



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:48 AM UTC

PDB ID : 3TYW / pdb_00003tyw
Title : Crystal Structure of CYP105N1 from Streptomyces coelicolor A3(2)
Authors : Zhao, B.; Waterman, M.R.
Deposited on : 2011-09-26
Resolution : 2.90 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

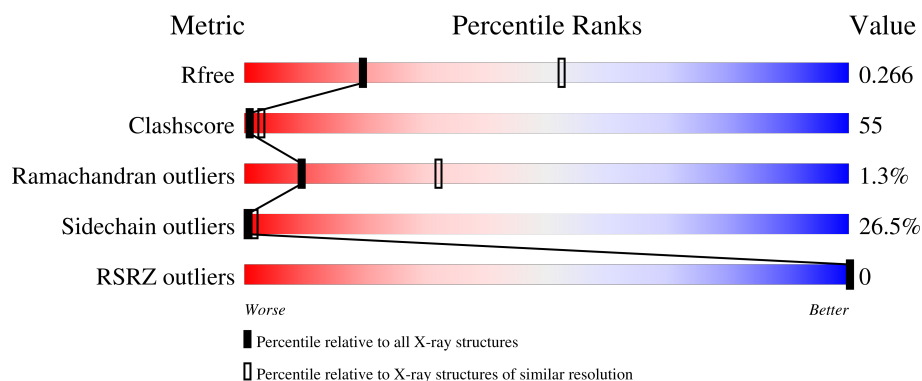
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	417	
1	B	417	
1	C	417	
1	D	417	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12633 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 Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3084	1927	567	581	9			
1	B	397	Total	C	N	O	S	0	0	0
			3084	1927	567	581	9			
1	C	398	Total	C	N	O	S	0	0	0
			3094	1933	570	582	9			
1	D	399	Total	C	N	O	S	0	0	0
			3104	1939	573	583	9			

There are 24 discrepancies between the modelled and reference sequences:

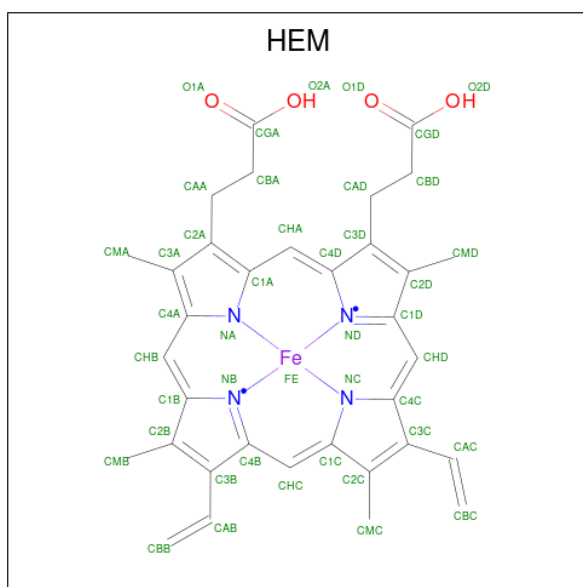
Chain	Residue	Modelled	Actual	Comment	Reference
A	412	HIS	-	expression tag	UNP Q9EWP1
A	413	HIS	-	expression tag	UNP Q9EWP1
A	414	HIS	-	expression tag	UNP Q9EWP1
A	415	HIS	-	expression tag	UNP Q9EWP1
A	416	HIS	-	expression tag	UNP Q9EWP1
A	417	HIS	-	expression tag	UNP Q9EWP1
B	412	HIS	-	expression tag	UNP Q9EWP1
B	413	HIS	-	expression tag	UNP Q9EWP1
B	414	HIS	-	expression tag	UNP Q9EWP1
B	415	HIS	-	expression tag	UNP Q9EWP1
B	416	HIS	-	expression tag	UNP Q9EWP1
B	417	HIS	-	expression tag	UNP Q9EWP1
C	412	HIS	-	expression tag	UNP Q9EWP1
C	413	HIS	-	expression tag	UNP Q9EWP1
C	414	HIS	-	expression tag	UNP Q9EWP1
C	415	HIS	-	expression tag	UNP Q9EWP1
C	416	HIS	-	expression tag	UNP Q9EWP1
C	417	HIS	-	expression tag	UNP Q9EWP1
D	412	HIS	-	expression tag	UNP Q9EWP1
D	413	HIS	-	expression tag	UNP Q9EWP1
D	414	HIS	-	expression tag	UNP Q9EWP1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	415	HIS	-	expression tag	UNP Q9EWP1
D	416	HIS	-	expression tag	UNP Q9EWP1
D	417	HIS	-	expression tag	UNP Q9EWP1

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	23	Total O 23 23	0	0
3	C	30	Total O 30 30	0	0

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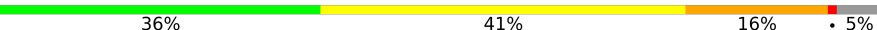
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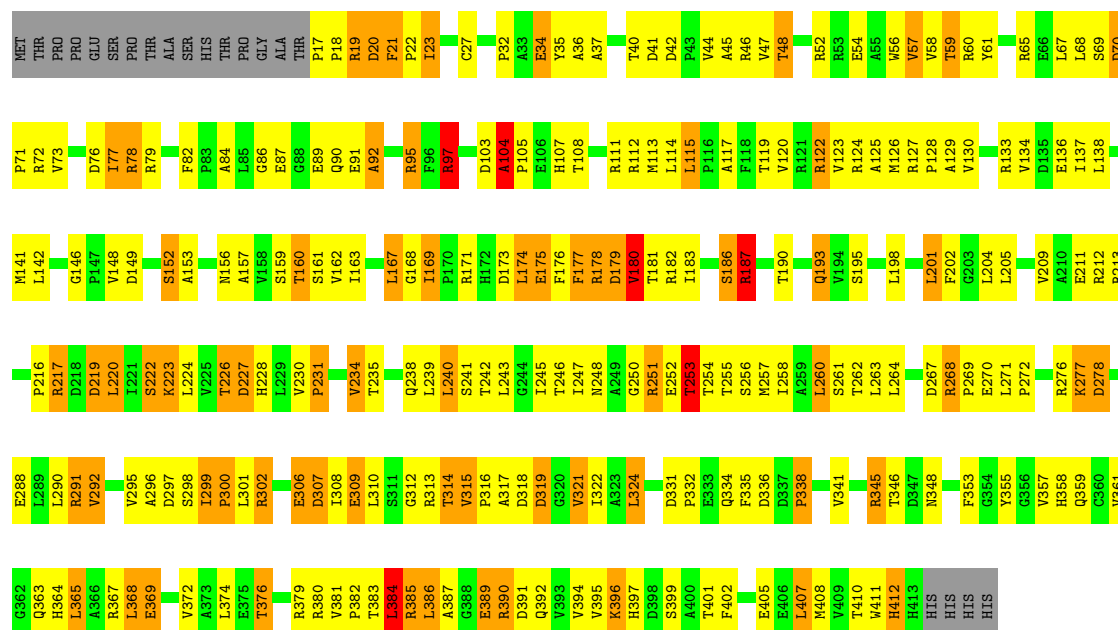
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	20	Total	O	0	0
			20	20		

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.

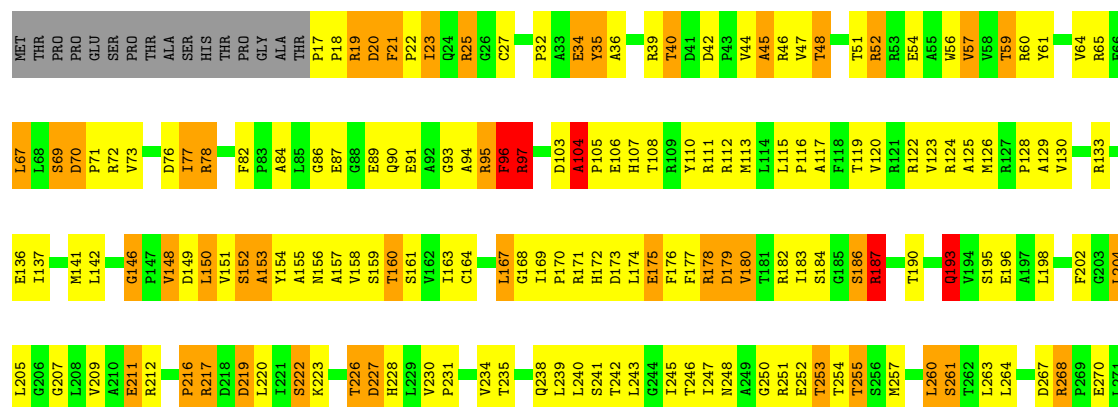
• Molecule 1: Putative cytochrome P450

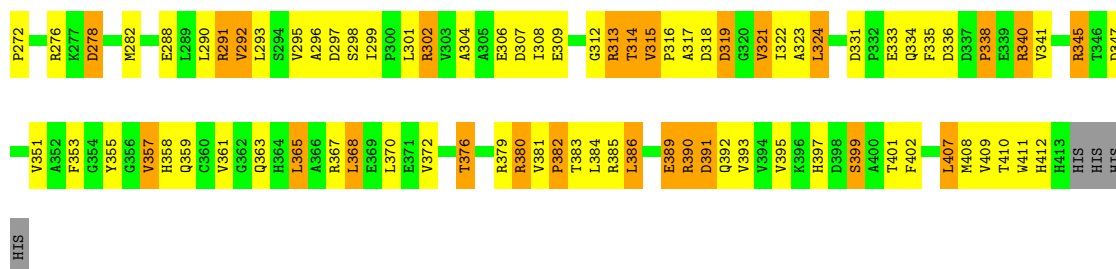
Chain A: 



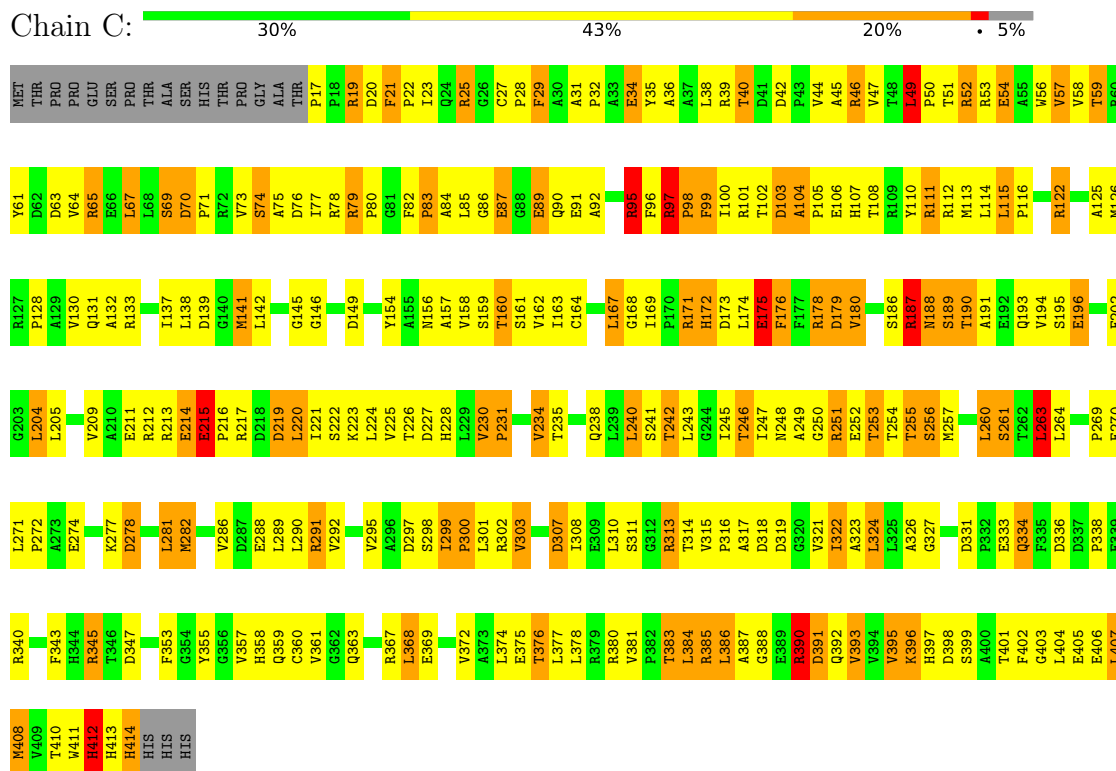
• Molecule 1: Putative cytochrome P450

Chain B: 

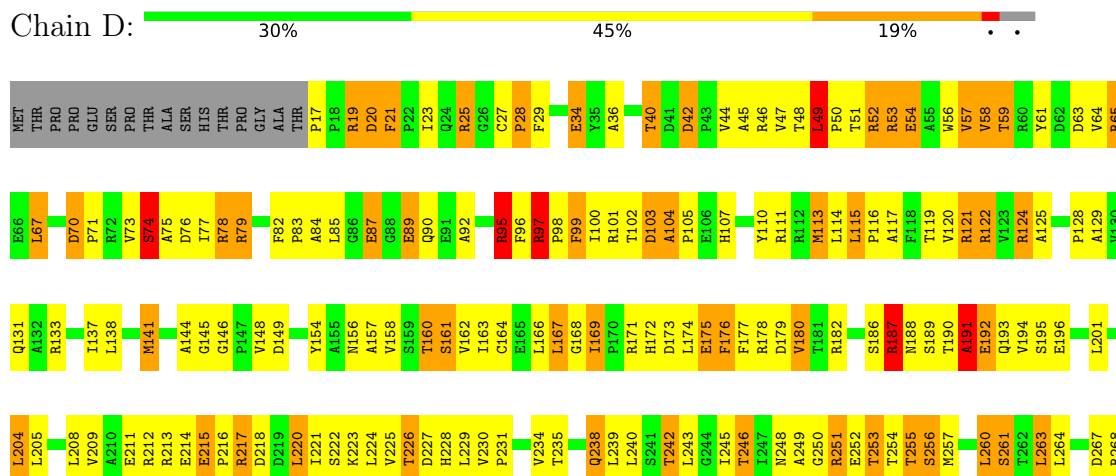




• Molecule 1: Putative cytochrome P450



• Molecule 1: Putative cytochrome P450





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	134.54Å 134.54Å 230.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.90) 99.5 (30.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.300 0.254 , 0.266	Depositor DCC
R_{free} test set	2646 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	6/3144 (0.2%)	1.30	45/4280 (1.1%)
1	B	1.08	2/3144 (0.1%)	1.27	32/4280 (0.7%)
1	C	1.08	3/3155 (0.1%)	1.31	47/4295 (1.1%)
1	D	1.09	3/3166 (0.1%)	1.32	45/4310 (1.0%)
All	All	1.09	14/12609 (0.1%)	1.30	169/17165 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	ARG	CZ-NH2	16.06	1.54	1.33
1	D	95	ARG	CZ-NH2	15.30	1.53	1.33
1	D	95	ARG	CZ-NH1	12.82	1.50	1.32
1	C	95	ARG	CZ-NH1	10.14	1.47	1.32
1	A	193	GLN	CD-NE2	9.82	1.53	1.33
1	B	193	GLN	CG-CD	8.82	1.74	1.52
1	B	193	GLN	CD-NE2	8.25	1.50	1.33
1	A	193	GLN	CD-OE1	7.60	1.38	1.23
1	C	22	PRO	CA-C	-6.55	1.45	1.52
1	A	278	ASP	C-N	6.14	1.39	1.33
1	D	319	ASP	C-O	-5.60	1.16	1.23
1	A	230	VAL	C-N	5.38	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	ASP	C-N	5.18	1.37	1.33
1	A	60	ARG	CA-C	-5.08	1.46	1.52

