	2.46	0.61
1:A:32:ASP:O	1:A:37:LEU:HD11	2.01	0.60
1:A:181:HIS:CD2	1:A:212:HIS:NE2	2.69	0.60
1:A:205:ASP:OD1	1:A:206:PRO:N	2.34	0.60
1:B:259:ASN:OD1	1:B:262:THR:HB	2.02	0.60
1:C:5:LYS:HG2	1:C:6:SER:N	2.15	0.60
1:C:8:ARG:CZ	1:C:103:PRO:HG3	2.31	0.60
1:B:299:ILE:O	1:B:300:ASN:C	2.43	0.60
1:B:324:ASP:HB3	1:B:339:TYR:HB3	1.82	0.60
1:C:129:ILE:H	1:C:129:ILE:HD12	1.64	0.60
1:C:198:HIS:CE1	1:C:200:HIS:H	2.20	0.60
1:A:50:PRO:HD3	1:A:252:PHE:CE2	2.36	0.60
1:A:221:LEU:O	1:A:224:GLU:N	2.35	0.60
1:B:208:PHE:O	1:B:209:ILE:C	2.43	0.60
1:C:5:LYS:HA	1:C:283:ASP:OD1	2.00	0.60
1:A:104:ALA:O	1:A:106:PHE:N	2.33	0.60
1:A:371:ASP:OD1	1:A:373:HIS:N	2.35	0.60
1:A:32:ASP:OD1	1:A:37:LEU:HD21	2.02	0.60
1:A:179:ILE:HG21	1:A:357:TYR:CZ	2.36	0.60
1:B:342:VAL:CG1	1:B:343:LEU:H	2.06	0.60
1:C:259:ASN:HD21	1:C:262:THR:H	1.50	0.60
1:A:11:SER:OG	1:A:13:ALA:HB3	2.02	0.60
1:A:43:GLN:HG2	1:A:131:PHE:CZ	2.36	0.60
1:A:182:ASN:ND2	1:A:342:VAL:HA	2.09	0.60
1:A:199:LEU:HB3	1:A:345:GLY:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:O	1:C:36:SER:N	2.34	0.60
1:C:248:LYS:HB3	1:C:252:PHE:CE1	2.37	0.60
1:B:165:LEU:HD23	1:B:222:TRP:CD1	2.33	0.60
1:B:211:HIS:C	1:B:213:SER:H	2.08	0.60
1:B:291:ASN:O	1:B:295:LEU:HG	2.02	0.60
1:A:156:TRP:O	1:A:158:PHE:N	2.35	0.59
1:A:156:TRP:NE1	1:A:339:TYR:CE2	2.70	0.59
1:A:286:GLU:OE1	1:A:289:GLY:C	2.45	0.59
1:B:148:GLU:HG3	1:B:155:THR:HA	1.84	0.59
1:C:-2:HIS:CG	1:C:-1:ARG:HE	2.12	0.59
1:C:163:TYR:HD2	1:C:176:GLN:NE2	2.00	0.59
1:B:257:ASN:HD21	1:B:262:THR:CG2	2.15	0.59
1:A:7:VAL:HA	1:A:10:LEU:HD11	1.84	0.59
1:C:-1:ARG:CB	1:C:1:ASN:N	2.62	0.59
1:B:44:PRO:HD3	1:B:131:PHE:CE2	2.37	0.59
1:B:104:ALA:O	1:B:105:PHE:C	2.46	0.59
1:A:25:LEU:HA	1:A:84:HIS:CE1	2.38	0.59
1:B:145:LEU:CD1	1:B:146:ALA:N	2.62	0.59
1:B:219:PHE:O	1:B:223:GLN:HG3	2.03	0.59
1:C:149:GLY:C	1:C:151:LYS:N	2.57	0.59
1:A:1:ASN:CB	1:A:279:HIS:HB3	2.32	0.59
1:A:238:CYS:O	1:A:239:ALA:C	2.41	0.59
1:B:-2:HIS:NE2	1:B:-1:ARG:CG	2.66	0.59
1:C:347:LEU:HD22	1:C:347:LEU:H	1.66	0.59
1:A:400:VAL:HG12	1:A:400:VAL:O	2.02	0.59
1:B:132:ASN:ND2	1:B:132:ASN:O	2.35	0.59
1:B:365:LEU:HD12	1:B:370:LEU:HB3	1.84	0.59
1:B:262:THR:CG2	1:B:263:LYS:N	2.66	0.59
1:A:291:ASN:O	1:A:295:LEU:CG	2.50	0.59
1:B:361:ILE:HG13	1:B:365:LEU:HD23	1.85	0.59
1:A:34:PHE:O	1:A:35:GLN:C	2.46	0.59
1:C:122:ASN:O	1:C:125:ASN:N	2.36	0.59
1:A:60:VAL:C	1:A:61:HIS:CD2	2.81	0.58
1:A:286:GLU:OE1	1:A:289:GLY:O	2.20	0.58
1:B:361:ILE:O	1:B:362:THR:C	2.43	0.58
1:B:402:TYR:C	1:B:402:TYR:CD2	2.81	0.58
1:C:160:GLN:HA	1:C:160:GLN:OE1	2.03	0.58
1:C:217:ARG:NH1	1:C:286:GLU:O	2.36	0.58
1:A:129:ILE:HD11	1:A:136:ILE:HG13	1.85	0.58
1:A:136:ILE:HG23	1:A:137:ALA:H	1.67	0.58
1:A:136:ILE:HG22	1:A:137:ALA:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:O	1:A:194:TYR:N	2.36	0.58
1:B:198:HIS:NE2	1:B:200:HIS:CD2	2.71	0.58
1:C:259:ASN:HD21	1:C:262:THR:N	1.99	0.58
1:A:140:ILE:HG22	1:A:142:VAL:C	2.28	0.58
1:A:325:PHE:HB3	1:A:380:ILE:HG22	1.83	0.58
1:C:401:ILE:CG2	1:C:402:TYR:N	2.66	0.58
1:A:60:VAL:O	1:A:61:HIS:HD2	1.85	0.58
1:A:162:ILE:HA	1:A:165:LEU:HD12	1.84	0.58
1:B:249:PRO:C	1:B:251:SER:N	2.61	0.58
1:C:247:LEU:O	1:C:250:PHE:HB2	2.04	0.58
1:C:263:LYS:O	1:C:266:SER:OG	2.21	0.58
1:C:376:PHE:CD1	1:C:376:PHE:C	2.81	0.58
1:A:380:ILE:HD13	1:A:392:THR:HG21	1.86	0.58
1:B:97:VAL:HG12	1:B:97:VAL:O	2.02	0.58
1:B:259:ASN:OD1	1:B:259:ASN:C	2.47	0.58
1:C:210:LEU:HD12	1:C:210:LEU:N	2.14	0.58
1:B:238:CYS:O	1:B:239:ALA:HB3	2.03	0.58
1:C:136:ILE:HD11	1:C:204:TYR:HB3	1.86	0.58
1:B:263:LYS:O	1:B:264:GLU:C	2.44	0.57
1:C:386:ASP:O	1:C:387:ASN:C	2.47	0.57
1:A:159:LYS:O	1:A:162:ILE:HG22	2.04	0.57
1:B:-1:ARG:HA	1:B:1:ASN:N	2.18	0.57
1:A:62:GLY:HA2	1:A:353:PHE:CE2	2.38	0.57
1:B:180:ALA:C	1:B:182:ASN:N	2.62	0.57
1:C:306:ASP:C	1:C:307:ARG:HG3	2.27	0.57
1:A:207:VAL:O	1:A:208:PHE:C	2.46	0.57
1:C:382:GLN:HB3	1:C:390:ILE:HB	1.87	0.57
1:A:33:GLY:O	1:A:34:PHE:C	2.46	0.57
1:A:72:LEU:HD22	1:A:250:PHE:CD1	2.40	0.57
1:A:184:ILE:HD13	1:A:211:HIS:CE1	2.39	0.57
1:C:44:PRO:O	1:C:44:PRO:HG2	2.04	0.57
1:B:113:ASP:O	1:B:114:ALA:C	2.47	0.57
1:B:142:VAL:HG12	1:B:145:LEU:N	2.19	0.57
1:A:249:PRO:O	1:A:250:PHE:C	2.43	0.57
1:A:368:LYS:O	1:A:370:LEU:HG	2.04	0.57
1:B:70:HIS:HD2	1:B:212:HIS:CD2	2.23	0.57
1:C:401:ILE:CG2	1:C:402:TYR:H	2.17	0.57
1:A:224:GLU:O	1:A:227:LYS:CB	2.52	0.57
1:A:363:ASP:O	1:A:364:VAL:C	2.47	0.57
1:B:208:PHE:CE1	1:B:212:HIS:CE1	2.93	0.57
1:C:4:ARG:NH1	1:C:282:TYR:OH	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASN:HB2	1:A:279:HIS:C	2.30	0.57
1:B:127:ALA:H	1:B:136:ILE:HD11	1.69	0.57
1:B:206:PRO:O	1:B:207:VAL:C	2.42	0.57
1:C:174:GLU:O	1:C:175:VAL:C	2.46	0.57
1:A:238:CYS:O	1:A:240:LEU:HD12	2.05	0.57
1:A:267:LYS:O	1:A:268:PRO:C	2.47	0.57
1:A:140:ILE:HG23	1:A:187:TRP:O	2.04	0.56
1:B:299:ILE:O	1:B:302:GLN:N	2.28	0.56
1:B:323:LEU:HB3	1:B:382:GLN:HG3	1.87	0.56
1:C:291:ASN:O	1:C:294:ARG:N	2.38	0.56
1:A:299:ILE:O	1:A:300:ASN:C	2.45	0.56
1:A:365:LEU:O	1:A:368:LYS:HB3	2.04	0.56
1:B:35:GLN:HE22	1:B:129:ILE:HA	1.68	0.56
1:C:143:ASP:HA	1:C:145:LEU:CD2	2.36	0.56
1:A:104:ALA:O	1:A:105:PHE:C	2.48	0.56
1:A:200:HIS:NE2	1:A:347:LEU:HB2	2.21	0.56
1:B:140:ILE:O	1:B:143:ASP:N	2.39	0.56
1:B:251:SER:O	1:B:252:PHE:C	2.49	0.56
1:B:302:GLN:O	1:B:304:GLU:N	2.33	0.56
1:B:311:GLY:O	1:B:398:PRO:HA	2.06	0.56
1:C:5:LYS:HG2	1:C:6:SER:H	1.69	0.56
1:C:46:LEU:HB2	1:C:50:PRO:HA	1.87	0.56
1:C:198:HIS:ND1	1:C:200:HIS:N	2.53	0.56
1:C:259:ASN:ND2	1:C:260:PRO:C	2.63	0.56
1:A:59:CYS:HG	1:A:61:HIS:CE1	2.24	0.56
1:A:213:SER:O	1:A:217:ARG:HB2	2.05	0.56
1:B:141:ASN:CG	1:B:142:VAL:H	2.14	0.56
1:B:221:LEU:HD11	1:B:295:LEU:HD12	1.88	0.56
1:C:372:VAL:HG21	1:C:402:TYR:CE1	2.40	0.56
1:A:199:LEU:CB	1:A:345:GLY:H	2.18	0.56
1:A:290:MET:CB	1:A:294:ARG:CB	2.78	0.56
1:A:361:ILE:O	1:A:361:ILE:HG13	2.06	0.56
1:B:-1:ARG:C	1:B:1:ASN:N	2.64	0.56
1:C:15:ARG:O	1:C:16:ALA:C	2.46	0.56
1:C:114:ALA:HB2	1:C:119:ASN:OD1	2.06	0.56
1:C:259:ASN:ND2	1:C:260:PRO:N	2.54	0.56
1:A:39:SER:O	1:A:40:PHE:C	2.47	0.56
1:A:161:TYR:CZ	1:A:180:ALA:HB1	2.41	0.56
1:A:165:LEU:O	1:A:229:ARG:NH2	2.37	0.56
1:A:192:GLU:O	1:A:195:SER:OG	2.24	0.56
1:B:68:GLU:O	1:B:69:TRP:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:C	1:B:151:LYS:H	2.11	0.56
1:C:96:VAL:HG12	1:C:96:VAL:O	2.06	0.56
1:C:268:PRO:O	1:C:269:GLU:C	2.49	0.56
1:C:327:ILE:HD11	1:C:361:ILE:HD12	1.88	0.56
1:B:201:TYR:O	1:B:204:TYR:N	2.27	0.56
1:C:70:HIS:HD2	1:C:212:HIS:CD2	2.24	0.56
1:C:223:GLN:O	1:C:226:GLN:HB2	2.06	0.56
1:A:8:ARG:NH2	1:A:101:ASP:O	2.37	0.56
1:A:78:GLU:N	1:A:90:ILE:HD11	2.21	0.56
1:A:244:ARG:NH1	1:A:244:ARG:CG	2.58	0.56
1:C:77:PHE:C	1:C:80:ALA:HB3	2.31	0.56
1:C:198:HIS:ND1	1:C:198:HIS:C	2.64	0.56
1:A:144:LYS:C	1:A:146:ALA:H	2.13	0.56
1:A:170:TYR:O	1:A:171:CYS:C	2.44	0.56
1:A:228:PHE:CE1	1:A:293:GLN:HG3	2.41	0.56
1:C:291:ASN:HB3	1:C:294:ARG:HB2	1.86	0.56
1:C:380:ILE:CD1	1:C:392:THR:HB	2.34	0.56
1:B:320:SER:OG	1:B:344:GLY:N	2.38	0.55
1:C:34:PHE:O	1:C:37:LEU:N	2.38	0.55
1:C:145:LEU:HD23	1:C:145:LEU:N	2.15	0.55
1:A:292:VAL:CA	1:A:295:LEU:HD12	2.36	0.55
1:B:36:SER:C	1:B:38:ALA:N	2.63	0.55
1:B:234:ASN:OD1	1:B:273:ASP:HB2	2.05	0.55
1:B:211:HIS:C	1:B:213:SER:N	2.65	0.55
1:C:249:PRO:C	1:C:251:SER:N	2.63	0.55
1:C:267:LYS:H	1:C:267:LYS:HD2	1.72	0.55
1:A:93:TRP:HE1	1:A:99:GLN:NE2	2.05	0.55
1:B:63:MET:O	1:B:64:ALA:C	2.49	0.55
1:B:198:HIS:HD2	1:B:200:HIS:N	2.05	0.55
1:A:8:ARG:HH21	1:A:103:PRO:HD3	1.71	0.55
1:A:71:ARG:HH22	1:A:223:GLN:HE22	1.55	0.55
1:A:93:TRP:CD1	1:A:93:TRP:C	2.83	0.55
1:B:322:HIS:HA	1:B:341:ASP:HB3	1.88	0.55
1:C:153:TYR:O	1:C:155:THR:HG23	2.06	0.55
1:C:161:TYR:CE2	1:C:218:LEU:HD22	2.42	0.55
1:A:153:TYR:HB2	1:A:288:GLN:CD	2.32	0.55
1:A:228:PHE:CE2	1:A:296:HIS:HD2	2.23	0.55
1:B:250:PHE:O	1:B:263:LYS:HA	2.07	0.55
1:A:69:TRP:HE3	1:A:70:HIS:N	2.05	0.55
1:A:319:THR:HG1	1:A:385:TRP:NE1	2.05	0.55
1:B:36:SER:C	1:B:38:ALA:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASN:ND2	1:B:142:VAL:N	2.53	0.55
1:B:156:TRP:CZ3	1:B:183:ALA:HB2	2.42	0.55
1:B:32:ASP:OD2	1:B:37:LEU:HD21	2.06	0.54
1:C:78:GLU:O	1:C:81:LEU:N	2.32	0.54
1:A:386:ASP:C	1:A:387:ASN:CG	2.75	0.54
1:B:90:ILE:HG21	1:B:209:ILE:CG2	2.37	0.54
1:C:161:TYR:O	1:C:162:ILE:C	2.48	0.54
1:C:205:ASP:OD1	1:C:207:VAL:N	2.37	0.54
1:C:268:PRO:C	1:C:270:ASP:N	2.65	0.54
1:C:290:MET:SD	1:C:294:ARG:HD2	2.48	0.54
1:C:217:ARG:HG2	1:C:282:TYR:CD2	2.42	0.54
1:A:4:ARG:N	1:A:281:GLU:O	2.38	0.54
1:B:35:GLN:NE2	1:B:130:ASP:H	2.06	0.54
1:C:47:CYS:C	1:C:49:ALA:N	2.60	0.54
1:A:341:ASP:OD2	1:A:341:ASP:N	2.39	0.54
1:C:136:ILE:H	1:C:136:ILE:CD1	2.12	0.54
1:C:347:LEU:N	1:C:347:LEU:CD2	2.70	0.54
1:C:378:ILE:HG22	1:C:379:LYS:N	2.22	0.54
1:A:7:VAL:HA	1:A:10:LEU:HD12	1.90	0.54
1:A:87:VAL:C	1:A:88:VAL:HG13	2.31	0.54
1:A:155:THR:O	1:A:158:PHE:HB3	2.08	0.54
1:B:-2:HIS:CD2	1:B:-1:ARG:HG2	2.43	0.54
1:C:4:ARG:HB2	1:C:282:TYR:HD1	1.72	0.54
1:A:-2:HIS:CE1	1:A:-1:ARG:HG2	2.43	0.54
1:C:85:GLY:O	1:C:87:VAL:N	2.39	0.54
1:A:319:THR:O	1:A:320:SER:C	2.49	0.54
1:B:95:THR:C	1:B:97:VAL:N	2.65	0.54
1:B:164:ALA:O	1:B:173:PHE:HD1	1.91	0.54
1:A:22:LEU:HD23	1:A:26:GLN:HG3	1.90	0.54
1:B:28:ASP:OD1	1:B:28:ASP:C	2.45	0.54
1:B:202:ALA:C	1:B:204:TYR:H	2.16	0.54
1:C:68:GLU:H	1:C:68:GLU:CD	2.15	0.54
1:C:81:LEU:HD12	1:C:90:ILE:CG1	2.37	0.54
1:C:130:ASP:O	1:C:131:PHE:C	2.48	0.54
1:C:322:HIS:ND1	1:C:322:HIS:C	2.65	0.54
1:A:319:THR:HG1	1:A:385:TRP:CD1	2.26	0.54
1:B:234:ASN:CG	1:B:273:ASP:HB2	2.33	0.54
1:B:-1:ARG:NH1	1:B:-1:ARG:CG	2.60	0.53
1:B:155:THR:O	1:B:156:TRP:C	2.51	0.53
1:C:42:ALA:HA	1:C:57:ALA:HB1	1.88	0.53
1:B:345:GLY:O	1:B:346:SER:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-2:HIS:C	1:C:-1:ARG:HG2	2.33	0.53
1:C:175:VAL:CG2	1:C:176:GLN:N	2.71	0.53
1:C:238:CYS:O	1:C:239:ALA:CB	2.47	0.53
1:C:293:GLN:O	1:C:297:ASP:HB2	2.07	0.53
1:A:78:GLU:HB2	1:A:90:ILE:CD1	2.38	0.53
1:A:136:ILE:HD13	1:A:205:ASP:N	2.23	0.53
1:A:351:TRP:O	1:A:351:TRP:CD2	2.60	0.53
1:B:-2:HIS:CD2	1:B:-1:ARG:CG	2.91	0.53
1:A:236:VAL:CG2	1:A:272:PHE:CZ	2.91	0.53
1:C:267:LYS:HD2	1:C:267:LYS:N	2.22	0.53
1:A:163:TYR:O	1:A:164:ALA:C	2.50	0.53
1:B:2:LEU:O	1:B:281:GLU:N	2.39	0.53
1:B:164:ALA:HB1	1:B:173:PHE:CD1	2.43	0.53
1:C:95:THR:HA	1:C:99:GLN:OE1	2.09	0.53
1:C:122:ASN:O	1:C:123:PRO:C	2.52	0.53
1:C:198:HIS:HE1	1:C:200:HIS:CG	2.26	0.53
1:C:233:PRO:HG2	1:C:234:ASN:N	2.21	0.53
1:A:28:ASP:OD1	1:A:28:ASP:C	2.52	0.53
1:A:82:ARG:O	1:A:84:HIS:N	2.42	0.53
1:B:262:THR:HG22	1:B:263:LYS:H	1.73	0.53
1:C:129:ILE:HD11	1:C:136:ILE:N	2.24	0.53
1:A:330:ILE:HD12	1:A:330:ILE:N	2.18	0.53
1:A:383:THR:HG22	1:A:389:ASP:HA	1.91	0.53
1:B:97:VAL:O	1:B:98:PRO:C	2.49	0.53
1:C:25:LEU:HG	1:C:34:PHE:HB2	1.90	0.53
1:C:96:VAL:C	1:C:97:VAL:HG22	2.34	0.53
1:A:9:ASN:ND2	2:A:600:NAG:H5	2.24	0.53
1:A:81:LEU:O	1:A:82:ARG:C	2.50	0.53
1:A:293:GLN:C	1:A:295:LEU:N	2.64	0.53
1:B:13:ALA:O	1:B:16:ALA:HB3	2.09	0.53
1:B:33:GLY:O	1:B:37:LEU:HG	2.09	0.53
1:B:221:LEU:HD12	1:B:221:LEU:O	2.09	0.53
1:C:4:ARG:NH2	1:C:75:VAL:HG22	2.24	0.53
1:A:174:GLU:C	1:A:176:GLN:H	2.17	0.52
1:A:322:HIS:HD2	1:A:341:ASP:OD1	1.92	0.52
1:B:66:PHE:CE1	1:B:178:GLU:HG3	2.44	0.52
1:C:-2:HIS:O	1:C:-1:ARG:CD	2.57	0.52
1:C:260:PRO:CG	1:C:261:THR:H	2.20	0.52
1:A:286:GLU:OE2	1:A:290:MET:N	2.42	0.52
1:A:325:PHE:CD2	1:A:337:ALA:CB	2.91	0.52
1:C:309:PHE:N	1:C:309:PHE:CD1	2.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:HG2	1:A:131:PHE:HZ	1.73	0.52
1:A:57:ALA:O	1:A:58:CYS:CB	2.46	0.52
1:A:291:ASN:CG	1:A:292:VAL:N	2.67	0.52
1:A:338:GLY:HA3	1:A:359:TYR:CE2	2.43	0.52
1:B:2:LEU:O	1:B:280:TYR:HA	2.08	0.52
1:B:149:GLY:C	1:B:151:LYS:N	2.62	0.52
1:B:164:ALA:HB1	1:B:173:PHE:HD1	1.74	0.52
1:B:238:CYS:O	1:B:239:ALA:C	2.49	0.52
1:C:138:ARG:NH2	1:C:207:VAL:HG13	2.24	0.52
1:C:71:ARG:HD2	1:C:280:TYR:OH	2.09	0.52
1:C:113:ASP:O	1:C:116:PHE:C	2.53	0.52
1:C:268:PRO:O	1:C:271:THR:N	2.43	0.52
1:C:335:THR:CG2	1:C:368:LYS:HE3	2.38	0.52
1:A:259:ASN:OD1	1:A:259:ASN:C	2.52	0.52
1:B:196:MET:HE2	1:B:207:VAL:CG1	2.32	0.52
1:C:59:CYS:O	1:C:60:VAL:C	2.52	0.52
1:A:134:GLN:HG3	1:A:194:TYR:CZ	2.45	0.52
1:A:386:ASP:O	1:A:387:ASN:OD1	2.27	0.52
1:B:202:ALA:C	1:B:204:TYR:N	2.61	0.52
1:C:94:ASP:OD1	1:C:96:VAL:HG23	2.09	0.52
1:C:129:ILE:HD11	1:C:136:ILE:HD12	1.92	0.52
1:A:22:LEU:HA	1:A:25:LEU:HB3	1.91	0.52
1:B:163:TYR:HD2	1:B:176:GLN:HG2	1.73	0.52
1:B:259:ASN:OD1	1:B:260:PRO:N	2.42	0.52