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	PHE	N-CA-C	-9.26	101.27	111.36
1	B	153	ALA	N-CA-C	8.38	120.50	111.36
1	C	89	GLU	N-CA-C	7.98	119.98	111.28
1	B	97	ARG	CA-C-N	-7.94	112.53	120.31
1	B	97	ARG	C-N-CA	-7.94	112.53	120.31
1	A	299	ILE	CB-CA-C	-7.71	106.17	114.35
1	A	92	ALA	N-CA-C	-7.48	104.39	113.97
1	D	21	PHE	CA-C-N	-7.34	112.07	119.93
1	D	21	PHE	C-N-CA	-7.34	112.07	119.93
1	C	21	PHE	CA-C-N	-7.30	111.51	119.98
1	C	21	PHE	C-N-CA	-7.30	111.51	119.98
1	A	153	ALA	N-CA-C	7.30	119.32	111.36
1	D	387	ALA	N-CA-C	7.11	119.03	111.28
1	B	172	HIS	N-CA-C	6.94	118.63	111.14
1	C	189	SER	N-CA-C	6.91	119.07	108.42
1	A	87	GLU	N-CA-C	6.79	118.69	111.28
1	A	146	GLY	CA-C-N	-6.76	113.00	119.76
1	A	146	GLY	C-N-CA	-6.76	113.00	119.76
1	B	146	GLY	CA-C-N	-6.68	113.08	119.76
1	B	146	GLY	C-N-CA	-6.68	113.08	119.76
1	D	144	ALA	N-CA-C	-6.66	104.02	111.28
1	D	89	GLU	N-CA-C	6.51	118.92	111.11
1	D	280	ASP	N-CA-C	-6.42	105.41	113.18
1	B	87	GLU	N-CA-C	6.35	118.20	111.28
1	D	113	MET	N-CA-C	6.34	118.27	111.36
1	C	97	ARG	CA-C-N	-6.22	114.24	120.21
1	C	97	ARG	C-N-CA	-6.22	114.24	120.21
1	D	282	MET	CA-C-N	-6.22	112.15	119.05
1	D	282	MET	C-N-CA	-6.22	112.15	119.05
1	C	54	GLU	N-CA-C	6.20	118.72	110.53
1	D	394	VAL	N-CA-C	6.12	116.68	107.80
1	D	389	GLU	N-CA-C	-6.08	101.92	110.50
1	C	19	ARG	N-CA-C	6.04	118.98	110.23
1	A	315	VAL	CA-C-N	-6.03	114.06	120.03
1	A	315	VAL	C-N-CA	-6.03	114.06	120.03
1	A	390	ARG	N-CA-C	-6.03	102.00	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CA-C-N	-6.02	114.02	121.00
1	A	230	VAL	C-N-CA	-6.02	114.02	121.00
1	D	97	ARG	CA-C-N	-5.96	114.13	120.03
1	D	97	ARG	C-N-CA	-5.96	114.13	120.03
1	A	278	ASP	CA-C-N	-5.93	113.71	120.89
1	A	278	ASP	C-N-CA	-5.93	113.71	120.89
1	B	70	ASP	CA-C-N	-5.93	114.13	121.00
1	B	70	ASP	C-N-CA	-5.93	114.13	121.00
1	C	282	MET	CA-C-N	-5.88	112.52	119.05
1	C	282	MET	C-N-CA	-5.88	112.52	119.05
1	B	21	PHE	CB-CA-C	-5.87	104.35	113.57
1	A	21	PHE	N-CA-C	5.85	120.45	112.55
1	C	278	ASP	CA-C-N	-5.85	114.27	120.94
1	C	278	ASP	C-N-CA	-5.85	114.27	120.94
1	D	115	LEU	CA-C-N	-5.80	114.13	119.82
1	D	115	LEU	C-N-CA	-5.80	114.13	119.82
1	D	270	GLU	N-CA-C	5.80	118.38	111.71
1	D	27	CYS	CA-C-N	-5.77	113.73	119.56
1	D	27	CYS	C-N-CA	-5.77	113.73	119.56
1	C	390	ARG	N-CA-C	-5.75	99.82	108.96
1	D	57	VAL	N-CA-C	5.69	116.48	108.17
1	B	40	THR	N-CA-C	5.68	117.55	111.36
1	B	338	PRO	N-CA-C	5.64	121.26	113.98
1	D	49	LEU	CA-C-N	-5.64	113.86	119.56
1	D	49	LEU	C-N-CA	-5.64	113.86	119.56
1	A	193	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	D	58	VAL	N-CA-C	5.62	115.95	107.80
1	A	271	LEU	CA-C-N	-5.62	113.89	119.56
1	A	271	LEU	C-N-CA	-5.62	113.89	119.56
1	A	79	ARG	CA-C-N	-5.61	114.04	119.87
1	A	79	ARG	C-N-CA	-5.61	114.04	119.87
1	A	17	PRO	CA-C-N	-5.61	113.98	119.76
1	A	17	PRO	C-N-CA	-5.61	113.98	119.76
1	B	35	TYR	N-CA-C	5.61	117.39	111.28
1	C	263	LEU	N-CA-C	-5.60	105.27	111.71
1	C	397	HIS	N-CA-C	-5.60	106.12	113.12
1	B	399	SER	N-CA-C	5.58	118.58	109.59
1	D	268	ARG	CA-C-N	-5.55	113.95	119.56
1	D	268	ARG	C-N-CA	-5.55	113.95	119.56
1	D	218	ASP	N-CA-C	5.55	117.51	108.63
1	C	79	ARG	CA-C-N	-5.53	113.97	119.56
1	C	79	ARG	C-N-CA	-5.53	113.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	VAL	CA-C-N	-5.53	114.56	120.03
1	B	315	VAL	C-N-CA	-5.53	114.56	120.03
1	C	57	VAL	N-CA-C	5.52	116.07	108.12
1	D	95	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	B	104	ALA	CA-C-N	-5.48	114.02	119.56
1	B	104	ALA	C-N-CA	-5.48	114.02	119.56
1	A	338	PRO	N-CA-C	5.48	120.77	114.03
1	B	17	PRO	CA-C-N	-5.48	113.92	119.83
1	B	17	PRO	C-N-CA	-5.48	113.92	119.83
1	A	97	ARG	CA-C-N	-5.46	115.11	120.52
1	A	97	ARG	C-N-CA	-5.46	115.11	120.52
1	A	332	PRO	N-CA-C	5.45	120.73	114.03
1	A	70	ASP	CA-C-N	-5.45	114.68	121.00
1	A	70	ASP	C-N-CA	-5.45	114.68	121.00
1	A	27	CYS	CA-C-N	-5.45	113.01	119.05
1	A	27	CYS	C-N-CA	-5.45	113.01	119.05
1	A	268	ARG	CA-C-N	-5.43	114.17	120.04
1	A	268	ARG	C-N-CA	-5.43	114.17	120.04
1	C	17	PRO	CA-C-N	-5.42	113.98	119.83
1	C	17	PRO	C-N-CA	-5.42	113.98	119.83
1	A	180	VAL	N-CA-C	5.39	116.17	110.72
1	C	230	VAL	CA-C-N	-5.38	114.39	120.89
1	C	230	VAL	C-N-CA	-5.38	114.39	120.89
1	D	17	PRO	CA-C-N	-5.37	114.03	119.83
1	D	17	PRO	C-N-CA	-5.37	114.03	119.83
1	D	146	GLY	CA-C-N	-5.33	114.27	119.76
1	D	146	GLY	C-N-CA	-5.33	114.27	119.76
1	D	316	PRO	N-CA-C	5.31	119.66	111.21
1	B	331	ASP	CA-C-N	-5.30	114.57	120.45
1	B	331	ASP	C-N-CA	-5.30	114.57	120.45
1	D	54	GLU	N-CA-C	5.29	117.96	110.50
1	C	106	GLU	N-CA-C	5.29	116.85	111.14
1	D	20	ASP	N-CA-C	-5.26	103.20	110.35
1	D	70	ASP	CA-C-N	-5.25	114.54	120.89
1	D	70	ASP	C-N-CA	-5.25	114.54	120.89
1	D	331	ASP	CA-C-N	-5.24	114.27	119.56
1	D	331	ASP	C-N-CA	-5.24	114.27	119.56
1	C	70	ASP	CA-C-N	-5.24	114.55	120.89
1	C	70	ASP	C-N-CA	-5.24	114.55	120.89
1	A	115	LEU	CA-C-N	-5.23	114.22	119.56
1	A	115	LEU	C-N-CA	-5.23	114.22	119.56
1	A	104	ALA	CA-C-N	-5.23	114.43	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ALA	C-N-CA	-5.23	114.43	119.87
1	B	27	CYS	CA-C-N	-5.22	113.25	119.05
1	B	27	CYS	C-N-CA	-5.22	113.25	119.05
1	D	74	SER	N-CA-C	5.22	118.07	109.72
1	C	27	CYS	CA-C-N	-5.21	113.55	119.28
1	C	27	CYS	C-N-CA	-5.21	113.55	119.28
1	B	45	ALA	N-CA-C	5.21	118.30	109.76
1	C	146	GLY	CA-C-N	-5.20	114.41	119.76
1	C	146	GLY	C-N-CA	-5.20	114.41	119.76
1	C	171	ARG	N-CA-C	5.19	116.63	110.97
1	A	384	LEU	N-CA-C	5.19	117.87	110.24
1	A	306	GLU	N-CA-C	-5.18	101.41	109.24
1	A	213	ARG	N-CA-C	-5.18	105.76	111.71
1	C	196	GLU	N-CA-C	-5.17	105.65	111.28
1	B	390	ARG	N-CA-C	-5.16	102.84	110.48
1	C	331	ASP	CA-C-N	-5.16	114.51	119.87
1	C	331	ASP	C-N-CA	-5.16	114.51	119.87
1	B	268	ARG	CA-C-N	-5.15	114.51	119.87
1	B	268	ARG	C-N-CA	-5.15	114.51	119.87
1	C	74	SER	N-CA-C	5.15	117.96	109.72
1	C	20	ASP	N-CA-C	-5.15	102.77	110.23
1	D	215	GLU	CA-C-N	-5.14	114.94	120.03
1	D	215	GLU	C-N-CA	-5.14	114.94	120.03
1	D	191	ALA	N-CA-C	-5.13	99.86	110.80
1	D	19	ARG	N-CA-C	5.12	117.31	110.35
1	A	169	ILE	CA-C-N	-5.12	114.49	119.76
1	A	169	ILE	C-N-CA	-5.12	114.49	119.76
1	C	29	PHE	N-CA-C	5.11	119.14	113.01
1	C	49	LEU	CA-C-N	-5.11	113.66	119.28
1	C	49	LEU	C-N-CA	-5.11	113.66	119.28
1	C	31	ALA	CA-C-N	-5.10	114.69	119.89
1	C	31	ALA	C-N-CA	-5.10	114.69	119.89
1	B	282	MET	CA-C-N	-5.10	113.67	119.28
1	B	282	MET	C-N-CA	-5.10	113.67	119.28
1	D	347	ASP	N-CA-C	5.09	116.89	108.49
1	A	253	THR	N-CA-C	5.08	116.89	111.36
1	C	115	LEU	CA-C-N	-5.08	114.48	120.12
1	C	115	LEU	C-N-CA	-5.08	114.48	120.12
1	B	278	ASP	CA-C-N	-5.05	114.62	119.87
1	B	278	ASP	C-N-CA	-5.05	114.62	119.87
1	C	215	GLU	CA-C-N	-5.04	115.04	120.03
1	C	215	GLU	C-N-CA	-5.04	115.04	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ILE	CA-C-N	-5.04	113.54	119.84
1	C	299	ILE	C-N-CA	-5.04	113.54	119.84
1	A	331	ASP	CA-C-N	-5.03	114.64	119.87
1	A	331	ASP	C-N-CA	-5.03	114.64	119.87
1	A	180	VAL	CB-CA-C	-5.02	105.29	112.22
1	D	79	ARG	CA-C-N	-5.02	114.44	119.56
1	D	79	ARG	C-N-CA	-5.02	114.44	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	94	ALA	Peptide
1	C	412	HIS	Peptide

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	3084	0	3078	287	11
1	B	3084	0	3079	275	16
1	C	3094	0	3083	405	20
1	D	3104	0	3093	430	15
2	A	43	0	30	5	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	6	0
3	A	22	0	0	3	0
3	B	23	0	0	4	0
3	C	30	0	0	4	0
3	D	20	0	0	4	0
All	All	12633	0	12453	1381	31

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 55.