1:C:112:ASP:C	1:C:114:ALA:N	2.63	0.52
1:A:298:TYR:O	1:A:299:ILE:C	2.52	0.52
1:B:94:ASP:HA	1:B:214:ASN:CG	2.35	0.52
1:C:39:SER:OG	1:C:44:PRO:CD	2.57	0.52
1:C:178:GLU:O	1:C:181:HIS:HB3	2.09	0.52
1:A:81:LEU:O	1:A:84:HIS:N	2.35	0.52
1:B:59:CYS:SG	1:B:199:LEU:HD11	2.50	0.52
1:C:61:HIS:NE2	1:C:70:HIS:HE1	2.06	0.52
1:C:129:ILE:HD12	1:C:134:GLN:O	2.10	0.52
1:A:50:PRO:HG2	1:A:256:TYR:CE2	2.45	0.51
1:A:286:GLU:CG	1:A:290:MET:O	2.57	0.51
1:C:90:ILE:O	1:C:90:ILE:HG22	2.09	0.51
1:C:163:TYR:O	1:C:164:ALA:C	2.52	0.51
1:C:186:ALA:C	1:C:188:VAL:H	2.18	0.51
1:A:8:ARG:HH21	1:A:103:PRO:CD	2.22	0.51
1:A:9:ASN:HD22	2:A:600:NAG:C5	2.23	0.51
1:C:28:ASP:C	1:C:30:SER:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ALA:C	1:C:66:PHE:H	2.17	0.51
1:C:163:TYR:CD2	1:C:176:GLN:NE2	2.79	0.51
1:C:306:ASP:N	1:C:405:LYS:O	2.42	0.51
1:A:95:THR:HG21	1:A:184:ILE:CG1	2.40	0.51
1:A:95:THR:OG1	1:A:184:ILE:HD11	2.10	0.51
1:A:156:TRP:O	1:A:159:LYS:N	2.43	0.51
1:A:358:LYS:HG2	1:A:401:ILE:HD12	1.91	0.51
1:A:386:ASP:O	1:A:387:ASN:ND2	2.42	0.51
1:B:19:VAL:HG12	1:B:19:VAL:O	2.10	0.51
1:B:205:ASP:OD1	1:B:205:ASP:C	2.54	0.51
1:B:208:PHE:O	1:B:211:HIS:N	2.43	0.51
1:C:47:CYS:H	1:C:48:PRO:HD2	1.74	0.51
1:C:82:ARG:HA	1:C:86:SER:H	1.76	0.51
1:C:94:ASP:HA	1:C:214:ASN:ND2	2.25	0.51
1:C:113:ASP:O	1:C:116:PHE:O	2.27	0.51
1:A:184:ILE:C	1:A:186:ALA:N	2.64	0.51
1:B:127:ALA:H	1:B:136:ILE:CG1	2.23	0.51
1:C:47:CYS:O	1:C:48:PRO:C	2.53	0.51
1:C:249:PRO:HA	1:C:252:PHE:CD1	2.46	0.51
1:C:384:SER:C	1:C:386:ASP:H	2.16	0.51
1:A:4:ARG:NE	1:A:280:TYR:CD1	2.79	0.51
1:A:25:LEU:CD1	1:A:34:PHE:H	2.24	0.51
1:A:101:ASP:OD1	1:A:101:ASP:C	2.53	0.51
1:A:324:ASP:N	1:A:381:THR:O	2.39	0.51
1:C:86:SER:C	1:C:88:VAL:N	2.69	0.51
1:B:181:HIS:CD2	1:B:212:HIS:NE2	2.58	0.51
1:B:366:GLU:OE2	1:B:366:GLU:HA	2.11	0.51
1:B:-2:HIS:NE2	1:B:-1:ARG:NH1	2.59	0.51
1:C:102:LEU:CD1	1:C:140:ILE:HD13	2.40	0.51
1:C:43:GLN:HB3	1:C:131:PHE:CZ	2.46	0.51
1:C:65:THR:HG21	1:C:242:MET:HB3	1.93	0.51
1:C:239:ALA:C	1:C:241:GLU:H	2.18	0.51
1:C:259:ASN:HD21	1:C:261:THR:CA	2.24	0.51
1:C:305:ALA:C	1:C:405:LYS:O	2.53	0.51
1:A:11:SER:O	1:A:14:GLU:N	2.44	0.51
1:A:12:PRO:O	1:A:13:ALA:C	2.50	0.50
1:B:8:ARG:O	1:B:10:LEU:N	2.43	0.50
1:C:1:ASN:HD22	1:C:281:GLU:HG2	1.76	0.50
1:C:307:ARG:C	1:C:308:VAL:HG23	2.35	0.50
1:A:32:ASP:HA	1:A:37:LEU:HD21	1.93	0.50
1:B:257:ASN:ND2	1:B:259:ASN:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:HG21	1:B:402:TYR:HB2	1.93	0.50
1:B:384:SER:HB3	1:B:386:ASP:OD2	2.11	0.50
1:A:226:GLN:HA	1:A:229:ARG:HD2	1.92	0.50
1:B:240:LEU:HD12	1:B:240:LEU:N	2.26	0.50
1:C:131:PHE:CE1	1:C:132:ASN:OD1	2.64	0.50
1:C:66:PHE:CB	1:C:67:PRO:HD3	2.41	0.50
1:C:384:SER:C	1:C:386:ASP:N	2.67	0.50
1:A:-2:HIS:ND1	1:A:-1:ARG:HG2	2.26	0.50
1:A:66:PHE:CB	1:A:67:PRO:CD	2.84	0.50
1:B:71:ARG:HH22	1:B:223:GLN:NE2	2.06	0.50
1:B:141:ASN:ND2	1:B:187:TRP:HA	2.26	0.50
1:C:47:CYS:H	1:C:48:PRO:CD	2.25	0.50
1:C:102:LEU:O	1:C:103:PRO:C	2.53	0.50
1:C:161:TYR:O	1:C:164:ALA:HB3	2.11	0.50
1:C:257:ASN:OD1	1:C:259:ASN:HB3	2.12	0.50
1:B:148:GLU:CD	1:B:156:TRP:H	2.20	0.50
1:B:198:HIS:CD2	1:B:200:HIS:H	2.25	0.50
1:A:174:GLU:C	1:A:176:GLN:N	2.66	0.50
1:A:402:TYR:CD2	1:A:403:VAL:N	2.80	0.50
1:B:6:SER:C	1:B:8:ARG:H	2.18	0.50
1:A:220:ALA:O	1:A:221:LEU:C	2.55	0.50
1:A:291:ASN:C	1:A:295:LEU:HD12	2.37	0.50
1:A:339:TYR:O	1:A:339:TYR:CG	2.63	0.50
1:B:178:GLU:O	1:B:179:ILE:C	2.54	0.50
1:C:6:SER:C	1:C:8:ARG:N	2.68	0.50
1:C:187:TRP:N	1:C:187:TRP:CD1	2.77	0.50
1:C:323:LEU:C	1:C:323:LEU:HD12	2.37	0.50
1:A:156:TRP:CE3	1:A:157:SER:N	2.79	0.50
1:A:263:LYS:C	1:A:265:HIS:H	2.19	0.50
1:B:35:GLN:NE2	1:B:129:ILE:HA	2.27	0.50
1:B:78:GLU:HA	1:B:90:ILE:HD11	1.94	0.50
1:B:107:ASN:O	1:B:108:ASP:C	2.54	0.50
1:B:188:VAL:O	1:B:188:VAL:CG1	2.59	0.50
1:B:318:GLY:HA2	1:B:348:GLU:OE2	2.11	0.50
1:A:184:ILE:O	1:A:186:ALA:N	2.45	0.49
1:B:82:ARG:O	1:B:85:GLY:N	2.44	0.49
1:B:119:ASN:O	1:B:120:PHE:CD2	2.65	0.49
1:C:184:ILE:O	1:C:185:HIS:C	2.53	0.49
1:A:-3:GLY:CA	1:A:1:ASN:N	2.72	0.49
1:A:205:ASP:OD1	1:A:207:VAL:N	2.33	0.49
1:A:327:ILE:HD11	1:A:364:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLU:OE2	1:B:366:GLU:CA	2.59	0.49
1:C:65:THR:CG2	1:C:242:MET:CB	2.91	0.49
1:C:294:ARG:O	1:C:294:ARG:HD3	2.11	0.49
1:A:144:LYS:C	1:A:146:ALA:N	2.71	0.49
1:A:372:VAL:HG21	1:A:402:TYR:CD1	2.48	0.49
1:C:113:ASP:OD2	1:C:118:ALA:HB3	2.11	0.49
1:A:319:THR:OG1	1:A:385:TRP:NE1	2.40	0.49
1:B:22:LEU:HA	1:B:25:LEU:HB3	1.94	0.49
1:B:184:ILE:CD1	1:B:184:ILE:H	2.23	0.49
1:C:361:ILE:HD12	1:C:365:LEU:HD22	1.95	0.49
1:A:92:TYR:HA	1:A:213:SER:HB3	1.94	0.49
1:A:162:ILE:HG23	1:A:163:TYR:N	2.27	0.49
1:A:291:ASN:O	1:A:292:VAL:C	2.54	0.49
1:B:111:TRP:CZ2	1:B:113:ASP:HA	2.47	0.49
1:B:150:PRO:O	1:B:151:LYS:CD	2.61	0.49
1:B:185:HIS:CE1	1:B:212:HIS:HE1	2.30	0.49
1:C:68:GLU:CB	1:C:268:PRO:HB3	2.43	0.49
1:C:153:TYR:O	1:C:155:THR:N	2.44	0.49
1:C:259:ASN:ND2	1:C:259:ASN:C	2.70	0.49
1:A:228:PHE:CZ	1:A:293:GLN:HG3	2.48	0.49
1:C:-2:HIS:C	1:C:-1:ARG:CG	2.85	0.49
1:C:129:ILE:CG1	1:C:136:ILE:CD1	2.91	0.49
1:C:150:PRO:CG	1:C:154:ASP:HB3	2.43	0.49
1:B:70:HIS:CD2	1:B:212:HIS:CD2	2.99	0.49
1:B:127:ALA:H	1:B:136:ILE:CD1	2.25	0.49
1:B:268:PRO:O	1:B:269:GLU:C	2.51	0.49
1:B:290:MET:HE3	1:B:294:ARG:HH11	1.77	0.49
1:C:68:GLU:HB3	1:C:271:THR:HG21	1.94	0.49
1:C:349:THR:O	1:C:350:PRO:C	2.55	0.49
1:A:179:ILE:HG21	1:A:357:TYR:OH	2.11	0.49
1:A:182:ASN:ND2	1:A:343:LEU:H	2.11	0.49
1:C:19:VAL:O	1:C:23:LYS:HB2	2.13	0.49
1:C:161:TYR:O	1:C:164:ALA:N	2.46	0.49
1:C:384:SER:OG	1:C:385:TRP:N	2.45	0.49
1:B:87:VAL:C	1:B:88:VAL:CG1	2.86	0.49
1:C:6:SER:O	1:C:7:VAL:C	2.56	0.49
1:C:66:PHE:HZ	1:C:181:HIS:ND1	2.11	0.49
1:C:404:PRO:C	1:C:405:LYS:O	2.56	0.49
1:A:71:ARG:HH22	1:A:223:GLN:NE2	2.11	0.48
1:A:162:ILE:O	1:A:163:TYR:C	2.56	0.48
1:A:195:SER:C	1:A:197:GLY:N	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:O	1:A:246:PRO:HD3	2.12	0.48
1:B:94:ASP:OD2	1:B:96:VAL:N	2.45	0.48
1:C:225:LEU:HD11	1:C:296:HIS:HB2	1.95	0.48
1:C:349:THR:O	1:C:350:PRO:O	2.30	0.48
1:C:59:CYS:O	1:C:61:HIS:N	2.46	0.48
1:C:71:ARG:HD3	1:C:216:ASP:CG	2.38	0.48
1:A:9:ASN:ND2	2:A:600:NAG:C5	2.76	0.48
1:A:153:TYR:CD1	1:A:154:ASP:OD1	2.65	0.48
1:A:180:ALA:O	1:A:181:HIS:C	2.56	0.48
1:A:254:ALA:HB1	1:A:255:PRO:HA	1.95	0.48
1:B:320:SER:CA	1:B:344:GLY:H	2.24	0.48
1:C:184:ILE:HB	1:C:211:HIS:CE1	2.48	0.48
1:A:43:GLN:HB3	1:A:200:HIS:HB3	1.95	0.48
1:B:184:ILE:H	1:B:184:ILE:HD13	1.77	0.48
1:C:97:VAL:CG1	1:C:98:PRO:HD2	2.27	0.48
1:C:268:PRO:O	1:C:271:THR:HG22	2.14	0.48
1:A:155:THR:OG1	1:A:156:TRP:N	2.46	0.48
1:A:281:GLU:CG	1:A:282:TYR:N	2.76	0.48
1:A:345:GLY:O	1:A:348:GLU:HG2	2.14	0.48
1:B:259:ASN:OD1	1:B:261:THR:N	2.46	0.48
1:A:189:GLY:O	1:A:191:THR:N	2.45	0.48
1:B:114:ALA:O	1:B:115:LEU:HB2	2.14	0.48
1:B:372:VAL:CB	1:B:402:TYR:HD1	2.27	0.48
1:C:2:LEU:H	1:C:280:TYR:HA	1.79	0.48
1:C:87:VAL:HG12	1:C:88:VAL:HG13	1.95	0.48
1:C:243:MET:O	1:C:268:PRO:HD2	2.13	0.48
1:A:22:LEU:HD23	1:A:26:GLN:CG	2.42	0.48
1:B:7:VAL:HG12	1:B:93:TRP:HA	1.96	0.48
1:B:8:ARG:C	1:B:10:LEU:H	2.22	0.48
1:B:112:ASP:O	1:B:114:ALA:CB	2.61	0.48
1:B:163:TYR:O	1:B:164:ALA:C	2.52	0.48
1:C:4:ARG:HD3	1:C:282:TYR:HE1	1.78	0.48
1:A:39:SER:C	1:A:41:HIS:N	2.70	0.48
1:C:6:SER:OG	1:C:8:ARG:HB2	2.14	0.48
1:C:129:ILE:CD1	1:C:136:ILE:CD1	2.92	0.48
1:B:54:LYS:HG3	1:C:387:ASN:ND2	2.29	0.48
1:B:299:ILE:O	1:B:302:GLN:HB2	2.14	0.48
1:C:68:GLU:CG	1:C:268:PRO:HB3	2.41	0.48
1:A:122:ASN:O	1:A:123:PRO:C	2.54	0.47
1:A:184:ILE:HD12	1:A:184:ILE:H	1.78	0.47
1:A:247:LEU:HD11	1:A:268:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASN:O	1:A:295:LEU:HG	2.12	0.47
1:B:95:THR:O	1:B:96:VAL:C	2.52	0.47
1:B:111:TRP:CD1	1:B:111:TRP:O	2.66	0.47
1:C:202:ALA:O	1:C:204:TYR:N	2.46	0.47
1:C:237:ASN:C	1:C:240:LEU:HD21	2.39	0.47
1:A:90:ILE:HG21	1:A:209:ILE:HG22	1.96	0.47
1:B:156:TRP:O	1:B:157:SER:C	2.55	0.47
1:A:136:ILE:CD1	1:A:205:ASP:N	2.77	0.47
1:A:170:TYR:O	1:A:173:PHE:N	2.46	0.47
1:A:198:HIS:C	1:A:200:HIS:N	2.71	0.47
1:A:221:LEU:O	1:A:222:TRP:C	2.58	0.47
1:B:104:ALA:O	1:B:106:PHE:N	2.48	0.47
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.78	0.47
1:B:350:PRO:O	1:B:350:PRO:HG2	2.15	0.47
1:C:29:SER:O	1:C:29:SER:OG	2.32	0.47
1:C:59:CYS:SG	1:C:61:HIS:NE2	2.81	0.47
1:C:132:ASN:C	1:C:134:GLN:HE22	2.23	0.47
1:C:176:GLN:O	1:C:177:PHE:C	2.56	0.47
1:A:243:MET:O	1:A:269:GLU:HB2	2.14	0.47
1:A:274:TYR:HB2	1:A:280:TYR:CE2	2.48	0.47
1:A:339:TYR:N	1:A:339:TYR:CD2	2.80	0.47
1:A:343:LEU:C	1:A:343:LEU:HD23	2.40	0.47
1:B:42:ALA:CB	1:B:57:ALA:HB1	2.45	0.47
1:B:335:THR:HG21	1:B:368:LYS:HE3	1.95	0.47
1:B:400:VAL:O	1:B:400:VAL:HG12	2.14	0.47
1:C:13:ALA:O	1:C:14:GLU:C	2.58	0.47
1:C:200:HIS:O	1:C:201:TYR:CD2	2.68	0.47
1:C:283:ASP:O	1:C:284:HIS:ND1	2.48	0.47
1:C:312:PHE:HB2	1:C:357:TYR:HB3	1.97	0.47
1:A:50:PRO:HD3	1:A:252:PHE:HE2	1.79	0.47
1:A:195:SER:C	1:A:197:GLY:H	2.22	0.47
1:A:199:LEU:HA	1:A:343:LEU:HD21	1.95	0.47
1:A:296:HIS:C	1:A:298:TYR:H	2.20	0.47
1:B:188:VAL:O	1:B:188:VAL:HG12	2.13	0.47
1:B:369:GLY:O	1:B:370:LEU:HD23	2.14	0.47
1:B:153:TYR:O	1:B:155:THR:HG23	2.15	0.47
1:B:218:LEU:O	1:B:221:LEU:HB3	2.15	0.47
1:A:-2:HIS:ND1	1:A:-2:HIS:C	2.72	0.47
1:A:315:GLU:O	1:A:316:GLY:C	2.58	0.47
1:A:319:THR:HG23	1:A:320:SER:O	2.15	0.47
1:B:135:LYS:O	1:B:136:ILE:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PHE:C	1:B:177:PHE:CD2	2.92	0.47
1:B:206:PRO:O	1:B:208:PHE:N	2.48	0.47
1:C:7:VAL:C	1:C:10:LEU:HG	2.40	0.47
1:C:8:ARG:HG2	1:C:8:ARG:NH1	2.29	0.47
1:C:39:SER:HB3	1:C:46:LEU:HD21	1.96	0.47
1:C:65:THR:CG2	1:C:242:MET:HB3	2.43	0.47
1:C:74:THR:O	1:C:77:PHE:HB2	2.15	0.47
1:C:196:MET:HA	1:C:202:ALA:CB	2.45	0.47
1:C:200:HIS:C	1:C:201:TYR:CD2	2.93	0.47
1:A:19:VAL:HG12	1:A:19:VAL:O	2.11	0.47
1:A:42:ALA:CB	1:A:200:HIS:HA	2.45	0.47
1:A:205:ASP:CG	1:A:207:VAL:HG22	2.40	0.47
1:A:281:GLU:HG2	1:A:282:TYR:O	2.15	0.47
1:A:293:GLN:C	1:A:295:LEU:H	2.23	0.47
1:B:164:ALA:O	1:B:173:PHE:CD1	2.68	0.47
1:C:198:HIS:HE1	1:C:200:HIS:CB	2.27	0.47
1:C:326:SER:OG	1:C:336:HIS:HA	2.15	0.47
1:A:342:VAL:O	1:A:342:VAL:HG23	2.12	0.47
1:A:366:GLU:O	1:A:368:LYS:N	2.42	0.47
1:B:196:MET:HE3	1:B:207:VAL:HG13	1.88	0.47
1:B:220:ALA:O	1:B:221:LEU:C	2.53	0.47
1:A:207:VAL:O	1:A:210:LEU:N	2.48	0.47
1:A:209:ILE:HD13	1:A:209:ILE:HG21	1.39	0.47
1:A:236:VAL:HG21	1:A:272:PHE:CE2	2.49	0.47
1:B:11:SER:O	1:B:14:GLU:HB2	2.15	0.47
1:B:94:ASP:OD2	1:B:94:ASP:C	2.57	0.47
1:B:136:ILE:O	1:B:136:ILE:CD1	2.63	0.47
1:B:78:GLU:HG3	1:B:90:ILE:HG13	1.97	0.46
1:B:127:ALA:O	1:B:136:ILE:HG13	2.15	0.46
1:C:327:ILE:HD11	1:C:361:ILE:HD13	1.97	0.46
1:C:397:PRO:HA	1:C:398:PRO:HD3	1.60	0.46
1:B:71:ARG:HD2	1:B:280:TYR:OH	2.15	0.46
1:B:72:LEU:HD12	1:B:247:LEU:HD13	1.97	0.46
1:B:110:ILE:N	1:B:110:ILE:CD1	2.70	0.46
1:B:247:LEU:HD11	1:B:268:PRO:HG3	1.98	0.46
1:B:401:ILE:CG2	1:B:402:TYR:H	2.25	0.46
1:C:95:THR:O	1:C:97:VAL:N	2.48	0.46
1:C:311:GLY:C	1:C:356:LEU:HD22	2.40	0.46
1:A:6:SER:O	1:A:10:LEU:HG	2.16	0.46
1:A:368:LYS:HB3	1:A:370:LEU:HD12	1.97	0.46
1:C:68:GLU:O	1:C:69:TRP:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:H	1:C:347:LEU:CD2	2.26	0.46
1:A:43:GLN:CB	1:A:200:HIS:HB3	2.45	0.46
1:A:225:LEU:O	1:A:228:PHE:N	2.49	0.46
1:B:78:GLU:C	1:B:80:ALA:N	2.72	0.46
1:B:112:ASP:C	1:B:114:ALA:N	2.74	0.46
1:B:260:PRO:HG2	1:B:261:THR:N	2.30	0.46
1:B:365:LEU:HD12	1:B:370:LEU:CB	2.46	0.46
1:A:199:LEU:HB3	1:A:345:GLY:H	1.78	0.46
1:A:263:LYS:C	1:A:265:HIS:N	2.72	0.46
1:A:268:PRO:O	1:A:269:GLU:C	2.58	0.46
1:A:371:ASP:O	1:A:372:VAL:C	2.55	0.46
1:B:302:GLN:C	1:B:304:GLU:N	2.74	0.46
1:C:90:ILE:HG21	1:C:209:ILE:HG22	1.98	0.46
1:C:347:LEU:HD13	1:C:347:LEU:HA	1.62	0.46
1:A:22:LEU:HD12	1:A:81:LEU:HD21	1.97	0.46
1:A:214:ASN:OD1	1:A:217:ARG:NE	2.43	0.46
1:B:149:GLY:O	1:B:151:LYS:N	2.49	0.46
1:C:8:ARG:NH2	1:C:103:PRO:HG3	2.30	0.46
1:C:11:SER:O	1:C:14:GLU:N	2.49	0.46
1:C:132:ASN:C	1:C:134:GLN:NE2	2.73	0.46
1:C:144:LYS:HD3	1:C:144:LYS:N	2.29	0.46
1:A:92:TYR:CD2	1:A:214:ASN:OD1	2.68	0.46
1:A:198:HIS:HE1	1:A:200:HIS:ND1	2.13	0.46
1:B:280:TYR:C	1:B:281:GLU:OE1	2.58	0.46
1:C:347:LEU:O	1:C:348:GLU:C	2.55	0.46
1:A:112:ASP:HA	1:A:119:ASN:HA	1.97	0.46
1:A:217:ARG:HA	1:A:282:TYR:CZ	2.51	0.46
1:C:119:ASN:HD22	2:C:650:NAG:H4	1.81	0.46
1:C:327:ILE:O	1:C:327:ILE:HG22	2.14	0.46
1:A:4:ARG:CZ	1:A:280:TYR:CE1	2.99	0.46
1:A:11:SER:N	1:A:14:GLU:OE2	2.48	0.46