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:190:THR:CG2	1:A:193:GLN:HB2	1.30	1.57
1:A:190:THR:HG21	1:A:193:GLN:CB	1.42	1.49
1:C:171:ARG:HD2	1:C:172:HIS:CE1	1.49	1.45
1:C:107:HIS:NE2	1:C:358:HIS:CD2	1.84	1.45
1:A:190:THR:CG2	1:A:193:GLN:CB	1.92	1.40
1:C:92:ALA:O	1:C:95:ARG:HD3	1.17	1.31
1:C:234:VAL:HG12	1:C:238:GLN:NE2	1.46	1.30
1:D:107:HIS:NE2	1:D:358:HIS:CD2	1.97	1.30
1:C:104:ALA:HB1	1:C:105:PRO:CD	1.62	1.29
1:B:65:ARG:NH1	1:B:355:TYR:CZ	2.01	1.29
1:C:374:LEU:O	1:C:378:LEU:CD1	1.81	1.27
1:B:136:GLU:OE2	1:B:171:ARG:NH1	1.68	1.25
1:C:291:ARG:NH2	1:C:338:PRO:O	1.68	1.25
1:C:234:VAL:CG1	1:C:238:GLN:HE21	1.50	1.22
1:C:299:ILE:HD11	1:C:401:THR:CG2	1.71	1.21
1:C:107:HIS:CD2	1:C:358:HIS:HE2	1.59	1.21
1:D:133:ARG:NH1	1:D:161:SER:O	1.74	1.20
1:D:77:ILE:HA	1:D:82:PHE:CD2	1.76	1.19
1:D:98:PRO:HB3	1:D:245:ILE:CD1	1.71	1.19
1:C:74:SER:OG	1:C:103:ASP:OD2	1.60	1.19
1:B:341:VAL:O	3:B:602:HOH:O	1.63	1.17
1:A:169:ILE:HD13	1:A:178:ARG:CD	1.74	1.16
1:C:299:ILE:HD11	1:C:401:THR:HG22	1.19	1.16
1:D:98:PRO:CB	1:D:245:ILE:CD1	2.24	1.16
1:D:302:ARG:NH2	1:D:358:HIS:ND1	1.93	1.16
1:D:386:LEU:HD23	1:D:408:MET:O	1.41	1.16
1:C:104:ALA:CB	1:C:105:PRO:HD2	1.76	1.15
1:C:77:ILE:HA	1:C:82:PHE:CD2	1.80	1.15
1:D:49:LEU:CD1	1:D:84:ALA:O	1.94	1.15
1:D:138:LEU:HD23	1:D:141:MET:HE2	1.30	1.14
1:D:92:ALA:O	1:D:95:ARG:CD	1.96	1.13
1:D:107:HIS:NE2	1:D:358:HIS:HD2	1.39	1.13
1:A:383:THR:HG21	1:A:412:HIS:HB2	1.22	1.13
1:D:57:VAL:CG2	1:D:322:ILE:HD12	1.78	1.13
1:C:392:GLN:O	3:C:606:HOH:O	1.67	1.12
1:C:77:ILE:O	1:C:90:GLN:NE2	1.80	1.12
1:C:191:ALA:O	3:C:603:HOH:O	1.66	1.11
1:A:169:ILE:HD13	1:A:178:ARG:HD3	1.25	1.11
1:D:104:ALA:HB1	1:D:105:PRO:HD2	1.29	1.10
1:C:299:ILE:CD1	1:C:401:THR:HG22	1.81	1.09
1:A:190:THR:CG2	1:A:193:GLN:HB3	1.83	1.08
1:C:92:ALA:O	1:C:95:ARG:CD	2.01	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:PRO:HB3	1:D:245:ILE:HD11	1.32	1.08
1:A:190:THR:HG22	1:A:193:GLN:CB	1.79	1.08
1:B:383:THR:HG21	1:B:412:HIS:HB2	1.33	1.07
1:C:303:VAL:HG13	1:C:319:ASP:O	1.52	1.07
1:C:171:ARG:CD	1:C:172:HIS:CE1	2.38	1.07
1:D:301:LEU:HD23	1:D:322:ILE:HG23	1.11	1.07
1:C:374:LEU:O	1:C:378:LEU:HD12	1.46	1.06
1:C:372:VAL:O	1:C:376:THR:HG23	1.53	1.06
1:A:288:GLU:OE1	1:A:291:ARG:NH1	1.89	1.06
1:D:216:PRO:O	1:D:217:ARG:NH1	1.89	1.06
1:D:250:GLY:HA3	2:D:501:HEM:HBC2	1.29	1.06
1:D:98:PRO:CB	1:D:245:ILE:HD13	1.85	1.05
1:B:251:ARG:O	1:B:255:THR:HG23	1.57	1.04
1:A:302:ARG:HG3	1:A:302:ARG:HH11	1.18	1.04
1:C:303:VAL:CG1	1:C:319:ASP:O	2.04	1.04
1:A:381:VAL:HG12	1:A:384:LEU:HB2	1.39	1.04
1:A:190:THR:HG21	1:A:193:GLN:HB3	1.35	1.04
1:B:250:GLY:HA3	2:B:501:HEM:HBC2	1.38	1.04
1:D:386:LEU:HD21	1:D:408:MET:SD	1.98	1.03
1:D:74:SER:HB3	1:D:103:ASP:OD2	1.58	1.03
1:C:171:ARG:HD2	1:C:172:HIS:ND1	1.73	1.03
1:B:288:GLU:OE1	1:B:291:ARG:NH1	1.91	1.03
1:C:98:PRO:CB	1:C:245:ILE:HD13	1.89	1.03
1:C:113:MET:SD	1:C:228:HIS:ND1	2.30	1.03
1:C:99:PHE:HD2	1:C:110:TYR:HB2	1.20	1.03
1:C:386:LEU:HD23	1:C:408:MET:O	1.59	1.02
1:C:301:LEU:HD23	1:C:322:ILE:HG23	1.39	1.02
1:C:104:ALA:HB1	1:C:105:PRO:HD2	1.04	1.02
1:C:107:HIS:CD2	1:C:358:HIS:NE2	2.26	1.02
1:C:174:LEU:HD13	1:C:204:LEU:HD21	1.07	1.02
1:D:77:ILE:HA	1:D:82:PHE:CE2	1.95	1.02
1:D:190:THR:OG1	1:D:193:GLN:N	1.90	1.02
1:C:99:PHE:HD2	1:C:110:TYR:CB	1.73	1.01
1:D:301:LEU:CD2	1:D:322:ILE:HG23	1.89	1.01
1:C:250:GLY:HA3	2:C:501:HEM:HBC2	1.37	1.01
1:C:174:LEU:CD1	1:C:204:LEU:HD21	1.91	1.00
1:D:176:PHE:O	1:D:180:VAL:HG23	1.61	0.99
1:B:169:ILE:HD13	1:B:178:ARG:HD3	1.43	0.99
1:C:75:ALA:O	1:C:101:ARG:O	1.81	0.99
1:A:18:PRO:HG2	1:A:54:GLU:OE2	1.61	0.99
1:D:251:ARG:O	1:D:255:THR:HG23	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ARG:HG3	1:D:78:ARG:HH11	1.28	0.98
1:D:386:LEU:CD2	1:D:408:MET:O	2.12	0.97
1:D:121:ARG:HG2	1:D:121:ARG:HH11	1.28	0.97
1:D:217:ARG:CZ	1:D:217:ARG:HA	1.93	0.97
1:B:104:ALA:HB1	1:B:105:PRO:HD2	1.43	0.97
1:A:250:GLY:HA3	2:A:501:HEM:HBC2	1.45	0.97
1:B:21:PHE:HB3	1:B:22:PRO:HD3	1.45	0.96
1:C:138:LEU:CD2	1:C:141:MET:HE2	1.95	0.96
1:C:84:ALA:HB1	1:C:89:GLU:OE1	1.63	0.96
1:C:49:LEU:CD1	1:C:84:ALA:O	2.14	0.96
1:C:77:ILE:HA	1:C:82:PHE:CE2	2.00	0.96
1:A:291:ARG:NH2	1:A:338:PRO:O	2.00	0.95
1:C:107:HIS:NE2	1:C:358:HIS:NE2	2.12	0.95
1:B:34:GLU:N	1:B:34:GLU:OE2	2.00	0.95
1:C:282:MET:O	1:C:286:VAL:HG23	1.66	0.95
1:D:92:ALA:O	1:D:95:ARG:HD2	1.64	0.95
1:C:171:ARG:HD2	1:C:172:HIS:HE1	1.14	0.95
1:D:190:THR:HG21	1:D:193:GLN:HB2	1.49	0.94
1:A:190:THR:HG23	1:A:193:GLN:HB2	1.48	0.94
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.32	0.94
1:B:372:VAL:O	1:B:376:THR:OG1	1.86	0.94
1:A:173:ASP:C	1:A:174:LEU:HD23	1.93	0.93
1:A:372:VAL:O	1:A:376:THR:OG1	1.86	0.93
1:D:98:PRO:HB2	1:D:245:ILE:HD13	1.50	0.93
1:A:104:ALA:HB1	1:A:105:PRO:HD2	1.48	0.93
1:D:267:ASP:OD2	1:D:390:ARG:NH2	2.01	0.93
1:C:98:PRO:HB2	1:C:245:ILE:HD13	1.50	0.93
1:D:75:ALA:CB	1:D:358:HIS:HE1	1.81	0.93
1:D:190:THR:CB	1:D:193:GLN:HB2	1.99	0.93
1:A:381:VAL:CG1	1:A:384:LEU:HB2	1.98	0.93
1:D:57:VAL:HG22	1:D:322:ILE:HD12	1.49	0.93
1:A:169:ILE:CD1	1:A:178:ARG:CD	2.47	0.93
1:B:65:ARG:NH1	1:B:355:TYR:CE1	2.34	0.93
1:C:257:MET:O	1:C:261:SER:OG	1.87	0.93
1:A:21:PHE:HB3	1:A:22:PRO:HD3	1.51	0.92
1:D:173:ASP:HB3	1:D:174:LEU:CD2	2.00	0.92
1:D:303:VAL:HG13	1:D:320:GLY:HA2	1.48	0.92
1:B:169:ILE:HD13	1:B:178:ARG:CD	1.99	0.92
1:D:131:GLN:OE1	1:D:376:THR:HG21	1.69	0.92
1:C:234:VAL:CG1	1:C:238:GLN:NE2	2.21	0.92
1:D:383:THR:OG1	1:D:413:HIS:HB3	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ASP:O	1:D:345:ARG:NH2	2.03	0.92
1:A:175:GLU:OE2	1:A:179:ASP:OD2	1.89	0.91
1:B:222:SER:O	1:B:226:THR:OG1	1.88	0.91
1:D:92:ALA:O	1:D:95:ARG:HD3	1.67	0.91
1:D:104:ALA:HB1	1:D:105:PRO:CD	2.01	0.90
1:B:219:ASP:OD1	1:B:222:SER:HB3	1.71	0.90
1:C:156:ASN:O	1:C:160:THR:OG1	1.89	0.90
1:D:313:ARG:HG2	1:D:313:ARG:HH11	1.36	0.90
1:D:395:VAL:HG12	1:D:396:LYS:H	1.36	0.90
1:D:76:ASP:OD1	1:D:78:ARG:NH1	2.05	0.90
1:D:190:THR:HG23	1:D:191:ALA:H	1.35	0.90
1:A:104:ALA:HB1	1:A:105:PRO:CD	2.03	0.89
1:B:257:MET:O	1:B:261:SER:OG	1.88	0.89
1:C:75:ALA:CB	1:C:358:HIS:HE1	1.85	0.89
1:D:257:MET:O	1:D:261:SER:OG	1.88	0.89
1:D:190:THR:CG2	1:D:193:GLN:HB2	2.03	0.89
1:C:133:ARG:NH1	1:C:161:SER:O	2.06	0.89
1:D:107:HIS:CE1	1:D:358:HIS:CD2	2.60	0.89
1:D:138:LEU:CD2	1:D:141:MET:HE2	2.02	0.89
1:A:205:LEU:O	1:A:209:VAL:HG23	1.73	0.89
1:B:90:GLN:O	1:B:90:GLN:NE2	2.05	0.89
1:B:302:ARG:HG3	1:B:302:ARG:HH11	1.38	0.89
1:C:395:VAL:HG12	1:C:396:LYS:H	1.35	0.89
1:D:173:ASP:C	1:D:174:LEU:HD23	1.98	0.88
1:A:169:ILE:CD1	1:A:178:ARG:HD3	2.01	0.88
1:D:49:LEU:HD12	1:D:84:ALA:O	1.73	0.88
1:C:138:LEU:HD23	1:C:141:MET:HE2	1.55	0.88
1:B:73:VAL:CG2	1:B:308:ILE:CD1	2.51	0.88
1:C:393:VAL:CG1	1:C:407:LEU:HD21	2.04	0.88
1:C:99:PHE:CD2	1:C:110:TYR:CB	2.57	0.87
1:C:234:VAL:HG12	1:C:238:GLN:HE21	0.72	0.87
1:C:98:PRO:HB3	1:C:245:ILE:HD13	1.55	0.87
1:D:385:ARG:HG3	1:D:386:LEU:N	1.88	0.86
1:A:219:ASP:OD1	1:A:222:SER:HB2	1.75	0.86
1:C:50:PRO:HG3	1:C:85:LEU:O	1.75	0.86
1:B:104:ALA:HB1	1:B:105:PRO:CD	2.06	0.86
1:D:263:LEU:HD12	1:D:404:LEU:HD11	1.54	0.86
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.39	0.86
1:B:123:VAL:HG22	1:B:365:LEU:HD12	1.58	0.86
1:C:49:LEU:HD13	1:C:84:ALA:O	1.74	0.86
1:C:107:HIS:NE2	1:C:358:HIS:HD2	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ARG:CD	1:C:172:HIS:HE1	1.81	0.85
1:D:257:MET:CE	1:D:290:LEU:HD23	2.06	0.85
1:A:379:ARG:NH1	1:B:276:ARG:O	2.09	0.85
1:B:212:ARG:O	1:B:216:PRO:HB3	1.75	0.85