1:B:66:PHE:HB3	1:B:67:PRO:HD3	1.98	0.46
1:B:140:ILE:O	1:B:142:VAL:C	2.59	0.46
1:B:224:GLU:O	1:B:225:LEU:C	2.59	0.46
1:C:123:PRO:C	1:C:125:ASN:H	2.24	0.46
1:C:267:LYS:O	1:C:268:PRO:C	2.56	0.46
1:A:31:ALA:HB3	1:A:258:LEU:HD11	1.97	0.46
1:A:136:ILE:HG23	1:A:137:ALA:N	2.21	0.46
1:B:324:ASP:OD1	1:B:324:ASP:N	2.49	0.46
1:C:97:VAL:O	1:C:98:PRO:C	2.54	0.46
1:C:163:TYR:O	1:C:166:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ASN:CA	1:C:240:LEU:HD21	2.40	0.46
1:C:329:ALA:HB3	1:C:333:GLU:HB3	1.98	0.46
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.62	0.46
1:A:195:SER:O	1:A:197:GLY:N	2.49	0.45
1:A:232:ASP:OD2	1:A:232:ASP:C	2.58	0.45
1:A:319:THR:CA	1:A:344:GLY:O	2.62	0.45
1:B:71:ARG:HD3	1:B:216:ASP:CG	2.41	0.45
1:B:263:LYS:C	1:B:265:HIS:N	2.74	0.45
1:C:122:ASN:ND2	1:C:124:PHE:H	2.14	0.45
1:C:194:TYR:HA	1:C:201:TYR:CD1	2.52	0.45
1:C:307:ARG:HB2	1:C:309:PHE:HE1	1.80	0.45
1:A:11:SER:C	1:A:13:ALA:N	2.71	0.45
1:A:67:PRO:O	1:A:68:GLU:C	2.55	0.45
1:A:295:LEU:O	1:A:298:TYR:HB3	2.16	0.45
1:B:34:PHE:O	1:B:35:GLN:C	2.59	0.45
1:B:329:ALA:C	1:B:331:ASP:N	2.67	0.45
1:C:43:GLN:HA	1:C:44:PRO:C	2.41	0.45
1:C:47:CYS:N	1:C:48:PRO:CD	2.79	0.45
1:C:149:GLY:HA2	1:C:154:ASP:O	2.17	0.45
1:C:180:ALA:O	1:C:181:HIS:C	2.59	0.45
1:C:242:MET:CE	1:C:242:MET:CG	2.94	0.45
1:A:156:TRP:HE3	1:A:157:SER:N	2.15	0.45
1:A:226:GLN:NE2	1:A:229:ARG:HH11	2.15	0.45
1:B:181:HIS:CD2	1:B:212:HIS:CD2	3.03	0.45
1:C:99:GLN:O	1:C:100:GLU:C	2.58	0.45
1:C:112:ASP:HA	1:C:119:ASN:OD1	2.15	0.45
1:C:175:VAL:CG2	1:C:176:GLN:H	2.17	0.45
1:C:291:ASN:C	1:C:294:ARG:H	2.24	0.45
1:A:47:CYS:C	1:A:49:ALA:N	2.69	0.45
1:A:104:ALA:C	1:A:106:PHE:N	2.73	0.45
1:A:241:GLU:H	1:A:241:GLU:HG3	1.42	0.45
1:C:96:VAL:C	1:C:97:VAL:CG2	2.86	0.45
1:C:162:ILE:O	1:C:163:TYR:C	2.58	0.45
1:C:268:PRO:C	1:C:270:ASP:H	2.24	0.45
1:A:169:ASP:HB3	1:A:172:ASP:HB2	1.99	0.45
1:A:211:HIS:C	1:A:213:SER:N	2.75	0.45
1:A:380:ILE:HD12	1:A:380:ILE:C	2.41	0.45
1:B:153:TYR:HB2	1:B:288:GLN:NE2	2.31	0.45
1:B:298:TYR:O	1:B:301:GLN:HB3	2.16	0.45
1:B:302:GLN:C	1:B:304:GLU:H	2.19	0.45
1:C:41:HIS:NE2	1:C:59:CYS:SG	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:VAL:O	1:C:87:VAL:CG1	2.65	0.45
1:C:131:PHE:CD1	1:C:132:ASN:OD1	2.70	0.45
1:C:150:PRO:HG2	1:C:154:ASP:HB3	1.97	0.45
1:C:399:SER:C	1:C:400:VAL:HG23	2.42	0.45
1:A:80:ALA:O	1:A:81:LEU:C	2.57	0.45
1:A:286:GLU:CD	1:A:289:GLY:O	2.59	0.45
1:B:299:ILE:C	1:B:301:GLN:N	2.69	0.45
1:B:311:GLY:N	1:B:399:SER:O	2.49	0.45
1:A:138:ARG:NE	1:A:205:ASP:OD2	2.50	0.45
1:A:236:VAL:CG2	1:A:272:PHE:CE2	2.99	0.45
1:A:242:MET:O	1:A:244:ARG:N	2.49	0.45
1:B:116:PHE:C	1:B:117:HIS:ND1	2.75	0.45
1:B:363:ASP:O	1:B:364:VAL:C	2.57	0.45
1:C:86:SER:C	1:C:88:VAL:H	2.24	0.45
1:A:-3:GLY:O	1:A:-2:HIS:C	2.59	0.45
1:A:96:VAL:CG1	1:A:287:LEU:HD11	2.30	0.45
1:A:157:SER:O	1:A:161:TYR:N	2.36	0.45
1:A:286:GLU:OE2	1:A:290:MET:O	2.34	0.45
1:A:323:LEU:HD21	1:A:380:ILE:CG2	2.47	0.45
1:A:362:THR:HG22	1:A:363:ASP:N	2.32	0.45
1:C:187:TRP:CD1	1:C:187:TRP:H	2.35	0.45
1:A:36:SER:C	1:A:38:ALA:N	2.63	0.45
1:A:184:ILE:HD13	1:A:211:HIS:HE1	1.82	0.45
1:A:216:ASP:OD2	1:A:282:TYR:OH	2.32	0.45
1:B:-1:ARG:CA	1:B:1:ASN:N	2.80	0.45
1:B:22:LEU:HD11	1:B:34:PHE:CE1	2.52	0.45
1:B:211:HIS:O	1:B:214:ASN:N	2.40	0.45
1:A:34:PHE:O	1:A:37:LEU:N	2.50	0.45
1:A:98:PRO:CB	1:A:147:LYS:HB2	2.47	0.45
1:A:136:ILE:HD11	1:A:204:TYR:CA	2.43	0.45
1:A:211:HIS:O	1:A:213:SER:N	2.50	0.45
1:A:232:ASP:OD1	1:A:235:GLU:HB2	2.17	0.45
1:A:287:LEU:O	1:A:287:LEU:HG	2.16	0.45
1:A:299:ILE:HD13	1:A:299:ILE:HA	1.82	0.45
1:A:322:HIS:HA	1:A:341:ASP:HB3	1.99	0.45
1:B:148:GLU:HG3	1:B:149:GLY:N	2.32	0.45
1:C:59:CYS:O	1:C:61:HIS:CG	2.70	0.45
1:A:97:VAL:O	1:A:97:VAL:HG23	2.14	0.44
1:A:140:ILE:HD12	1:A:140:ILE:N	2.22	0.44
1:A:208:PHE:O	1:A:212:HIS:HB2	2.16	0.44
1:A:228:PHE:CE2	1:A:296:HIS:CD2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:CYS:C	1:B:240:LEU:HD12	2.42	0.44
1:B:382:GLN:OE1	1:B:390:ILE:HG21	2.16	0.44
1:A:71:ARG:NE	1:A:216:ASP:OD1	2.32	0.44
1:B:72:LEU:HD12	1:B:247:LEU:CD1	2.47	0.44
1:B:140:ILE:HD12	1:B:140:ILE:HG23	1.73	0.44
1:B:241:GLU:H	1:B:241:GLU:HG3	1.38	0.44
1:C:151:LYS:HB2	1:C:154:ASP:HB2	1.99	0.44
1:B:145:LEU:O	1:B:146:ALA:C	2.61	0.44
1:B:224:GLU:C	1:B:226:GLN:N	2.71	0.44
1:B:236:VAL:CG1	1:B:238:CYS:HB3	2.47	0.44
1:B:274:TYR:O	1:B:278:PHE:N	2.43	0.44
1:C:22:LEU:O	1:C:26:GLN:N	2.40	0.44
1:C:275:LYS:HG3	1:C:276:GLY:N	2.32	0.44
1:B:65:THR:HG23	1:B:242:MET:HG3	1.99	0.44
1:B:77:PHE:CD1	1:B:209:ILE:HD11	2.52	0.44
1:B:139:ASP:C	1:B:139:ASP:OD2	2.56	0.44
1:B:202:ALA:O	1:B:203:SER:C	2.56	0.44
1:B:388:GLU:O	1:B:389:ASP:C	2.58	0.44
1:C:59:CYS:SG	1:C:61:HIS:ND1	2.65	0.44
1:C:61:HIS:CD2	1:C:70:HIS:HE1	2.35	0.44
1:C:139:ASP:O	1:C:140:ILE:C	2.58	0.44
1:C:145:LEU:CD2	1:C:145:LEU:N	2.76	0.44
1:C:247:LEU:HD12	1:C:247:LEU:HA	1.67	0.44
1:A:143:ASP:O	1:A:146:ALA:HB2	2.17	0.44
1:B:299:ILE:O	1:B:301:GLN:N	2.51	0.44
1:B:309:PHE:CE2	1:B:360:GLU:HB2	2.52	0.44
1:B:323:LEU:HD11	1:B:340:PHE:CZ	2.53	0.44
1:C:4:ARG:HH21	1:C:75:VAL:HG22	1.83	0.44
1:C:20:ALA:O	1:C:21:ALA:C	2.58	0.44
1:C:42:ALA:O	1:C:45:PRO:HA	2.18	0.44
1:C:69:TRP:HE3	1:C:70:HIS:N	2.15	0.44
1:C:404:PRO:O	1:C:405:LYS:C	2.61	0.44
1:A:156:TRP:HE3	1:A:157:SER:H	1.66	0.44
1:A:168:GLU:HA	1:A:226:GLN:HE22	1.83	0.44
1:A:199:LEU:CB	1:A:345:GLY:N	2.78	0.44
1:B:-1:ARG:C	1:B:1:ASN:H3	2.24	0.44
1:C:27:GLU:H	1:C:27:GLU:HG3	1.55	0.44
1:C:66:PHE:HE2	1:C:70:HIS:CE1	2.36	0.44
1:C:235:GLU:CD	1:C:237:ASN:HD21	2.25	0.44
1:C:396:PRO:HA	1:C:397:PRO:HD2	1.74	0.44
1:B:78:GLU:O	1:B:81:LEU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LEU:HD11	1:B:376:PHE:CE2	2.52	0.44
1:C:16:ALA:O	1:C:17:SER:C	2.57	0.44
1:C:136:ILE:HG23	1:C:195:SER:HA	2.00	0.44
1:A:90:ILE:HG21	1:A:90:ILE:HD13	1.77	0.44
1:A:293:GLN:O	1:A:295:LEU:N	2.51	0.44
1:A:370:LEU:HD23	1:A:374:ASP:OD1	2.17	0.44
1:B:318:GLY:O	1:B:345:GLY:C	2.61	0.44
1:B:327:ILE:O	1:B:327:ILE:CG2	2.51	0.44
1:C:93:TRP:CD1	1:C:103:PRO:HG2	2.53	0.44
1:A:201:TYR:C	1:A:203:SER:N	2.76	0.44
1:A:268:PRO:C	1:A:270:ASP:N	2.76	0.44
1:A:339:TYR:O	1:A:339:TYR:CD2	2.70	0.44
1:A:392:THR:O	1:A:393:ASP:C	2.61	0.44
1:B:222:TRP:O	1:B:224:GLU:N	2.50	0.44
1:C:90:ILE:HA	1:C:91:PRO:HD2	1.72	0.44
1:A:181:HIS:ND1	1:A:182:ASN:OD1	2.50	0.43
1:B:135:LYS:C	1:B:136:ILE:O	2.58	0.43
1:B:238:CYS:N	1:B:240:LEU:HD11	2.33	0.43
1:B:397:PRO:HA	1:B:398:PRO:HD3	1.79	0.43
1:C:95:THR:C	1:C:97:VAL:H	2.26	0.43
1:C:169:ASP:O	1:C:170:TYR:C	2.60	0.43
1:C:211:HIS:O	1:C:215:THR:HG23	2.18	0.43
1:C:312:PHE:N	1:C:356:LEU:HD22	2.33	0.43
1:A:257:ASN:OD1	1:A:259:ASN:HB3	2.18	0.43
1:B:94:ASP:HA	1:B:214:ASN:ND2	2.32	0.43
1:B:368:LYS:HE2	1:B:368:LYS:HB2	1.81	0.43
1:B:185:HIS:NE2	1:B:212:HIS:CE1	2.86	0.43
1:C:38:ALA:C	1:C:40:PHE:N	2.75	0.43
1:C:305:ALA:O	1:C:307:ARG:HG3	2.18	0.43
1:C:315:GLU:O	1:C:316:GLY:C	2.59	0.43
1:A:104:ALA:O	1:A:107:ASN:N	2.47	0.43
1:A:167:GLN:HG2	1:A:172:ASP:HB3	2.01	0.43
1:B:107:ASN:O	1:B:107:ASN:ND2	2.52	0.43
1:B:202:ALA:O	1:B:204:TYR:N	2.52	0.43
1:B:307:ARG:O	1:B:308:VAL:CG2	2.63	0.43
1:C:41:HIS:CD2	1:C:59:CYS:SG	3.12	0.43
1:C:65:THR:HG23	1:C:242:MET:CB	2.49	0.43
1:C:95:THR:HG21	1:C:184:ILE:HG12	1.99	0.43
1:C:186:ALA:C	1:C:188:VAL:N	2.76	0.43
1:B:123:PRO:C	1:B:125:ASN:H	2.26	0.43
1:C:42:ALA:CB	1:C:200:HIS:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:MET:HB3	1:C:196:MET:HE3	1.54	0.43
1:C:245:GLU:C	1:C:246:PRO:O	2.53	0.43
1:C:282:TYR:HB2	1:C:285:LEU:HD23	1.99	0.43
1:A:136:ILE:HG21	1:A:205:ASP:HB2	2.00	0.43
1:A:167:GLN:HE21	1:A:167:GLN:HB2	1.70	0.43
1:A:192:GLU:HB2	1:A:195:SER:HG	1.83	0.43
1:C:65:THR:CG2	1:C:242:MET:HB2	2.49	0.43
1:C:71:ARG:NH2	1:C:272:PHE:O	2.52	0.43
1:C:82:ARG:C	1:C:84:HIS:N	2.75	0.43
1:C:232:ASP:OD2	1:C:232:ASP:C	2.62	0.43
1:C:309:PHE:N	1:C:309:PHE:HD1	2.15	0.43
1:A:61:HIS:HE2	1:A:70:HIS:HE1	1.66	0.43
1:A:218:LEU:HD12	1:A:218:LEU:C	2.43	0.43
1:A:301:GLN:HG3	1:A:304:GLU:OE1	2.19	0.43
1:C:4:ARG:NH2	1:C:75:VAL:CG2	2.82	0.43
1:C:8:ARG:NH1	1:C:103:PRO:HG3	2.34	0.43
1:C:8:ARG:HH22	1:C:103:PRO:HD3	1.82	0.43
1:C:404:PRO:O	1:C:405:LYS:O	2.37	0.43
1:A:4:ARG:CZ	1:A:280:TYR:CD1	3.01	0.43
1:A:32:ASP:C	1:A:37:LEU:HD11	2.43	0.43
1:A:128:ASP:OD1	1:A:128:ASP:N	2.51	0.43
1:B:127:ALA:N	1:B:136:ILE:HD11	2.33	0.43
1:B:128:ASP:C	1:B:129:ILE:HG13	2.42	0.43
1:C:234:ASN:CG	1:C:273:ASP:HB2	2.41	0.43
1:A:6:SER:C	1:A:8:ARG:N	2.72	0.43
1:A:219:PHE:O	1:A:223:GLN:HG3	2.18	0.43
1:A:329:ALA:O	1:A:330:ILE:C	2.62	0.43
1:B:279:HIS:O	1:B:280:TYR:HB3	2.19	0.43
1:C:295:LEU:HD23	1:C:295:LEU:HA	1.55	0.43
1:B:132:ASN:ND2	1:B:134:GLN:CB	2.81	0.43
1:B:242:MET:C	1:B:244:ARG:H	2.27	0.43
1:C:211:HIS:C	1:C:213:SER:N	2.74	0.43
1:B:37:LEU:HG	1:B:37:LEU:H	1.65	0.42
1:B:374:ASP:OD2	1:B:375:VAL:N	2.52	0.42
1:B:395:PHE:HA	1:B:396:PRO:HD2	1.84	0.42
1:B:401:ILE:H	1:B:401:ILE:HG13	1.64	0.42
1:C:149:GLY:C	1:C:151:LYS:H	2.27	0.42
1:C:303:LYS:C	1:C:303:LYS:CD	2.92	0.42
1:A:32:ASP:O	1:A:32:ASP:CG	2.60	0.42
1:A:143:ASP:O	1:A:146:ALA:CB	2.68	0.42
1:A:174:GLU:O	1:A:175:VAL:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:HA	1:B:123:PRO:HD3	1.78	0.42
1:C:283:ASP:C	1:C:284:HIS:ND1	2.76	0.42
1:A:22:LEU:O	1:A:26:GLN:N	2.45	0.42
1:C:-1:ARG:CB	1:C:1:ASN:H2	2.20	0.42
1:C:65:THR:HG23	1:C:242:MET:HB2	2.00	0.42
1:B:-1:ARG:CA	1:B:1:ASN:H3	2.32	0.42
1:B:263:LYS:HG2	1:B:264:GLU:N	2.33	0.42
1:A:87:VAL:C	1:A:88:VAL:CG1	2.92	0.42
1:A:299:ILE:O	1:A:302:GLN:HB2	2.19	0.42
1:A:366:GLU:O	1:A:369:GLY:N	2.50	0.42
1:B:39:SER:O	1:B:41:HIS:N	2.49	0.42
1:B:66:PHE:HE2	1:B:70:HIS:CE1	2.38	0.42
1:B:221:LEU:HD11	1:B:295:LEU:CD1	2.49	0.42
1:B:252:PHE:HD1	1:B:252:PHE:H	1.66	0.42
1:C:330:ILE:HD12	1:C:330:ILE:N	2.30	0.42
1:B:169:ASP:O	1:B:170:TYR:C	2.62	0.42
1:B:267:LYS:O	1:B:270:ASP:HB2	2.19	0.42
1:C:65:THR:HG21	1:C:242:MET:CB	2.49	0.42
1:C:254:ALA:HB1	1:C:255:PRO:HA	2.00	0.42
1:C:391:SER:HB2	1:C:393:ASP:OD2	2.20	0.42
1:A:145:LEU:HD12	1:A:145:LEU:C	2.44	0.42
1:B:150:PRO:O	1:B:151:LYS:CE	2.67	0.42
1:C:11:SER:C	1:C:13:ALA:N	2.74	0.42
1:C:139:ASP:C	1:C:141:ASN:N	2.76	0.42
1:C:275:LYS:HG3	1:C:276:GLY:H	1.85	0.42
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.21	0.42
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.72	0.42
1:A:173:PHE:O	1:A:173:PHE:CD1	2.72	0.42
1:A:249:PRO:O	1:A:251:SER:N	2.53	0.42
1:A:386:ASP:HB2	1:A:387:ASN:H	1.66	0.42
1:B:132:ASN:OD1	1:B:194:TYR:HE2	2.02	0.42
1:B:229:ARG:HH11	1:B:229:ARG:CB	2.33	0.42
1:B:245:GLU:HA	1:B:246:PRO:HD2	1.67	0.42
1:B:303:LYS:CE	1:B:405:LYS:HG2	2.41	0.42
1:C:-1:ARG:HG2	1:C:1:ASN:H3	1.85	0.42
1:A:-3:GLY:CA	1:A:1:ASN:H2	2.32	0.42
1:A:143:ASP:HA	1:A:145:LEU:HD23	2.01	0.42
1:A:309:PHE:N	1:A:309:PHE:CD1	2.86	0.42
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.93	0.42
1:B:229:ARG:HB2	1:B:229:ARG:HH11	1.84	0.42
1:C:-2:HIS:CB	1:C:1:ASN:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:PHE:CE1	1:C:177:PHE:HB2	2.55	0.42
1:C:184:ILE:N	1:C:184:ILE:HD12	2.34	0.42
1:A:25:LEU:C	1:A:27:GLU:N	2.76	0.42
1:A:66:PHE:CE2	1:A:178:GLU:HG3	2.54	0.42
1:A:106:PHE:HD1	1:A:138:ARG:HH12	1.67	0.42
1:A:170:TYR:C	1:A:170:TYR:CD2	2.98	0.42
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.97	0.42
1:B:47:CYS:HB3	1:B:48:PRO:CD	2.45	0.42
1:B:367:SER:O	1:B:368:LYS:HE2	2.20	0.42
1:A:53:ASN:HB2	1:B:322:HIS:NE2	2.35	0.41
1:A:92:TYR:CG	1:A:217:ARG:HD3	2.55	0.41
1:A:228:PHE:HE2	1:A:296:HIS:CD2	2.33	0.41
1:B:130:ASP:O	1:B:131:PHE:C	2.61	0.41
1:B:295:LEU:O	1:B:296:HIS:C	2.63	0.41
1:C:122:ASN:HD22	1:C:124:PHE:H	1.68	0.41
1:C:254:ALA:CB	1:C:255:PRO:HA	2.50	0.41
1:A:69:TRP:CE3	1:A:69:TRP:C	2.98	0.41
1:A:232:ASP:CG	1:A:235:GLU:HB2	2.45	0.41
1:A:252:PHE:N	1:A:252:PHE:CD1	2.86	0.41
1:A:349:THR:O	1:A:350:PRO:C	2.63	0.41
1:C:102:LEU:HD11	1:C:140:ILE:HD13	2.02	0.41
1:C:249:PRO:C	1:C:251:SER:H	2.26	0.41
1:A:199:LEU:HD22	1:A:348:GLU:HB3	2.02	0.41
1:A:286:GLU:OE2	1:A:289:GLY:C	2.63	0.41
1:B:17:SER:O	1:B:21:ALA:HB2	2.20	0.41
1:B:78:GLU:C	1:B:80:ALA:H	2.28	0.41
1:B:139:ASP:C	1:B:141:ASN:H	2.28	0.41
1:B:166:GLU:O	1:B:167:GLN:C	2.59	0.41
1:C:96:VAL:HG11	1:C:287:LEU:HD11	2.02	0.41
1:C:131:PHE:N	1:C:131:PHE:CD2	2.87	0.41
1:B:42:ALA:HA	1:B:57:ALA:HB1	2.03	0.41
1:A:94:ASP:HA	1:A:214:ASN:HD21	1.80	0.41
1:A:117:HIS:CD2	1:A:117:HIS:N	2.87	0.41
1:A:366:GLU:C	1:A:368:LYS:N	2.78	0.41
1:B:66:PHE:CE2	1:B:70:HIS:CE1	3.07	0.41