1:C:154:TYR:O	1:C:158:VAL:HG23	1.77	0.85
1:A:251:ARG:O	1:A:255:THR:HG23	1.75	0.85
1:C:381:VAL:HG12	1:C:384:LEU:HB2	1.59	0.85
1:B:217:ARG:O	1:B:222:SER:OG	1.95	0.84
1:C:98:PRO:CB	1:C:245:ILE:CD1	2.55	0.84
1:D:102:THR:O	1:D:107:HIS:HB2	1.76	0.84
1:C:77:ILE:HA	1:C:82:PHE:HD2	1.37	0.84
1:C:171:ARG:O	1:C:174:LEU:O	1.95	0.84
1:D:98:PRO:HB2	1:D:245:ILE:CD1	2.01	0.84
1:A:77:ILE:CG2	1:A:97:ARG:HG2	2.08	0.84
1:A:223:LYS:O	1:A:227:ASP:HB2	1.78	0.84
1:C:169:ILE:CD1	1:C:178:ARG:HD2	2.07	0.84
1:B:173:ASP:C	1:B:174:LEU:HD23	2.02	0.84
1:C:98:PRO:HB3	1:C:245:ILE:CD1	2.07	0.84
1:A:169:ILE:HD13	1:A:178:ARG:HD2	1.57	0.84
1:D:107:HIS:CE1	1:D:358:HIS:HD2	1.96	0.84
1:C:217:ARG:O	1:C:219:ASP:OD1	1.94	0.84
1:D:107:HIS:CD2	1:D:358:HIS:HE2	1.95	0.84
1:B:205:LEU:O	1:B:209:VAL:HG23	1.79	0.83
1:A:174:LEU:CD1	1:A:204:LEU:HD21	2.06	0.83
1:C:313:ARG:HH11	1:C:313:ARG:HG2	1.40	0.83
1:D:84:ALA:HB1	1:D:89:GLU:HB2	1.60	0.83
1:C:374:LEU:O	1:C:378:LEU:HD13	1.76	0.83
1:C:99:PHE:CE1	1:C:100:ILE:HG13	2.13	0.83
1:C:297:ASP:OD2	1:C:326:ALA:HB3	1.79	0.83
1:D:385:ARG:HG3	1:D:386:LEU:H	1.44	0.83
1:D:394:VAL:HG12	1:D:405:GLU:HB2	1.59	0.82
1:C:95:ARG:CZ	1:C:97:ARG:HD3	2.09	0.82
1:D:75:ALA:HB2	1:D:358:HIS:HE1	1.43	0.82
1:D:381:VAL:HG12	1:D:384:LEU:HB2	1.61	0.82
1:D:190:THR:OG1	1:D:192:GLU:HG3	1.79	0.82
1:C:297:ASP:OD2	1:C:326:ALA:CB	2.28	0.82
1:D:99:PHE:HB3	1:D:110:TYR:HD2	1.45	0.82
1:D:77:ILE:HG21	1:D:97:ARG:HG2	1.61	0.82
1:D:158:VAL:O	1:D:162:VAL:HG23	1.79	0.82
1:C:386:LEU:HD21	1:C:408:MET:SD	2.19	0.81
1:C:107:HIS:CE1	1:C:358:HIS:CD2	2.67	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:NH2	1:B:338:PRO:O	2.14	0.81
1:C:363:GLN:OE1	1:C:367:ARG:NH1	2.13	0.81
1:D:98:PRO:HB3	1:D:245:ILE:HD13	1.51	0.81
1:D:257:MET:HE3	1:D:290:LEU:HD23	1.60	0.81
1:C:251:ARG:O	1:C:255:THR:HG23	1.80	0.81
1:A:92:ALA:HA	1:A:95:ARG:CG	2.10	0.81
1:C:368:LEU:HD12	1:C:368:LEU:O	1.79	0.81
1:A:212:ARG:O	1:A:216:PRO:HB3	1.79	0.81
1:D:175:GLU:OE1	3:D:612:HOH:O	1.98	0.81
1:D:234:VAL:HG13	1:D:238:GLN:HE21	1.45	0.81
1:A:73:VAL:HG23	1:A:308:ILE:CD1	2.11	0.80
1:A:239:LEU:HD23	1:A:239:LEU:O	1.81	0.80
1:C:176:PHE:O	1:C:180:VAL:HG23	1.82	0.80
1:D:238:GLN:O	1:D:242:THR:HG23	1.82	0.80
1:B:239:LEU:O	1:B:239:LEU:HD23	1.81	0.80
1:C:175:GLU:O	1:C:179:ASP:HB2	1.82	0.80
1:C:408:MET:N	1:C:408:MET:HE3	1.96	0.80
1:D:154:TYR:O	1:D:158:VAL:HG23	1.80	0.80
1:B:107:HIS:NE2	1:B:358:HIS:CD2	2.49	0.80
1:A:190:THR:HG21	1:A:193:GLN:CG	2.12	0.80
1:D:205:LEU:O	1:D:209:VAL:HG23	1.82	0.80
1:A:368:LEU:HD12	1:A:368:LEU:O	1.83	0.79
1:B:242:THR:O	1:B:246:THR:HG23	1.82	0.79
1:D:99:PHE:HB3	1:D:110:TYR:CD2	2.16	0.79
1:D:121:ARG:HG2	1:D:121:ARG:NH1	1.96	0.79
1:D:408:MET:SD	1:D:408:MET:N	2.55	0.79
1:D:57:VAL:HG23	1:D:322:ILE:HD12	1.64	0.79
1:C:190:THR:HG22	1:C:193:GLN:H	1.48	0.79
1:D:74:SER:CB	1:D:103:ASP:OD2	2.30	0.79
1:D:171:ARG:HG3	1:D:172:HIS:N	1.95	0.79
1:D:234:VAL:CG1	1:D:238:GLN:HB3	2.12	0.79
1:C:190:THR:CG2	1:C:193:GLN:HB2	2.12	0.79
1:C:190:THR:HB	1:C:193:GLN:HB2	1.65	0.79
1:C:254:THR:HG21	1:C:369:GLU:OE2	1.83	0.79
1:C:110:TYR:O	1:C:113:MET:HB3	1.82	0.79
1:C:158:VAL:O	1:C:162:VAL:HG23	1.82	0.79
1:C:299:ILE:CD1	1:C:401:THR:CG2	2.49	0.79
1:A:268:ARG:HB3	1:A:270:GLU:OE2	1.83	0.79
1:D:44:VAL:HG21	1:D:313:ARG:HB2	1.65	0.79
1:A:190:THR:HG22	1:A:193:GLN:HB2	1.44	0.78
1:B:340:ARG:NH1	3:B:621:HOH:O	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ARG:HG2	1:D:379:ARG:HH11	1.48	0.78
1:C:99:PHE:HB3	1:C:110:TYR:CD2	2.18	0.78
1:C:138:LEU:CD2	1:C:141:MET:CE	2.62	0.78
1:A:73:VAL:CG2	1:A:308:ILE:CD1	2.61	0.78
1:C:131:GLN:OE1	1:C:376:THR:HG21	1.84	0.78
1:C:378:LEU:HD12	1:C:378:LEU:H	1.48	0.78
1:D:46:ARG:HH21	1:D:54:GLU:CB	1.97	0.78
1:B:73:VAL:HG23	1:B:308:ILE:CD1	2.13	0.78
1:D:168:GLY:O	1:D:212:ARG:NH2	2.17	0.78
1:D:414:HIS:O	1:D:415:HIS:HB2	1.84	0.78
1:A:381:VAL:HG12	1:A:384:LEU:CB	2.14	0.78
1:C:260:LEU:HD11	1:C:402:PHE:HE1	1.49	0.78
1:A:107:HIS:NE2	1:A:358:HIS:CD2	2.52	0.78
1:B:302:ARG:HG3	1:B:302:ARG:NH1	1.98	0.78
1:B:316:PRO:O	1:B:319:ASP:HB2	1.83	0.78
1:D:46:ARG:HH21	1:D:54:GLU:HB2	1.48	0.78
1:D:347:ASP:OD1	3:D:601:HOH:O	2.01	0.78
1:D:394:VAL:HG12	1:D:405:GLU:CB	2.14	0.77
1:B:93:GLY:O	1:B:95:ARG:HA	1.83	0.77
1:B:253:THR:HG23	1:B:401:THR:HG21	1.67	0.77
1:D:78:ARG:HG3	1:D:78:ARG:NH1	1.99	0.77
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.84	0.77
1:A:111:ARG:NH1	1:A:359:GLN:O	2.15	0.77
1:C:107:HIS:CE1	1:C:358:HIS:HD2	2.03	0.77
1:D:111:ARG:NH1	1:D:359:GLN:O	2.15	0.77
1:D:167:LEU:HD23	1:D:221:ILE:HG13	1.67	0.77
1:D:190:THR:HG21	1:D:193:GLN:CB	2.14	0.77
1:A:242:THR:O	1:A:246:THR:HG23	1.86	0.76
1:B:111:ARG:NH1	1:B:359:GLN:O	2.17	0.76
1:A:202:PHE:HD1	1:A:240:LEU:HD12	1.49	0.76
1:B:65:ARG:O	1:B:69:SER:HB2	1.84	0.76
1:C:248:ASN:OD1	3:C:604:HOH:O	2.03	0.76
1:A:277:LYS:HE2	1:B:380:ARG:NH2	2.00	0.76
1:C:99:PHE:CD2	1:C:110:TYR:HB3	2.20	0.76
1:A:77:ILE:O	1:A:90:GLN:NE2	2.19	0.76
1:B:383:THR:HG21	1:B:412:HIS:CB	2.14	0.76
1:C:188:ASN:O	1:C:189:SER:OG	2.03	0.76
1:C:234:VAL:HG12	1:C:238:GLN:HB3	1.68	0.76
1:B:264:LEU:HD12	1:B:264:LEU:O	1.84	0.76
1:D:97:ARG:HG3	1:D:98:PRO:HD2	1.67	0.75
1:C:49:LEU:HB2	1:C:53:ARG:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:THR:HG21	1:C:412:HIS:O	1.84	0.75
1:D:381:VAL:CG1	1:D:384:LEU:HB2	2.16	0.75
1:D:395:VAL:HG12	1:D:396:LYS:N	2.00	0.75
1:A:179:ASP:O	1:A:183:ILE:HD12	1.86	0.75
1:C:174:LEU:HD13	1:C:204:LEU:CD2	2.03	0.75
1:A:253:THR:HG23	1:A:401:THR:HG21	1.67	0.75
1:B:65:ARG:NH1	1:B:355:TYR:CE2	2.40	0.75
1:C:303:VAL:HG12	1:C:319:ASP:O	1.85	0.75
1:B:78:ARG:HH11	1:B:78:ARG:HB2	1.51	0.74
1:A:242:THR:HA	1:A:245:ILE:HD12	1.69	0.74
1:D:302:ARG:HH21	1:D:358:HIS:CG	2.05	0.74
1:A:78:ARG:CB	1:A:78:ARG:HH11	1.99	0.74
1:A:92:ALA:HA	1:A:95:ARG:HD3	1.68	0.74
1:C:385:ARG:HG3	1:C:386:LEU:N	2.02	0.74
1:C:99:PHE:CD2	1:C:110:TYR:HB2	2.12	0.74
1:B:149:ASP:OD1	1:B:152:SER:OG	2.05	0.74
1:B:242:THR:HA	1:B:245:ILE:HD12	1.70	0.74
1:C:99:PHE:HB3	1:C:110:TYR:HD2	1.53	0.74
1:D:410:THR:HG22	1:D:411:TRP:N	2.02	0.74
1:A:368:LEU:O	1:A:372:VAL:HG23	1.87	0.74
1:D:156:ASN:O	1:D:160:THR:OG1	2.04	0.74
1:A:149:ASP:OD1	1:A:152:SER:OG	2.06	0.74
1:C:75:ALA:CB	1:C:358:HIS:CE1	2.69	0.74
1:A:216:PRO:HB2	1:A:222:SER:OG	1.88	0.74
1:A:258:ILE:O	1:A:262:THR:OG1	2.03	0.74
1:C:133:ARG:HD3	1:C:161:SER:OG	1.87	0.74
1:D:75:ALA:CB	1:D:358:HIS:CE1	2.69	0.74
1:D:122:ARG:NH1	1:D:122:ARG:HG2	2.02	0.73
1:D:75:ALA:O	1:D:101:ARG:O	2.07	0.73
1:D:107:HIS:NE2	1:D:358:HIS:NE2	2.34	0.73
1:D:234:VAL:CG1	1:D:238:GLN:HE21	2.01	0.73
1:D:235:THR:H	1:D:238:GLN:NE2	1.86	0.73
1:D:44:VAL:HG11	1:D:315:VAL:HG12	1.68	0.73
1:D:76:ASP:HB3	1:D:79:ARG:HG3	1.71	0.73
1:A:107:HIS:CD2	1:A:358:HIS:NE2	2.57	0.73
1:C:393:VAL:CG1	1:C:407:LEU:CD2	2.66	0.73
1:A:302:ARG:HG3	1:A:302:ARG:NH1	1.93	0.73
1:B:18:PRO:HG3	1:B:54:GLU:OE2	1.88	0.72
1:B:163:ILE:HG22	1:B:167:LEU:HD12	1.70	0.72
1:C:313:ARG:HG2	1:C:313:ARG:NH1	1.99	0.72
1:C:387:ALA:HB2	1:C:410:THR:OG1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:VAL:HG12	1:C:396:LYS:N	2.02	0.72
1:D:251:ARG:O	1:D:255:THR:CG2	2.38	0.72
1:B:133:ARG:HD3	1:B:161:SER:OG	1.89	0.72
1:C:95:ARG:HD3	1:C:97:ARG:HG2	1.70	0.72
1:D:368:LEU:O	1:D:372:VAL:HG23	1.90	0.72
1:D:124:ARG:HG3	1:D:124:ARG:HH11	1.53	0.72
1:D:317:ALA:O	1:D:318:ASP:HB2	1.89	0.72
1:C:381:VAL:CG1	1:C:384:LEU:HB2	2.18	0.72
1:C:107:HIS:HD2	1:C:358:HIS:HE2	1.35	0.72
1:D:107:HIS:CD2	1:D:358:HIS:NE2	2.57	0.72
1:D:122:ARG:HG2	1:D:122:ARG:HH11	1.52	0.72
1:C:225:VAL:O	1:C:230:VAL:HG23	1.89	0.72
1:D:49:LEU:HD13	1:D:84:ALA:O	1.90	0.72
1:A:92:ALA:O	1:A:95:ARG:HG3	1.90	0.71
1:B:368:LEU:O	1:B:372:VAL:HG23	1.90	0.71
1:A:190:THR:HG22	1:A:193:GLN:H	1.55	0.71
1:B:253:THR:HB	2:B:501:HEM:HBB2	1.72	0.71
1:C:32:PRO:HG2	1:C:35:TYR:CD1	2.25	0.71
1:C:86:GLY:N	1:C:89:GLU:OE2	2.23	0.71
1:D:190:THR:HG23	1:D:191:ALA:N	2.05	0.71
1:D:217:ARG:HG2	1:D:217:ARG:HH11	1.54	0.71
1:D:138:LEU:HD23	1:D:141:MET:CE	2.16	0.71
1:A:341:VAL:O	3:A:605:HOH:O	2.08	0.71
1:A:159:SER:CB	1:A:255:THR:HG22	2.19	0.71
1:B:126:MET:O	1:B:130:VAL:HG23	1.91	0.71
1:B:73:VAL:HG22	1:B:308:ILE:CD1	2.19	0.71
1:C:104:ALA:HB1	1:C:105:PRO:HD3	1.71	0.71
1:A:383:THR:CG2	1:A:412:HIS:HB2	2.14	0.71
1:C:190:THR:CB	1:C:193:GLN:HB2	2.20	0.71
1:D:301:LEU:HD23	1:D:322:ILE:CG2	2.07	0.71
1:A:190:THR:HG21	1:A:193:GLN:HB2	1.08	0.71
1:B:76:ASP:OD1	1:B:78:ARG:HG3	1.90	0.71
1:B:168:GLY:O	1:B:212:ARG:NH2	2.24	0.71
1:C:95:ARG:NE	1:C:97:ARG:HD3	2.06	0.71
1:C:368:LEU:HD12	1:C:372:VAL:HG23	1.72	0.71
1:D:75:ALA:HB2	1:D:358:HIS:CE1	2.26	0.71
1:A:217:ARG:HG3	1:A:217:ARG:NH1	2.02	0.71
1:A:368:LEU:HD12	1:A:372:VAL:HG23	1.73	0.71
1:A:159:SER:HB2	1:A:255:THR:HG22	1.73	0.70
1:C:125:ALA:O	1:C:128:PRO:HD2	1.90	0.70
1:D:42:ASP:OD1	1:D:42:ASP:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:GLU:OE2	1:D:376:THR:HG22	1.91	0.70
1:C:253:THR:HG23	1:C:401:THR:HG21	1.72	0.70
1:D:190:THR:HG1	1:D:193:GLN:H	1.36	0.70
1:A:276:ARG:O	1:B:379:ARG:NH1	2.24	0.70
1:A:228:HIS:C	1:A:231:PRO:HD2	2.17	0.70
1:B:136:GLU:CD	1:B:171:ARG:NH1	2.49	0.70
1:D:303:VAL:HG13	1:D:320:GLY:CA	2.22	0.70
1:D:313:ARG:HG2	1:D:313:ARG:NH1	1.99	0.70
1:B:239:LEU:HD23	1:B:239:LEU:C	2.16	0.70
1:C:99:PHE:CD1	1:C:100:ILE:HG13	2.26	0.70
1:C:149:ASP:OD2	1:C:407:LEU:N	2.25	0.69
1:D:77:ILE:HA	1:D:82:PHE:HD2	1.50	0.69
1:A:156:ASN:O	1:A:160:THR:OG1	2.10	0.69
1:B:136:GLU:CD	1:B:171:ARG:HH11	1.99	0.69
1:D:98:PRO:CB	1:D:245:ILE:HD11	2.08	0.69
1:D:23:ILE:HD13	1:D:34:GLU:HG3	1.75	0.69
1:C:299:ILE:HD11	1:C:401:THR:HG23	1.70	0.69
1:A:163:ILE:HG22	1:A:167:LEU:HD12	1.74	0.69
1:A:174:LEU:HD12	1:A:204:LEU:HD21	1.72	0.69
1:D:412:HIS:O	1:D:413:HIS:HB2	1.93	0.69
1:B:268:ARG:HB3	1:B:270:GLU:OE2	1.92	0.69
1:B:383:THR:HG21	1:B:412:HIS:H	1.58	0.69
1:B:357:VAL:HG12	3:D:609:HOH:O	1.91	0.69
1:C:75:ALA:HB3	1:C:358:HIS:HE1	1.58	0.69
1:D:186:SER:O	1:D:187:ARG:HB2	1.93	0.69
1:D:372:VAL:O	1:D:376:THR:HG23	1.93	0.69
1:D:413:HIS:CG	1:D:414:HIS:H	2.11	0.69
1:B:78:ARG:HH11	1:B:78:ARG:CB	2.06	0.69
1:A:125:ALA:O	1:A:128:PRO:HD2	1.93	0.68
1:B:410:THR:HG22	1:B:411:TRP:N	2.09	0.68
1:D:110:TYR:HD1	1:D:113:MET:CE	2.06	0.68
1:B:363:GLN:O	1:B:367:ARG:HG3	1.93	0.68
1:C:297:ASP:O	1:C:300:PRO:HD3	1.93	0.68
1:A:383:THR:HG21	1:A:412:HIS:H	1.59	0.68
1:D:110:TYR:HD1	1:D:113:MET:HE2	1.59	0.68
1:D:302:ARG:NH2	1:D:358:HIS:CG	2.60	0.68
1:C:234:VAL:HG12	1:C:238:GLN:CB	2.24	0.68
1:A:92:ALA:HA	1:A:95:ARG:CD	2.23	0.68
1:C:190:THR:HG21	1:C:193:GLN:CG	2.24	0.68
1:D:51:THR:O	1:D:52:ARG:HB2	1.94	0.68
1:C:99:PHE:CB	1:C:110:TYR:HD2	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:LEU:HD23	1:D:289:LEU:CD2	2.23	0.67
1:C:76:ASP:HB3	1:C:79:ARG:HG3	1.76	0.67
1:C:307:ASP:OD2	1:C:307:ASP:N	2.26	0.67
1:D:254:THR:HG21	1:D:369:GLU:OE2	1.95	0.67
1:D:413:HIS:O	1:D:414:HIS:ND1	2.28	0.67
1:D:217:ARG:HA	1:D:217:ARG:NE	2.09	0.67
1:A:171:ARG:O	1:A:175:GLU:HB2	1.95	0.67
1:A:20:ASP:OD2	1:A:20:ASP:N	2.19	0.67
1:A:129:ALA:O	1:A:133:ARG:HG3	1.95	0.67
1:D:138:LEU:CD2	1:D:141:MET:CE	2.73	0.67
1:A:78:ARG:HH11	1:A:78:ARG:HB2	1.60	0.67
1:A:133:ARG:O	1:A:137:ILE:HG13	1.95	0.67
1:A:241:SER:O	1:A:245:ILE:HG13	1.94	0.66
1:C:45:ALA:HB3	1:C:57:VAL:CG1	2.25	0.66
1:C:163:ILE:O	1:C:167:LEU:HB2	1.95	0.66
1:A:71:PRO:HB2	1:C:71:PRO:HB3	1.78	0.66
1:A:301:LEU:HD23	1:A:322:ILE:HG12	1.77	0.66
1:C:216:PRO:HB2	1:C:222:SER:OG	1.95	0.66
1:C:316:PRO:HG2	1:C:319:ASP:CG	2.20	0.66
1:B:383:THR:CG2	1:B:412:HIS:HB2	2.20	0.66
1:C:393:VAL:HG11	1:C:407:LEU:HD21	1.75	0.66
1:D:65:ARG:HD2	1:D:355:TYR:CE1	2.30	0.66
1:B:21:PHE:CB	1:B:22:PRO:HD3	2.21	0.66
1:D:110:TYR:O	1:D:113:MET:HB3	1.96	0.66
1:B:44:VAL:HB	1:B:313:ARG:HG3	1.76	0.66
1:D:163:ILE:O	1:D:167:LEU:HB2	1.96	0.66
1:B:108:THR:O	1:B:112:ARG:HB2	1.96	0.66
1:B:142:LEU:HD23	1:B:411:TRP:NE1	2.11	0.66
1:C:253:THR:HB	2:C:501:HEM:HBB2	1.78	0.66
1:D:52:ARG:HG3	1:D:52:ARG:NH1	1.95	0.66
1:A:235:THR:H	1:A:238:GLN:HE21	1.44	0.65
1:D:84:ALA:HB1	1:D:89:GLU:CB	2.26	0.65
1:C:50:PRO:CG	1:C:85:LEU:O	2.44	0.65
1:D:253:THR:HB	2:D:501:HEM:HBB2	1.78	0.65
1:C:89:GLU:O	1:C:92:ALA:HB3	1.96	0.65
1:C:219:ASP:OD1	1:C:219:ASP:N	2.29	0.65
1:C:384:LEU:HD13	1:C:385:ARG:N	2.11	0.65
1:C:169:ILE:HD12	1:C:178:ARG:HD2	1.77	0.65
1:C:383:THR:OG1	1:C:413:HIS:O	2.13	0.65
1:D:173:ASP:HB3	1:D:174:LEU:HD21	1.76	0.65
1:A:190:THR:HG22	1:A:190:THR:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ALA:HB2	1:A:410:THR:OG1	1.97	0.65
1:C:173:ASP:O	1:C:174:LEU:HD23	1.97	0.65
1:A:239:LEU:HD23	1:A:239:LEU:C	2.22	0.65
1:B:20:ASP:HA	1:B:48:THR:O	1.97	0.65
1:C:234:VAL:CG1	1:C:238:GLN:HB3	2.26	0.64
1:C:169:ILE:HD12	1:C:178:ARG:CD	2.27	0.64
1:D:84:ALA:HB1	1:D:89:GLU:OE1	1.97	0.64
1:D:99:PHE:CD2	1:D:110:TYR:HB2	2.31	0.64
1:D:394:VAL:CG1	1:D:405:GLU:HB3	2.28	0.64
1:C:390:ARG:O	1:C:391:ASP:HB2	1.98	0.64
1:A:84:ALA:HB1	1:A:89:GLU:HB3	1.79	0.64
1:A:92:ALA:C	1:A:95:ARG:HG3	2.21	0.64
1:B:52:ARG:NH1	1:B:52:ARG:HG3	2.13	0.64
1:C:102:THR:O	1:C:107:HIS:HB2	1.97	0.64
1:D:189:SER:C	1:D:190:THR:HG22	2.23	0.64
1:D:230:VAL:N	1:D:231:PRO:HD2	2.13	0.64
1:D:414:HIS:O	1:D:415:HIS:CB	2.45	0.64
1:A:190:THR:HG22	1:A:193:GLN:N	2.13	0.64
1:B:156:ASN:O	1:B:160:THR:OG1	2.15	0.64
1:B:234:VAL:HG13	1:B:238:GLN:HE21	1.62	0.64
1:D:46:ARG:NH2	1:D:54:GLU:CB	2.61	0.64
1:D:286:VAL:HG21	1:D:371:GLU:HB2	1.80	0.64
1:A:335:PHE:HB2	1:A:338:PRO:HB3	1.80	0.64
1:C:393:VAL:HG13	1:C:407:LEU:CD2	2.28	0.64
1:C:167:LEU:HD23	1:C:221:ILE:HG13	1.79	0.64
1:C:378:LEU:HD12	1:C:378:LEU:N	2.13	0.64
1:A:173:ASP:O	1:A:174:LEU:HD23	1.97	0.63
1:B:159:SER:O	1:B:163:ILE:HG13	1.98	0.63
1:D:52:ARG:HH11	1:D:52:ARG:CG	2.10	0.63
1:D:302:ARG:HG3	1:D:302:ARG:HH11	1.63	0.63
1:D:307:ASP:OD2	1:D:307:ASP:N	2.21	0.63
1:B:383:THR:CG2	1:B:412:HIS:H	2.11	0.63
1:C:145:GLY:HA2	1:C:411:TRP:CZ2	2.33	0.63
1:C:336:ASP:O	1:C:345:ARG:NH2	2.31	0.63
1:A:163:ILE:O	1:A:167:LEU:HB2	1.97	0.63
1:B:390:ARG:NH1	1:B:393:VAL:HG21	2.13	0.63
1:B:113:MET:HG3	1:B:228:HIS:CE1	2.33	0.63
1:A:73:VAL:HG23	1:A:308:ILE:HD13	1.80	0.63
1:A:77:ILE:HA	1:A:82:PHE:CD2	2.34	0.63
1:C:368:LEU:HD12	1:C:368:LEU:C	2.24	0.63
1:D:59:THR:HG22	1:D:327:GLY:HA3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLU:O	1:D:179:ASP:N	2.30	0.63
1:A:70:ASP:OD1	1:A:72:ARG:N	2.27	0.63
1:A:86:GLY:HA3	1:A:89:GLU:OE2	1.98	0.63
1:C:264:LEU:HD23	1:C:289:LEU:CD2	2.29	0.63
1:D:190:THR:CG2	1:D:191:ALA:H	2.05	0.63
1:D:386:LEU:CD2	1:D:408:MET:SD	2.84	0.63
1:D:63:ASP:O	1:D:67:LEU:HB2	1.98	0.63
1:A:169:ILE:CD1	1:A:178:ARG:HD2	2.24	0.62
1:C:169:ILE:HD13	1:C:178:ARG:HD2	1.80	0.62
1:C:248:ASN:OD1	1:C:249:ALA:N	2.32	0.62
1:A:190:THR:HG22	1:A:193:GLN:CA	2.28	0.62
1:A:235:THR:H	1:A:238:GLN:NE2	1.96	0.62
1:B:149:ASP:HA	1:B:407:LEU:O	2.00	0.62
1:C:169:ILE:CD1	1:C:178:ARG:CD	2.76	0.62
1:D:61:TYR:CE1	1:D:334:GLN:HG3	2.34	0.62
1:D:104:ALA:CB	1:D:105:PRO:HD2	2.19	0.62
1:C:396:LYS:HE2	1:C:399:SER:HB2	1.81	0.62
1:B:159:SER:CB	1:B:255:THR:HG22	2.29	0.62
1:C:110:TYR:HD1	1:C:113:MET:CE	2.10	0.62
1:D:133:ARG:HH12	1:D:164:CYS:HB2	1.62	0.62