1:B:97:VAL:HG13	1:B:98:PRO:CD	2.47	0.41
1:B:135:LYS:O	1:B:136:ILE:O	2.39	0.41
1:B:153:TYR:HB2	1:B:288:GLN:CD	2.46	0.41
1:B:181:HIS:O	1:B:181:HIS:CD2	2.70	0.41
1:C:241:GLU:H	1:C:241:GLU:HG3	1.55	0.41
1:A:72:LEU:HD22	1:A:250:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:CD1	1:A:204:TYR:O	2.69	0.41
1:A:166:GLU:HG3	1:A:299:ILE:HD12	2.01	0.41
1:B:28:ASP:HB2	1:B:84:HIS:CE1	2.56	0.41
1:B:87:VAL:C	1:B:88:VAL:HG13	2.45	0.41
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.84	0.41
1:B:337:ALA:HB1	1:B:361:ILE:HG22	2.02	0.41
1:C:149:GLY:HA3	1:C:152:GLY:O	2.21	0.41
1:A:73:TYR:O	1:A:76:GLN:HB3	2.20	0.41
1:A:285:LEU:HD13	1:A:285:LEU:HA	1.68	0.41
1:A:323:LEU:HD21	1:A:380:ILE:HB	2.01	0.41
1:B:132:ASN:ND2	1:B:134:GLN:HB2	2.35	0.41
1:B:200:HIS:CE1	1:B:347:LEU:H	2.39	0.41
1:B:232:ASP:O	1:B:233:PRO:C	2.60	0.41
1:B:299:ILE:HG22	1:B:300:ASN:N	2.35	0.41
1:B:314:LEU:H	1:B:314:LEU:HG	1.69	0.41
1:C:149:GLY:O	1:C:151:LYS:N	2.53	0.41
1:A:42:ALA:HB1	1:A:200:HIS:HA	2.02	0.41
1:A:325:PHE:O	1:A:337:ALA:CB	2.64	0.41
1:A:376:PHE:C	1:A:376:PHE:HD1	2.28	0.41
1:B:166:GLU:HB3	1:B:167:GLN:NE2	2.30	0.41
1:B:205:ASP:OD1	1:B:206:PRO:N	2.53	0.41
1:C:307:ARG:C	1:C:308:VAL:CG2	2.93	0.41
1:C:346:SER:O	1:C:348:GLU:N	2.54	0.41
1:A:10:LEU:HA	1:A:14:GLU:OE2	2.21	0.41
1:A:87:VAL:HG12	1:A:87:VAL:O	2.21	0.41
1:A:92:TYR:HA	1:A:210:LEU:O	2.21	0.41
1:A:260:PRO:O	1:A:262:THR:N	2.54	0.41
1:B:71:ARG:C	1:B:73:TYR:N	2.78	0.41
1:B:82:ARG:C	1:B:84:HIS:N	2.78	0.41
1:B:145:LEU:C	1:B:145:LEU:CD1	2.93	0.41
1:B:153:TYR:O	1:B:155:THR:N	2.54	0.41
1:B:198:HIS:O	1:B:199:LEU:C	2.62	0.41
1:B:269:GLU:C	1:B:271:THR:H	2.29	0.41
1:B:366:GLU:O	1:B:368:LYS:N	2.46	0.41
1:C:41:HIS:CD2	1:C:59:CYS:CB	3.04	0.41
1:C:47:CYS:SG	1:C:248:LYS:HB2	2.60	0.41
1:C:99:GLN:NE2	1:C:103:PRO:HD3	2.36	0.41
1:C:182:ASN:O	1:C:185:HIS:N	2.54	0.41
1:C:323:LEU:HD21	1:C:340:PHE:CZ	2.55	0.41
1:C:346:SER:HB2	1:C:347:LEU:CD2	2.41	0.41
1:A:75:VAL:HG21	1:A:278:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:HB2	1:A:147:LYS:HB2	2.03	0.41
1:A:139:ASP:O	1:A:190:GLY:HA3	2.21	0.41
1:A:170:TYR:O	1:A:172:ASP:N	2.54	0.41
1:A:244:ARG:HH11	1:A:244:ARG:CG	2.06	0.41
1:B:32:ASP:O	1:B:37:LEU:HD11	2.21	0.41
1:B:78:GLU:O	1:B:79:ASP:C	2.64	0.41
1:B:95:THR:C	1:B:97:VAL:H	2.29	0.41
1:B:167:GLN:H	1:B:167:GLN:HG2	1.14	0.41
1:C:11:SER:HA	1:C:12:PRO:HD3	1.87	0.41
1:C:217:ARG:HG2	1:C:282:TYR:CG	2.55	0.41
1:A:149:GLY:O	1:A:150:PRO:C	2.64	0.40
1:A:156:TRP:C	1:A:158:PHE:N	2.79	0.40
1:B:161:TYR:O	1:B:162:ILE:C	2.63	0.40
1:B:184:ILE:HG21	1:B:211:HIS:CG	2.56	0.40
1:B:320:SER:OG	1:B:343:LEU:HA	2.20	0.40
1:C:131:PHE:CE2	1:C:204:TYR:OH	2.63	0.40
1:C:208:PHE:CD2	1:C:208:PHE:C	2.99	0.40
1:C:259:ASN:CG	1:C:260:PRO:HD2	2.46	0.40
1:A:11:SER:O	1:A:12:PRO:C	2.64	0.40
1:B:171:CYS:C	1:B:173:PHE:N	2.76	0.40
1:B:206:PRO:C	1:B:208:PHE:N	2.77	0.40
1:B:234:ASN:HA	1:B:272:PHE:CB	2.51	0.40
1:C:24:SER:HB3	1:C:84:HIS:ND1	2.36	0.40
1:C:48:PRO:HD3	1:C:56:PHE:O	2.21	0.40
1:A:43:GLN:HG3	1:A:44:PRO:N	2.36	0.40
1:A:130:ASP:O	1:A:131:PHE:C	2.64	0.40
1:A:155:THR:O	1:A:159:LYS:HG2	2.22	0.40
1:B:142:VAL:HA	1:B:144:LYS:CG	2.47	0.40
1:C:68:GLU:CD	1:C:68:GLU:N	2.78	0.40
1:C:327:ILE:HD13	1:C:365:LEU:HD13	2.03	0.40
1:A:143:ASP:C	1:A:145:LEU:N	2.76	0.40
1:B:48:PRO:O	1:B:248:LYS:HE2	2.20	0.40
1:C:150:PRO:HG2	1:C:154:ASP:CB	2.52	0.40
1:C:298:TYR:O	1:C:302:GLN:HG2	2.21	0.40
1:A:307:ARG:HB2	1:A:309:PHE:HE1	1.85	0.40
1:B:-2:HIS:NE2	1:B:-1:ARG:HG3	2.35	0.40
1:C:28:ASP:OD1	1:C:30:SER:HB3	2.21	0.40
1:C:81:LEU:HD12	1:C:90:ILE:HG12	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:HIS:CA	3:B:5503:CU:CU[6_456]	1.67	0.53
1:A:-2:HIS:O	3:B:5503:CU:CU[6_456]	1.69	0.51

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	404/408 (99%)	280 (69%)	86 (21%)	38 (9%)	0	3
1	B	404/408 (99%)	311 (77%)	70 (17%)	23 (6%)	1	9
1	C	404/408 (99%)	287 (71%)	83 (20%)	34 (8%)	0	4
All	All	1212/1224 (99%)	878 (72%)	239 (20%)	95 (8%)	1	5

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	34	PHE
1	A	57	ALA
1	A	58	CYS
1	A	105	PHE
1	A	113	ASP
1	A	114	ALA
1	A	156	TRP
1	A	157	SER
1	A	170	TYR
1	A	199	LEU
1	A	316	GLY
1	A	331	ASP
1	A	362	THR
1	B	113	ASP
1	B	115	LEU
1	B	116	PHE
1	B	124	PHE

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Mol	Chain	Res	Type
1	B	141	ASN
1	B	327	ILE
1	B	404	PRO
1	C	34	PHE
1	C	35	GLN
1	C	59	CYS
1	C	60	VAL
1	C	79	ASP
1	C	87	VAL
1	C	141	ASN
1	C	148	GLU
1	C	187	TRP
1	C	246	PRO
1	C	269	GLU
1	C	316	GLY
1	C	350	PRO
1	C	387	ASN
1	C	404	PRO
1	A	119	ASN
1	A	190	GLY
1	A	368	LYS
1	A	375	VAL
1	A	384	SER
1	A	387	ASN
1	B	47	CYS
1	B	117	HIS
1	B	200	HIS
1	B	234	ASN
1	B	264	GLU
1	B	303	LYS
1	B	368	LYS
1	B	387	ASN
1	C	96	VAL
1	C	100	GLU
1	C	115	LEU
1	C	250	PHE
1	C	260	PRO
1	A	37	LEU
1	A	64	ALA
1	A	193	GLU
1	A	196	MET
1	A	212	HIS

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Mol	Chain	Res	Type
1	A	239	ALA
1	A	269	GLU
1	A	386	ASP
1	B	154	ASP
1	B	250	PHE
1	B	270	ASP
1	C	46	LEU
1	C	51	ALA
1	C	86	SER
1	C	130	ASP
1	C	154	ASP
1	A	350	PRO
1	A	367	SER
1	B	190	GLY
1	B	233	PRO
1	C	132	ASN
1	C	133	HIS
1	C	194	TYR
1	C	304	GLU
1	C	384	SER
1	C	393	ASP
1	A	264	GLU
1	A	297	ASP
1	B	260	PRO
1	C	47	CYS
1	A	177	PHE
1	A	261	THR
1	C	203	SER
1	A	260	PRO
1	A	332	GLY
1	B	7	VAL
1	B	140	ILE
1	C	149	GLY
1	A	49	ALA
1	A	96	VAL

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	352/352 (100%)	299 (85%)	53 (15%)	3	13
1	B	352/352 (100%)	296 (84%)	56 (16%)	2	12
1	C	352/352 (100%)	284 (81%)	68 (19%)	1	6
All	All	1056/1056 (100%)	879 (83%)	177 (17%)	2	11

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	12	PRO
1	A	15	ARG
1	A	22	LEU
1	A	43	GLN
1	A	46	LEU
1	A	47	CYS
1	A	79	ASP
1	A	92	TYR
1	A	96	VAL
1	A	97	VAL
1	A	102	LEU
1	A	108	ASP
1	A	110	ILE
1	A	119	ASN
1	A	121	THR
1	A	140	ILE
1	A	145	LEU
1	A	155	THR
1	A	160	GLN
1	A	167	GLN
1	A	173	PHE
1	A	174	GLU
1	A	191	THR
1	A	201	TYR
1	A	209	ILE
1	A	218	LEU
1	A	234	ASN
1	A	241	GLU
1	A	243	MET
1	A	246	PRO
1	A	248	LYS

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Mol	Chain	Res	Type
1	A	255	PRO
1	A	263	LYS
1	A	268	PRO
1	A	285	LEU
1	A	286	GLU
1	A	287	LEU
1	A	290	MET
1	A	293	GLN
1	A	299	ILE
1	A	317	ILE
1	A	324	ASP
1	A	326	SER
1	A	327	ILE
1	A	330	ILE
1	A	341	ASP
1	A	355	ARG
1	A	366	GLU
1	A	368	LYS
1	A	372	VAL
1	A	380	ILE
1	A	399	SER
1	B	-1	ARG
1	B	2	LEU
1	B	12	PRO
1	B	30	SER
1	B	46	LEU
1	B	47	CYS
1	B	58	CYS
1	B	71	ARG
1	B	83	ARG
1	B	87	VAL
1	B	95	THR
1	B	96	VAL
1	B	100	GLU
1	B	102	LEU
1	B	110	ILE
1	B	111	TRP
1	B	136	ILE
1	B	151	LYS
1	B	154	ASP
1	B	173	PHE
1	B	176	GLN

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Mol	Chain	Res	Type
1	B	181	HIS
1	B	196	MET
1	B	217	ARG
1	B	229	ARG
1	B	233	PRO
1	B	241	GLU
1	B	243	MET
1	B	249	PRO
1	B	260	PRO
1	B	262	THR
1	B	274	TYR
1	B	280	TYR
1	B	286	GLU
1	B	301	GLN
1	B	304	GLU
1	B	308	VAL
1	B	323	LEU
1	B	324	ASP
1	B	341	ASP
1	B	342	VAL
1	B	343	LEU
1	B	347	LEU
1	B	349	THR
1	B	359	TYR
1	B	361	ILE
1	B	365	LEU
1	B	368	LYS
1	B	375	VAL
1	B	378	ILE
1	B	380	ILE
1	B	382	GLN
1	B	388	GLU
1	B	391	SER
1	B	392	THR
1	B	402	TYR
1	C	3	VAL
1	C	7	VAL
1	C	12	PRO
1	C	15	ARG
1	C	22	LEU
1	C	23	LYS
1	C	24	SER

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Mol	Chain	Res	Type
1	C	27	GLU
1	C	29	SER
1	C	43	GLN
1	C	46	LEU
1	C	47	CYS
1	C	50	PRO
1	C	58	CYS
1	C	71	ARG
1	C	95	THR
1	C	97	VAL
1	C	99	GLN
1	C	101	ASP
1	C	102	LEU
1	C	110	ILE
1	C	119	ASN
1	C	120	PHE
1	C	130	ASP
1	C	134	GLN
1	C	138	ARG
1	C	143	ASP
1	C	154	ASP
1	C	155	THR
1	C	162	ILE
1	C	184	ILE
1	C	191	THR
1	C	196	MET
1	C	203	SER
1	C	209	ILE
1	C	218	LEU
1	C	233	PRO
1	C	241	GLU
1	C	246	PRO
1	C	247	LEU
1	C	248	LYS
1	C	255	PRO
1	C	259	ASN
1	C	260	PRO
1	C	286	GLU
1	C	297	ASP
1	C	300	ASN
1	C	303	LYS
1	C	309	PHE

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Mol	Chain	Res	Type
1	C	314	LEU
1	C	315	GLU
1	C	322	HIS
1	C	323	LEU
1	C	330	ILE
1	C	334	CYS
1	C	341	ASP
1	C	349	THR
1	C	350	PRO
1	C	358	LYS
1	C	362	THR
1	C	364	VAL
1	C	365	LEU
1	C	372	VAL
1	C	380	ILE
1	C	381	THR
1	C	390	ILE
1	C	392	THR
1	C	401	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	76	GLN
1	A	84	HIS
1	A	99	GLN
1	A	117	HIS
1	A	119	ASN
1	A	122	ASN
1	A	160	GLN
1	A	167	GLN
1	A	182	ASN
1	A	198	HIS
1	A	211	HIS
1	A	223	GLN
1	A	226	GLN
1	A	291	ASN
1	A	296	HIS
1	A	322	HIS
1	B	-2	HIS
1	B	1	ASN

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Mol	Chain	Res	Type
1	B	35	GLN
1	B	53	ASN
1	B	107	ASN
1	B	119	ASN
1	B	132	ASN
1	B	141	ASN
1	B	160	GLN
1	B	167	GLN
1	B	176	GLN
1	B	200	HIS
1	B	211	HIS
1	B	223	GLN
1	B	226	GLN
1	B	234	ASN
1	B	265	HIS
1	B	277	HIS
1	B	300	ASN
1	B	302	GLN
1	B	373	HIS
1	B	387	ASN
1	C	-2	HIS
1	C	99	GLN
1	C	117	HIS
1	C	119	ASN
1	C	122	ASN
1	C	125	ASN
1	C	132	ASN
1	C	133	HIS
1	C	134	GLN
1	C	167	GLN
1	C	176	GLN
1	C	198	HIS
1	C	211	HIS
1	C	223	GLN
1	C	226	GLN
1	C	237	ASN
1	C	259	ASN
1	C	265	HIS
1	C	293	GLN
1	C	336	HIS
1	C	387	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	651	-	15,15,15	1.80	4 (26%)	21,21,21	4.28	11 (52%)
2	NAG	A	600	-	15,15,15	1.71	3 (20%)	21,21,21	1.96	6 (28%)
2	NAG	C	650	-	15,15,15	1.89	4 (26%)	21,21,21	1.82	6 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	651	-	-	4/6/26/26	0/1/1/1
2	NAG	A	600	-	-	3/6/26/26	0/1/1/1
2	NAG	C	650	-	-	2/6/26/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	650	NAG	O7-C7	4.74	1.33	1.23
2	A	600	NAG	C3-C2	3.62	1.59	1.53
2	C	650	NAG	C8-C7	3.14	1.57	1.50
2	C	651	NAG	C8-C7	2.92	1.56	1.50
2	C	651	NAG	O1-C1	2.74	1.48	1.39
2	A	600	NAG	C1-C2	2.48	1.55	1.52
2	C	650	NAG	C1-C2	2.42	1.55	1.52
2	C	650	NAG	O1-C1	2.38	1.47	1.39
2	C	651	NAG	C6-C5	2.28	1.59	1.51
2	C	651	NAG	C4-C5	2.25	1.57	1.53
2	A	600	NAG	C8-C7	2.25	1.55	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	651	NAG	C1-C2-C3	-13.28	92.43	110.54
2	C	651	NAG	O1-C1-C2	8.11	126.06	109.22
2	C	651	NAG	C1-O5-C5	-7.08	99.96	113.65
2	C	651	NAG	O5-C5-C6	4.81	118.36	106.44
2	A	600	NAG	C1-C2-N2	-4.63	105.37	110.73
2	A	600	NAG	C1-C2-C3	3.89	115.85	110.54
2	C	650	NAG	C1-C2-C3	3.58	115.42	110.54
2	C	650	NAG	O1-C1-C2	3.32	116.11	109.22
2	C	650	NAG	C2-N2-C7	-3.20	115.62	123.11
2	C	651	NAG	O1-C1-O5	3.19	119.89	110.41
2	C	650	NAG	O3-C3-C4	-3.17	102.89	110.38
2	A	600	NAG	O3-C3-C2	3.14	115.83	109.58
2	C	651	NAG	O5-C1-C2	-3.11	106.39	109.52
2	C	651	NAG	C2-N2-C7	2.96	130.03	123.11
2	C	651	NAG	C3-C4-C5	2.78	115.27	110.23
2	C	651	NAG	C1-C2-N2	2.71	113.86	110.73
2	A	600	NAG	O5-C5-C6	2.69	113.12	106.44
2	C	650	NAG	O3-C3-C2	2.58	114.73	109.58
2	C	651	NAG	C8-C7-N2	2.36	120.02	116.12
2	A	600	NAG	C2-N2-C7	-2.29	117.73	123.11
2	C	650	NAG	O5-C1-C2	-2.25	107.26	109.52
2	C	651	NAG	O3-C3-C2	2.11	113.79	109.58
2	A	600	NAG	C8-C7-N2	2.05	119.51	116.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NAG	C8-C7-N2-C2
2	A	600	NAG	O7-C7-N2-C2
2	C	650	NAG	C8-C7-N2-C2
2	C	650	NAG	O7-C7-N2-C2
2	C	651	NAG	C8-C7-N2-C2
2	C	651	NAG	O7-C7-N2-C2
2	C	651	NAG	C4-C5-C6-O6
2	A	600	NAG	O5-C5-C6-O6
2	C	651	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NAG	3	0
2	C	650	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	-1:ARG	C	1:ASN	N	5.08
1	C	-1:ARG	C	1:ASN	N	3.99
1	B	-1:ARG	C	1:ASN	N	2.64

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	408/408 (100%)	-0.01	4 (0%) 79 63	43, 43, 43, 78	0
1	B	408/408 (100%)	-0.09	6 (1%) 72 53	43, 43, 43, 78	0
1	C	408/408 (100%)	0.09	3 (0%) 84 70	31, 43, 43, 78	1 (0%)
All	All	1224/1224 (100%)	-0.00	13 (1%) 78 60	31, 43, 43, 78	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-3	GLY	7.5
1	B	141	ASN	4.8
1	B	132	ASN	3.2
1	C	132	ASN	3.2
1	B	148	GLU	2.9
1	C	297	ASP	2.5
1	A	-3	GLY	2.5
1	A	141	ASN	2.4
1	A	369	GLY	2.4
1	A	345	GLY	2.3
1	B	-3	GLY	2.2
1	B	111	TRP	2.2
1	B	-2	HIS	2.2

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	NAG	C	651	15/15	0.57	0.23	77,77,77,77	0
2	NAG	A	600	15/15	0.63	0.30	77,77,77,77	0
2	NAG	C	650	15/15	0.72	0.14	77,77,77,77	0
3	CU	A	5001	1/1	0.97	0.07	77,77,77,77	0
3	CU	B	5503	1/1	0.97	0.07	77,77,77,77	0
3	CU	B	5506	1/1	0.97	0.07	77,77,77,77	0
3	CU	A	5012	1/1	0.98	0.04	77,77,77,77	0
3	CU	C	5509	1/1	0.98	0.06	77,77,77,77	0
3	CU	B	5004	1/1	0.99	0.08	77,77,77,77	0
3	CU	C	5007	1/1	0.99	0.03	77,77,77,77	0
3	CU	C	5018	1/1	0.99	0.04	77,77,77,77	0
3	CU	B	5015	1/1	0.99	0.06	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.