1:C:241:SER:O	1:C:245:ILE:HG13	1.99	0.62
1:D:222:SER:O	1:D:226:THR:OG1	2.16	0.62
1:D:291:ARG:HG3	1:D:292:VAL:N	2.14	0.62
1:A:169:ILE:HG21	1:A:178:ARG:HD3	1.82	0.62
1:A:202:PHE:CD1	1:A:240:LEU:HD12	2.33	0.62
1:B:86:GLY:HA3	1:B:89:GLU:HG3	1.82	0.62
1:C:32:PRO:HG2	1:C:35:TYR:CE1	2.35	0.62
1:A:108:THR:O	1:A:112:ARG:HB2	2.00	0.62
1:C:122:ARG:HG2	1:C:122:ARG:HH11	1.64	0.61
1:D:57:VAL:CG2	1:D:322:ILE:CD1	2.69	0.61
1:A:71:PRO:CB	1:C:71:PRO:HB3	2.30	0.61
1:B:125:ALA:O	1:B:128:PRO:HD2	2.00	0.61
1:D:149:ASP:OD2	1:D:407:LEU:N	2.28	0.61
1:A:21:PHE:CB	1:A:22:PRO:HD3	2.29	0.61
1:B:18:PRO:O	1:B:48:THR:OG1	2.15	0.61
1:C:234:VAL:HA	1:C:238:GLN:NE2	2.16	0.61
1:D:73:VAL:CG2	1:D:308:ILE:CD1	2.78	0.61
1:D:190:THR:HB	1:D:193:GLN:HB2	1.82	0.61
1:D:396:LYS:HD2	1:D:399:SER:HB2	1.82	0.61
1:B:107:HIS:CD2	1:B:358:HIS:NE2	2.69	0.61
1:B:223:LYS:O	1:B:227:ASP:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ASP:C	1:C:228:HIS:HD2	2.08	0.61
1:C:386:LEU:CD2	1:C:408:MET:O	2.44	0.61
1:D:182:ARG:HE	1:D:251:ARG:HD3	1.66	0.61
1:D:190:THR:HG23	1:D:194:VAL:HG23	1.81	0.61
1:D:410:THR:HG22	1:D:411:TRP:H	1.64	0.61
1:B:230:VAL:CB	1:B:231:PRO:HD3	2.29	0.61
1:D:46:ARG:NH2	1:D:54:GLU:HB3	2.16	0.61
1:A:295:VAL:HG13	1:A:402:PHE:O	2.00	0.61
1:C:297:ASP:OD2	1:C:326:ALA:HB2	2.00	0.61
1:C:406:GLU:O	1:C:407:LEU:HD23	2.00	0.61
1:B:217:ARG:HG2	1:B:217:ARG:HH11	1.65	0.61
1:A:149:ASP:HA	1:A:407:LEU:O	2.01	0.61
1:A:335:PHE:O	1:A:338:PRO:HD3	1.99	0.61
1:C:52:ARG:CG	1:C:52:ARG:HH11	2.14	0.61
1:D:190:THR:HG1	1:D:192:GLU:HG3	1.65	0.61
1:A:92:ALA:HA	1:A:95:ARG:HG3	1.82	0.61
1:A:176:PHE:O	1:A:180:VAL:CG2	2.49	0.61
1:B:301:LEU:CD2	1:B:322:ILE:HG12	2.30	0.61
1:B:73:VAL:HG23	1:B:308:ILE:HD13	1.82	0.61
1:A:410:THR:HG22	1:A:411:TRP:H	1.66	0.60
1:C:44:VAL:HG12	1:C:44:VAL:O	2.00	0.60
1:C:235:THR:H	1:C:238:GLN:NE2	2.00	0.60
1:D:145:GLY:HA2	1:D:411:TRP:CZ2	2.37	0.60
1:A:202:PHE:HD1	1:A:240:LEU:CD1	2.12	0.60
1:B:73:VAL:HG22	1:B:308:ILE:HD12	1.84	0.60
1:A:264:LEU:HD12	1:A:264:LEU:O	2.00	0.60
1:A:383:THR:HG21	1:A:412:HIS:CB	2.14	0.60
1:C:95:ARG:NH2	1:C:96:PHE:O	2.33	0.60
1:C:291:ARG:HG3	1:C:292:VAL:N	2.15	0.60
1:C:190:THR:HG21	1:C:193:GLN:HG2	1.84	0.60
1:C:205:LEU:O	1:C:209:VAL:HG23	2.01	0.60
1:D:21:PHE:HB2	1:D:47:VAL:CG2	2.31	0.60
1:D:234:VAL:HG13	1:D:238:GLN:NE2	2.16	0.60
1:D:250:GLY:CA	2:D:501:HEM:HBC2	2.18	0.60
1:A:95:ARG:HB2	1:A:95:ARG:CZ	2.30	0.60
1:B:253:THR:CG2	1:B:401:THR:HG21	2.32	0.60
1:B:390:ARG:HH11	1:B:393:VAL:HG21	1.67	0.60
1:C:75:ALA:HB2	1:C:358:HIS:HE1	1.64	0.60
1:B:190:THR:HG22	1:B:193:GLN:CB	2.32	0.60
1:C:82:PHE:CD1	1:C:83:PRO:HD2	2.36	0.60
1:C:149:ASP:CG	1:C:406:GLU:HG2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:PHE:HD1	1:D:83:PRO:N	2.00	0.60
1:D:95:ARG:NE	1:D:96:PHE:O	2.33	0.60
1:D:316:PRO:O	1:D:319:ASP:HB2	2.01	0.60
1:C:111:ARG:NH2	1:C:359:GLN:O	2.34	0.60
1:D:264:LEU:HD23	1:D:289:LEU:HD21	1.82	0.60
1:D:394:VAL:CG1	1:D:405:GLU:CB	2.80	0.60
1:A:159:SER:O	1:A:163:ILE:HG13	2.02	0.60
1:A:162:VAL:HG11	1:A:369:GLU:HG3	1.83	0.60
1:B:291:ARG:HG3	1:B:292:VAL:N	2.16	0.60
1:C:299:ILE:HD12	1:C:401:THR:HG22	1.79	0.60
1:B:115:LEU:HD23	1:B:361:VAL:HG13	1.84	0.59
1:B:173:ASP:O	1:B:174:LEU:HD23	2.00	0.59
1:C:95:ARG:CD	1:C:97:ARG:HD3	2.31	0.59
1:C:113:MET:SD	1:C:228:HIS:CE1	2.95	0.59
1:D:77:ILE:CA	1:D:82:PHE:CD2	2.70	0.59
1:D:290:LEU:HD13	1:D:353:PHE:CE2	2.37	0.59
1:A:301:LEU:CD2	1:A:322:ILE:HG12	2.31	0.59
1:B:78:ARG:HD3	1:B:97:ARG:HE	1.66	0.59
1:D:178:ARG:NH1	1:D:178:ARG:HG2	2.17	0.59
1:D:302:ARG:HH11	1:D:302:ARG:CG	2.15	0.59
1:A:316:PRO:O	1:A:319:ASP:HB2	2.02	0.59
1:B:123:VAL:CG2	1:B:365:LEU:HD12	2.31	0.59
1:C:63:ASP:O	1:C:67:LEU:HB2	2.02	0.59
1:C:238:GLN:O	1:C:242:THR:HG23	2.02	0.59
1:C:316:PRO:O	1:C:319:ASP:HB2	2.01	0.59
1:D:174:LEU:CD1	1:D:204:LEU:HD21	2.32	0.59
1:A:59:THR:HG23	1:A:324:LEU:HD23	1.84	0.59
1:C:77:ILE:CA	1:C:82:PHE:HD2	2.13	0.59
1:D:49:LEU:HD11	1:D:84:ALA:O	1.96	0.59
1:D:84:ALA:CB	1:D:89:GLU:HB2	2.30	0.59
1:D:122:ARG:HH11	1:D:122:ARG:CG	2.16	0.59
1:A:307:ASP:OD2	1:A:307:ASP:N	2.35	0.59
1:A:336:ASP:O	1:A:345:ARG:NH2	2.35	0.59
1:B:20:ASP:OD2	1:B:20:ASP:N	2.24	0.59
1:B:111:ARG:HD2	2:B:501:HEM:O2D	2.02	0.59
1:B:117:ALA:O	1:B:122:ARG:HD3	2.03	0.59
1:B:243:LEU:O	1:B:247:ILE:HG13	2.03	0.59
1:C:209:VAL:HG13	1:C:225:VAL:CG2	2.33	0.59
1:C:234:VAL:HA	1:C:238:GLN:HE22	1.67	0.59
1:A:182:ARG:HH22	1:A:248:ASN:HD21	1.51	0.59
1:A:381:VAL:HG12	1:A:381:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ILE:HD12	1:C:82:PHE:CE2	2.37	0.59
1:B:52:ARG:HH11	1:B:52:ARG:CG	2.16	0.58
1:B:368:LEU:O	1:B:368:LEU:HD12	2.03	0.58
1:C:263:LEU:HD12	1:C:404:LEU:HD11	1.84	0.58
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.68	0.58
1:D:21:PHE:HB2	1:D:47:VAL:HB	1.85	0.58
1:B:190:THR:HG22	1:B:190:THR:O	2.03	0.58
1:B:235:THR:H	1:B:238:GLN:HE21	1.51	0.58
1:C:92:ALA:O	1:C:97:ARG:HG2	2.03	0.58
1:C:281:LEU:HD13	1:C:343:PHE:HB3	1.86	0.58
1:D:291:ARG:O	1:D:294:SER:OG	2.21	0.58
1:A:389:GLU:OE2	1:A:390:ARG:N	2.36	0.58
1:B:202:PHE:HD1	1:B:240:LEU:HD12	1.68	0.58
1:C:301:LEU:O	1:C:302:ARG:HG2	2.03	0.58
1:D:95:ARG:HD3	1:D:95:ARG:O	2.03	0.58
1:D:253:THR:HG23	1:D:401:THR:HG21	1.84	0.58
1:D:260:LEU:HD11	1:D:402:PHE:HE1	1.68	0.58
1:A:220:LEU:CD2	1:A:224:LEU:HG	2.33	0.58
1:A:309:GLU:O	1:A:310:LEU:HD23	2.04	0.58
1:C:82:PHE:HD1	1:C:83:PRO:N	2.02	0.58
1:B:46:ARG:HH11	1:B:56:TRP:NE1	2.01	0.58
1:D:388:GLY:HA3	1:D:408:MET:HE2	1.85	0.58
1:C:21:PHE:C	1:C:21:PHE:CD2	2.80	0.58
1:C:36:ALA:O	1:C:40:THR:OG1	2.22	0.58
1:C:167:LEU:O	1:C:221:ILE:HG13	2.04	0.58
1:D:242:THR:O	1:D:246:THR:HG23	2.03	0.58
1:D:248:ASN:OD1	1:D:249:ALA:N	2.37	0.58
1:D:307:ASP:HB3	1:D:316:PRO:HA	1.86	0.58
1:C:76:ASP:OD1	1:C:78:ARG:HD2	2.03	0.58
1:C:227:ASP:C	1:C:228:HIS:CD2	2.81	0.58
1:D:21:PHE:C	1:D:21:PHE:CD2	2.82	0.58
1:D:173:ASP:HB3	1:D:174:LEU:HD23	1.86	0.58
1:D:178:ARG:HG2	1:D:178:ARG:HH11	1.69	0.58
1:A:176:PHE:O	1:A:180:VAL:HG22	2.04	0.57
1:B:230:VAL:HB	1:B:231:PRO:HD3	1.84	0.57
1:C:99:PHE:CD1	1:C:100:ILE:N	2.71	0.57
1:D:149:ASP:HA	1:D:407:LEU:O	2.04	0.57
1:D:234:VAL:HG13	1:D:238:GLN:HB3	1.86	0.57
1:B:73:VAL:CG2	1:B:308:ILE:HD13	2.33	0.57
1:B:190:THR:CG2	1:B:193:GLN:CB	2.83	0.57
1:B:390:ARG:O	1:B:391:ASP:CG	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ASP:O	1:D:82:PHE:CD2	2.57	0.57
1:D:99:PHE:CB	1:D:110:TYR:HD2	2.14	0.57
1:B:70:ASP:OD1	1:B:72:ARG:N	2.32	0.57
1:B:234:VAL:CG1	1:B:238:GLN:HB2	2.34	0.57
1:B:390:ARG:O	1:B:391:ASP:OD2	2.22	0.57
1:D:121:ARG:HH11	1:D:121:ARG:CG	2.08	0.57
1:A:92:ALA:CA	1:A:95:ARG:HG3	2.34	0.57
1:B:207:GLY:O	1:B:211:GLU:HB2	2.04	0.57
1:C:23:ILE:HD13	1:C:34:GLU:HG3	1.85	0.57
1:C:75:ALA:HB2	1:C:358:HIS:CE1	2.38	0.57
1:C:408:MET:O	1:C:408:MET:HG2	2.04	0.57
1:C:65:ARG:O	1:C:69:SER:OG	2.23	0.57
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.19	0.57
1:D:379:ARG:HG2	1:D:379:ARG:NH1	2.17	0.57
1:A:104:ALA:CB	1:A:105:PRO:HD2	2.29	0.57
1:C:172:HIS:O	1:C:173:ASP:C	2.48	0.57
1:A:103:ASP:O	1:A:104:ALA:HB3	2.04	0.57
1:A:174:LEU:HD23	1:A:174:LEU:N	2.20	0.57
1:A:381:VAL:HG11	1:A:384:LEU:HB2	1.86	0.57
1:C:171:ARG:CD	1:C:172:HIS:ND1	2.59	0.57
1:D:95:ARG:HE	1:D:95:ARG:C	2.13	0.57
1:A:65:ARG:O	1:A:69:SER:CB	2.53	0.57
1:B:104:ALA:CB	1:B:105:PRO:HD2	2.26	0.57
1:A:65:ARG:O	1:A:69:SER:HB3	2.05	0.57
1:A:410:THR:HG22	1:A:411:TRP:N	2.19	0.57
1:B:260:LEU:HD11	1:B:402:PHE:CE1	2.39	0.57
1:D:75:ALA:HB3	1:D:358:HIS:HE1	1.69	0.57
1:A:21:PHE:O	1:A:23:ILE:CG1	2.53	0.56
1:A:186:SER:O	1:A:187:ARG:HB2	2.05	0.56
1:A:368:LEU:HD12	1:A:372:VAL:CG2	2.35	0.56
1:B:150:LEU:HD12	1:B:409:VAL:HG21	1.86	0.56
1:C:110:TYR:HD1	1:C:113:MET:HE2	1.69	0.56
1:C:317:ALA:O	1:C:318:ASP:HB2	2.04	0.56
1:D:282:MET:O	1:D:286:VAL:HG23	2.05	0.56
1:B:163:ILE:O	1:B:167:LEU:HB2	2.04	0.56
1:A:257:MET:HE2	1:A:295:VAL:HG23	1.86	0.56
1:A:300:PRO:HB3	2:A:501:HEM:O1A	2.06	0.56
1:D:297:ASP:O	1:D:299:ILE:N	2.35	0.56
1:C:73:VAL:HG22	1:C:308:ILE:CD1	2.35	0.56
1:D:99:PHE:HD1	1:D:99:PHE:H	1.54	0.56
1:B:129:ALA:O	1:B:133:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:THR:HG22	1:B:383:THR:O	2.04	0.56
1:C:103:ASP:O	1:C:104:ALA:HB3	2.05	0.56
1:D:227:ASP:C	1:D:228:HIS:CD2	2.84	0.56
1:A:44:VAL:HG12	1:A:44:VAL:O	2.06	0.56
1:A:288:GLU:OE2	1:A:345:ARG:HG3	2.04	0.56
1:C:61:TYR:CE1	1:C:334:GLN:HG3	2.41	0.56
1:C:175:GLU:HA	1:C:178:ARG:HB2	1.88	0.56
1:A:21:PHE:O	1:A:23:ILE:HG12	2.05	0.56
1:A:222:SER:O	1:A:226:THR:OG1	2.24	0.56
1:A:383:THR:CG2	1:A:412:HIS:H	2.18	0.56
1:D:167:LEU:CD2	1:D:221:ILE:HG13	2.35	0.56
1:D:301:LEU:CD2	1:D:322:ILE:CG2	2.74	0.56
1:A:382:PRO:HB2	1:B:382:PRO:HB2	1.88	0.56
1:B:56:TRP:O	1:B:321:VAL:HA	2.06	0.56
1:C:45:ALA:O	1:C:57:VAL:HG12	2.06	0.56
1:C:84:ALA:HB1	1:C:89:GLU:HB2	1.86	0.56
1:C:159:SER:CB	1:C:255:THR:HG22	2.35	0.56
1:C:209:VAL:HG13	1:C:225:VAL:HG22	1.87	0.56
1:A:104:ALA:CB	1:A:105:PRO:CD	2.81	0.56
1:C:99:PHE:CE1	1:C:100:ILE:CG1	2.87	0.56
1:A:46:ARG:HB2	1:A:56:TRP:CZ3	2.39	0.56
1:C:137:ILE:HD13	1:C:157:ALA:CB	2.36	0.56
1:A:78:ARG:HH11	1:A:78:ARG:CG	2.19	0.55
1:B:103:ASP:O	1:B:104:ALA:HB3	2.05	0.55
1:B:288:GLU:OE2	1:B:345:ARG:HD2	2.06	0.55
1:C:138:LEU:HD21	1:C:141:MET:HE2	1.85	0.55
1:D:25:ARG:HD3	1:D:402:PHE:CD2	2.41	0.55
1:D:76:ASP:O	1:D:82:PHE:HD2	1.89	0.55
1:D:124:ARG:HG3	1:D:124:ARG:NH1	2.21	0.55
1:B:104:ALA:CB	1:B:105:PRO:CD	2.82	0.55
1:B:179:ASP:O	1:B:183:ILE:HD12	2.06	0.55
1:C:98:PRO:HB3	1:C:245:ILE:HD11	1.86	0.55
1:B:171:ARG:O	1:B:175:GLU:HB2	2.07	0.55
1:C:261:SER:O	1:C:264:LEU:HB3	2.06	0.55
1:D:173:ASP:HB3	1:D:174:LEU:CG	2.36	0.55
1:D:296:ALA:O	1:D:299:ILE:HG12	2.06	0.55
1:A:253:THR:HB	2:A:501:HEM:HBB2	1.88	0.55
1:C:57:VAL:HG22	1:C:324:LEU:HD22	1.88	0.55
1:C:297:ASP:OD1	1:C:298:SER:N	2.39	0.55
1:D:261:SER:HB3	1:D:289:LEU:HD13	1.87	0.55
1:A:301:LEU:HD23	1:A:322:ILE:HG23	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:PHE:HB2	1:C:47:VAL:HB	1.89	0.55
1:A:182:ARG:NH2	1:A:248:ASN:ND2	2.55	0.55
1:B:234:VAL:HG13	1:B:238:GLN:NE2	2.22	0.55
1:C:227:ASP:HB3	1:C:228:HIS:HD2	1.72	0.55
1:D:260:LEU:O	1:D:260:LEU:HD23	2.06	0.55
1:A:32:PRO:HG2	1:A:35:TYR:CE1	2.42	0.55
1:C:132:ALA:HA	3:C:624:HOH:O	2.07	0.55
1:C:168:GLY:O	1:C:212:ARG:NH2	2.39	0.55
1:D:174:LEU:HD13	1:D:204:LEU:HD21	1.88	0.55
1:A:70:ASP:OD1	1:A:71:PRO:HD2	2.06	0.55
1:B:133:ARG:O	1:B:137:ILE:HG13	2.07	0.55
1:B:174:LEU:HD13	1:B:204:LEU:HD11	1.88	0.55
1:D:133:ARG:HH11	1:D:161:SER:C	2.11	0.55
1:D:169:ILE:HD13	1:D:208:LEU:CD1	2.37	0.55
1:A:123:VAL:HG22	1:A:365:LEU:HD12	1.89	0.55
1:A:130:VAL:O	1:A:134:VAL:HG23	2.07	0.55
1:B:368:LEU:HD12	1:B:372:VAL:HG23	1.89	0.55
1:C:188:ASN:OD1	1:C:188:ASN:N	2.38	0.55
1:B:73:VAL:HG23	1:B:308:ILE:HD11	1.86	0.54
1:C:56:TRP:NE1	1:C:316:PRO:HD2	2.22	0.54
1:C:159:SER:HB2	1:C:255:THR:HG22	1.88	0.54
1:C:386:LEU:HD23	1:C:387:ALA:H	1.73	0.54
1:D:212:ARG:O	1:D:216:PRO:HB3	2.07	0.54
1:A:73:VAL:CG1	1:A:302:ARG:HB3	2.38	0.54
1:B:59:THR:HG23	1:B:324:LEU:HD23	1.90	0.54
1:B:93:GLY:C	1:B:95:ARG:HA	2.32	0.54
1:B:217:ARG:HH11	1:B:217:ARG:CG	2.20	0.54
1:D:34:GLU:CD	1:D:34:GLU:H	2.14	0.54
1:A:56:TRP:HE1	1:A:316:PRO:HD2	1.71	0.54
1:C:59:THR:HG22	1:C:327:GLY:HA3	1.89	0.54
1:B:36:ALA:O	1:B:40:THR:HG23	2.06	0.54
1:C:299:ILE:H	1:C:300:PRO:HD3	1.72	0.54
1:D:173:ASP:O	1:D:174:LEU:HD23	2.06	0.54
1:A:73:VAL:HG23	1:A:308:ILE:HD11	1.86	0.54
1:B:96:PHE:CD1	1:B:96:PHE:C	2.85	0.54
1:B:115:LEU:N	1:B:116:PRO:HD2	2.21	0.54
1:C:73:VAL:CG2	1:C:308:ILE:HD13	2.38	0.54
1:A:256:SER:O	1:A:260:LEU:HB2	2.08	0.54
1:B:64:VAL:HG13	1:B:323:ALA:HB1	1.90	0.54
1:A:136:GLU:OE2	1:A:171:ARG:NH1	2.41	0.54
1:B:21:PHE:O	1:B:23:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PHE:O	1:B:180:VAL:HG23	2.08	0.54
1:D:217:ARG:NH1	1:D:217:ARG:HG2	2.22	0.54
1:A:126:MET:O	1:A:130:VAL:HG23	2.08	0.54
1:C:139:ASP:OD1	1:C:380:ARG:NH1	2.38	0.54
1:A:296:ALA:HB1	1:A:299:ILE:HG12	1.89	0.54
1:B:234:VAL:HG13	1:B:238:GLN:CB	2.38	0.54
1:C:408:MET:N	1:C:408:MET:CE	2.71	0.54
1:D:103:ASP:O	1:D:104:ALA:HB3	2.08	0.54
1:C:57:VAL:CG2	1:C:324:LEU:HD21	2.39	0.53
1:C:65:ARG:HD2	1:C:355:TYR:CE1	2.44	0.53
1:D:227:ASP:HB3	1:D:228:HIS:CD2	2.43	0.53
1:B:21:PHE:O	1:B:23:ILE:CG1	2.56	0.53
1:B:234:VAL:HG12	1:B:235:THR:O	2.08	0.53
1:C:126:MET:O	1:C:130:VAL:HG23	2.09	0.53
1:C:142:LEU:HA	1:C:411:TRP:CZ2	2.44	0.53
1:D:390:ARG:O	1:D:391:ASP:HB2	2.09	0.53
1:A:77:ILE:HG23	1:A:97:ARG:HG2	1.88	0.53
1:B:301:LEU:HD23	1:B:322:ILE:HG23	1.90	0.53
1:C:361:VAL:HG23	2:C:501:HEM:HBD2	1.90	0.53
1:D:234:VAL:CG1	1:D:238:GLN:CB	2.85	0.53
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.20	0.53
1:B:386:LEU:HD23	1:B:408:MET:O	2.09	0.53
1:C:313:ARG:HH11	1:C:313:ARG:CG	2.15	0.53
1:D:44:VAL:CG2	1:D:313:ARG:HB2	2.35	0.53
1:D:229:LEU:HD12	1:D:234:VAL:O	2.09	0.53
1:A:34:GLU:H	1:A:34:GLU:CD	2.16	0.53
1:A:138:LEU:O	1:A:142:LEU:HB2	2.08	0.53
1:C:25:ARG:HD3	1:C:402:PHE:CD2	2.43	0.53
1:D:410:THR:CG2	1:D:411:TRP:N	2.71	0.53
1:B:21:PHE:C	1:B:21:PHE:CD2	2.84	0.53
1:B:235:THR:H	1:B:238:GLN:NE2	2.06	0.53
1:C:46:ARG:NH2	1:C:54:GLU:HB3	2.23	0.53
1:C:110:TYR:HA	1:C:113:MET:HE2	1.91	0.53
1:C:82:PHE:HD1	1:C:82:PHE:C	2.17	0.53
1:C:149:ASP:HA	1:C:407:LEU:O	2.09	0.53
1:C:228:HIS:C	1:C:231:PRO:HD2	2.33	0.53
1:C:368:LEU:HD12	1:C:372:VAL:CG2	2.39	0.53
1:D:104:ALA:CB	1:D:105:PRO:CD	2.81	0.53
1:D:149:ASP:OD1	1:D:406:GLU:HG2	2.09	0.53
1:D:260:LEU:HD11	1:D:402:PHE:CE1	2.43	0.53
1:D:374:LEU:O	1:D:378:LEU:HG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD12	1:A:368:LEU:C	2.33	0.52
1:C:167:LEU:HD11	1:C:247:ILE:HD11	1.91	0.52
1:C:410:THR:HG22	1:C:411:TRP:N	2.25	0.52
1:A:73:VAL:HG22	1:A:308:ILE:CD1	2.39	0.52
1:B:190:THR:CG2	1:B:193:GLN:HB2	2.39	0.52
1:B:336:ASP:O	1:B:345:ARG:NH2	2.42	0.52
1:C:86:GLY:H	1:C:89:GLU:CD	2.17	0.52
1:C:190:THR:CG2	1:C:193:GLN:CB	2.86	0.52
1:D:138:LEU:HD13	1:D:380:ARG:HG3	1.92	0.52
1:A:56:TRP:HB2	1:A:321:VAL:HG13	1.92	0.52
1:C:57:VAL:HG13	1:C:57:VAL:O	2.09	0.52
1:C:242:THR:O	1:C:246:THR:HG23	2.09	0.52
1:A:21:PHE:C	1:A:21:PHE:CD2	2.85	0.52
1:A:389:GLU:HB3	1:A:392:GLN:HG3	1.91	0.52
1:B:21:PHE:HB3	1:B:22:PRO:CD	2.31	0.52
1:B:302:ARG:HH11	1:B:302:ARG:CG	2.15	0.52
1:D:82:PHE:CD1	1:D:83:PRO:CD	2.92	0.52
1:D:381:VAL:HG12	1:D:384:LEU:CB	2.37	0.52
1:B:71:PRO:HB3	1:D:71:PRO:HB3	1.91	0.52
1:B:190:THR:CG2	1:B:193:GLN:HB3	2.39	0.52
1:B:410:THR:CG2	1:B:411:TRP:N	2.72	0.52
1:C:301:LEU:CD2	1:C:322:ILE:HG23	2.27	0.52
1:D:316:PRO:HG2	1:D:319:ASP:CG	2.35	0.52
1:D:395:VAL:CG1	1:D:396:LYS:H	2.16	0.52
1:A:317:ALA:O	1:A:318:ASP:HB2	2.08	0.52
1:B:315:VAL:HG23	1:B:315:VAL:O	2.09	0.52
1:C:368:LEU:O	1:C:372:VAL:HG23	2.10	0.52
1:D:256:SER:OG	1:D:403:GLY:CA	2.58	0.52
1:B:39:ARG:O	1:B:60:ARG:NE	2.33	0.52
1:B:137:ILE:HD13	1:B:157:ALA:HB1	1.92	0.52
1:C:91:GLU:O	1:C:91:GLU:HG2	2.07	0.52
1:D:44:VAL:HG23	1:D:313:ARG:HG3	1.90	0.52
1:A:133:ARG:NH1	1:A:161:SER:O	2.43	0.52
1:A:312:GLY:HA3	3:A:616:HOH:O	2.10	0.52
1:B:183:ILE:O	1:B:187:ARG:HD3	2.10	0.52
1:C:299:ILE:N	1:C:300:PRO:HD3	2.24	0.52
1:C:353:PHE:HB3	1:C:360:CYS:HB3	1.92	0.52
1:A:117:ALA:O	1:A:122:ARG:HD2	2.10	0.52
1:C:301:LEU:C	1:C:302:ARG:CG	2.83	0.52
1:C:368:LEU:CD1	1:C:372:VAL:CG2	2.88	0.52
1:C:386:LEU:HD23	1:C:387:ALA:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:PHE:O	1:D:180:VAL:CG2	2.46	0.52
1:A:177:PHE:C	1:A:177:PHE:CD2	2.85	0.52
1:B:268:ARG:O	1:B:272:PRO:HD2	2.10	0.52
1:D:182:ARG:HE	1:D:251:ARG:CD	2.23	0.52
1:D:257:MET:HE3	1:D:290:LEU:CD2	2.36	0.52
1:D:261:SER:O	1:D:264:LEU:HB3	2.10	0.52
1:B:51:THR:O	1:B:52:ARG:HB2	2.10	0.51
1:D:82:PHE:CD1	1:D:82:PHE:C	2.87	0.51
1:D:302:ARG:NH2	1:D:358:HIS:CB	2.73	0.51
1:D:377:LEU:O	1:D:377:LEU:HD12	2.10	0.51
1:A:177:PHE:O	1:A:180:VAL:HG23	2.09	0.51
1:B:21:PHE:CB	1:B:22:PRO:CD	2.89	0.51
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.25	0.51
1:C:99:PHE:CB	1:C:110:TYR:CD2	2.88	0.51
1:D:95:ARG:CZ	1:D:97:ARG:HH11	2.23	0.51
1:D:138:LEU:CD1	1:D:380:ARG:HG3	2.40	0.51
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.74	0.51
1:A:238:GLN:O	1:A:241:SER:OG	2.26	0.51
1:C:402:PHE:CD1	1:C:402:PHE:C	2.88	0.51
1:D:124:ARG:HH11	1:D:124:ARG:CG	2.22	0.51
1:D:384:LEU:CD1	1:D:384:LEU:C	2.83	0.51
1:B:288:GLU:OE2	1:B:345:ARG:HG3	2.11	0.51
1:C:138:LEU:HD23	1:C:141:MET:CE	2.31	0.51
1:D:77:ILE:HD12	1:D:82:PHE:CE2	2.46	0.51
1:D:256:SER:O	1:D:260:LEU:HB2	2.11	0.51
1:A:61:TYR:CD1	1:A:61:TYR:C	2.89	0.51
1:B:44:VAL:HG12	1:B:44:VAL:O	2.11	0.51
1:B:46:ARG:NH1	1:B:56:TRP:NE1	2.59	0.51
1:D:220:LEU:HD22	1:D:220:LEU:O	2.10	0.51
1:D:256:SER:OG	1:D:403:GLY:HA2	2.10	0.51
1:C:87:GLU:N	1:C:87:GLU:CD	2.69	0.51
1:C:234:VAL:CA	1:C:238:GLN:NE2	2.74	0.51
1:B:57:VAL:HG22	1:B:324:LEU:HD11	1.93	0.51
1:B:120:VAL:O	1:B:124:ARG:HB2	2.11	0.51
1:B:381:VAL:HG12	1:B:381:VAL:O	2.10	0.51
1:C:84:ALA:CB	1:C:89:GLU:OE1	2.50	0.51
1:C:260:LEU:HD11	1:C:402:PHE:CE1	2.37	0.51
1:D:78:ARG:HH11	1:D:78:ARG:CG	2.10	0.51
1:D:99:PHE:CE1	1:D:100:ILE:HG13	2.46	0.51
1:A:175:GLU:CD	1:A:179:ASP:OD2	2.54	0.50
1:D:96:PHE:HD1	1:D:96:PHE:N	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLU:O	1:D:179:ASP:HB2	2.11	0.50
1:A:57:VAL:HG23	1:A:322:ILE:HB	1.93	0.50
1:C:82:PHE:CD1	1:C:82:PHE:C	2.87	0.50
1:D:82:PHE:HD1	1:D:82:PHE:C	2.19	0.50
1:D:208:LEU:O	1:D:212:ARG:HG2	2.11	0.50
1:A:137:ILE:HD13	1:A:157:ALA:HB1	1.94	0.50
1:B:347:ASP:OD1	3:B:610:HOH:O	2.18	0.50
1:C:384:LEU:CD1	1:C:384:LEU:C	2.84	0.50
1:B:77:ILE:HG13	1:B:77:ILE:O	2.11	0.50
1:B:169:ILE:HD13	1:B:178:ARG:HD2	1.88	0.50
1:B:395:VAL:HG23	1:B:395:VAL:O	2.10	0.50
1:C:49:LEU:HD11	1:C:84:ALA:O	2.07	0.50
1:B:73:VAL:CG2	1:B:308:ILE:HD11	2.34	0.50
1:B:390:ARG:HH11	1:B:393:VAL:CG2	2.24	0.50
1:C:52:ARG:CG	1:C:52:ARG:NH1	2.74	0.50
1:C:395:VAL:O	1:C:396:LYS:HG2	2.11	0.50
1:A:384:LEU:HD13	1:A:384:LEU:C	2.37	0.50
1:B:296:ALA:O	1:B:299:ILE:HG12	2.11	0.50
1:C:260:LEU:HD23	1:C:260:LEU:O	2.11	0.50
1:D:52:ARG:HD2	1:D:52:ARG:N	2.26	0.50
1:D:87:GLU:CD	1:D:87:GLU:N	2.70	0.50
1:D:361:VAL:HG23	2:D:501:HEM:HBD2	1.94	0.50
1:D:413:HIS:CG	1:D:414:HIS:N	2.79	0.50
1:A:107:HIS:CD2	1:A:358:HIS:CD2	3.00	0.50
1:A:365:LEU:O	1:A:369:GLU:HB2	2.10	0.50
1:B:234:VAL:HG13	1:B:238:GLN:HB2	1.94	0.50
1:C:257:MET:HE3	1:C:290:LEU:HD23	1.93	0.50
1:D:271:LEU:O	1:D:274:GLU:HB2	2.11	0.50
1:A:34:GLU:CD	1:A:34:GLU:N	2.70	0.50
1:A:182:ARG:NH2	1:A:248:ASN:HD21	2.10	0.50
1:C:77:ILE:HD12	1:C:82:PHE:CD2	2.47	0.50
1:C:95:ARG:CD	1:C:97:ARG:HG2	2.40	0.50
1:C:98:PRO:HB2	1:C:245:ILE:CD1	2.28	0.50
1:D:99:PHE:N	1:D:99:PHE:CD1	2.79	0.50
1:D:301:LEU:C	1:D:302:ARG:CG	2.85	0.50
1:B:241:SER:O	1:B:245:ILE:HD12	2.12	0.50
1:D:78:ARG:O	1:D:90:GLN:NE2	2.45	0.50
1:A:315:VAL:HG23	1:A:315:VAL:O	2.11	0.49
1:A:353:PHE:CD1	1:A:363:GLN:HB3	2.46	0.49
1:B:161:SER:O	1:B:164:CYS:HB2	2.11	0.49
1:B:193:GLN:HG3	1:B:196:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ARG:NH1	1:C:52:ARG:HG3	2.26	0.49
1:C:149:ASP:OD2	1:C:406:GLU:HG2	2.12	0.49
1:D:50:PRO:HG3	1:D:85:LEU:O	2.12	0.49
1:A:379:ARG:O	1:B:276:ARG:HD3	2.13	0.49
1:A:384:LEU:C	1:A:384:LEU:CD1	2.85	0.49
1:A:395:VAL:HG23	1:A:395:VAL:O	2.12	0.49
1:B:123:VAL:HG13	1:B:368:LEU:HD23	1.94	0.49
1:C:51:THR:O	1:C:52:ARG:HB2	2.10	0.49
1:D:46:ARG:NH2	1:D:54:GLU:HB2	2.21	0.49
1:C:75:ALA:O	1:C:101:ARG:C	2.53	0.49
1:C:169:ILE:HG21	1:C:178:ARG:HD3	1.92	0.49
1:C:299:ILE:N	1:C:300:PRO:CD	2.75	0.49
1:D:120:VAL:O	1:D:124:ARG:HB2	2.12	0.49
1:A:23:ILE:HD13	1:A:34:GLU:HG3	1.94	0.49
1:B:333:GLU:OE1	1:D:119:THR:HG21	2.13	0.49
1:C:368:LEU:CD1	1:C:372:VAL:HG23	2.42	0.49
1:D:174:LEU:C	1:D:176:PHE:H	2.20	0.49
1:A:68:LEU:CD2	1:A:302:ARG:NE	2.75	0.49
1:A:257:MET:HE2	1:A:295:VAL:CG2	2.43	0.49
1:B:177:PHE:C	1:B:177:PHE:CD2	2.88	0.49
1:C:220:LEU:HD22	1:C:224:LEU:HG	1.94	0.49
1:C:234:VAL:HG12	1:C:238:GLN:CD	2.27	0.49
1:C:383:THR:HG21	1:C:412:HIS:C	2.37	0.49
1:D:209:VAL:HG13	1:D:225:VAL:CG2	2.43	0.49
1:B:290:LEU:HD13	1:B:353:PHE:HE2	1.77	0.49
1:C:21:PHE:CE1	1:C:322:ILE:HD13	2.48	0.49
1:C:57:VAL:CG2	1:C:324:LEU:CD2	2.90	0.49
1:A:65:ARG:HA	1:A:355:TYR:HD1	1.77	0.49
1:B:230:VAL:N	1:B:231:PRO:CD	2.76	0.49
1:C:21:PHE:HB2	1:C:47:VAL:CG2	2.43	0.49
1:C:251:ARG:CG	1:C:251:ARG:HH11	2.26	0.49
1:A:120:VAL:HG11	1:C:347:ASP:OD2	2.12	0.48
1:B:56:TRP:HB2	1:B:321:VAL:HG13	1.93	0.48
1:D:96:PHE:N	1:D:96:PHE:CD1	2.78	0.48
1:A:239:LEU:C	1:A:239:LEU:CD2	2.85	0.48
1:B:217:ARG:CG	1:B:217:ARG:NH1	2.74	0.48
1:C:190:THR:HG22	1:C:193:GLN:N	2.24	0.48
1:C:214:GLU:OE2	1:C:215:GLU:N	2.46	0.48
1:D:299:ILE:N	1:D:300:PRO:CD	2.76	0.48
1:C:23:ILE:HG21	1:C:34:GLU:HG3	1.95	0.48
1:D:117:ALA:HA	1:D:122:ARG:HE	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:CG1	1:A:368:LEU:HD23	2.43	0.48
1:C:99:PHE:HD1	1:C:100:ILE:H	1.62	0.48
1:D:95:ARG:CZ	1:D:97:ARG:NH1	2.77	0.48
1:D:177:PHE:HD1	1:D:204:LEU:CD1	2.26	0.48
1:D:196:GLU:OE1	1:D:196:GLU:HA	2.14	0.48
1:D:269:PRO:O	1:D:272:PRO:HG2	2.13	0.48
1:C:113:MET:HG3	1:C:228:HIS:CE1	2.48	0.48
1:C:288:GLU:OE2	1:C:288:GLU:HA	2.14	0.48
1:D:20:ASP:HA	1:D:48:THR:HB	1.95	0.48
1:B:176:PHE:O	1:B:180:VAL:HG22	2.13	0.48
1:B:317:ALA:O	1:B:318:ASP:HB2	2.12	0.48
1:B:390:ARG:HG3	1:B:391:ASP:N	2.27	0.48
1:B:77:ILE:HD12	1:B:82:PHE:CE1	2.49	0.48
1:D:74:SER:HB3	1:D:103:ASP:CG	2.36	0.48
1:D:125:ALA:O	1:D:128:PRO:HD2	2.13	0.48
1:D:302:ARG:CG	1:D:302:ARG:NH1	2.74	0.48
1:A:78:ARG:CG	1:A:78:ARG:NH1	2.76	0.48
1:A:112:ARG:NH2	1:C:70:ASP:OD2	2.34	0.48
1:D:95:ARG:CZ	1:D:96:PHE:O	2.62	0.48
1:A:133:ARG:HG2	1:A:171:ARG:NH2	2.29	0.48
1:C:301:LEU:O	1:C:302:ARG:CG	2.61	0.48
1:D:73:VAL:HG23	1:D:308:ILE:CD1	2.44	0.48
1:D:271:LEU:HB3	1:D:343:PHE:HE2	1.79	0.48
1:A:201:LEU:HD23	1:A:201:LEU:O	2.13	0.48
1:B:234:VAL:CG1	1:B:238:GLN:CB	2.92	0.48
1:B:304:ALA:O	1:B:318:ASP:N	2.34	0.48
1:B:389:GLU:HB3	1:B:392:GLN:HG3	1.96	0.48
1:C:408:MET:CE	1:C:408:MET:H	2.27	0.48
1:A:167:LEU:HD21	1:A:243:LEU:HD22	1.96	0.47
1:B:301:LEU:HD23	1:B:322:ILE:HG12	1.96	0.47
1:B:309:GLU:HG3	1:B:314:THR:HB	1.96	0.47
1:B:312:GLY:HA3	3:B:605:HOH:O	2.14	0.47
1:B:335:PHE:O	1:B:338:PRO:HD3	2.13	0.47
1:C:353:PHE:HB3	1:C:360:CYS:CB	2.44	0.47
1:C:386:LEU:HD22	1:C:388:GLY:H	1.77	0.47
1:A:21:PHE:CB	1:A:22:PRO:CD	2.92	0.47
1:B:96:PHE:C	1:B:97:ARG:HG3	2.38	0.47
1:B:107:HIS:NE2	1:B:358:HIS:NE2	2.62	0.47
1:D:385:ARG:CG	1:D:386:LEU:N	2.70	0.47
1:A:389:GLU:CB	1:A:392:GLN:HG3	2.44	0.47
1:C:21:PHE:HB2	1:C:47:VAL:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:OG1	1:C:333:GLU:OE1	2.21	0.47
1:B:260:LEU:HD11	1:B:402:PHE:HE1	1.79	0.47
1:C:303:VAL:HG13	1:C:319:ASP:C	2.30	0.47
1:D:209:VAL:HG13	1:D:225:VAL:HG22	1.96	0.47
1:A:21:PHE:HB3	1:A:22:PRO:CD	2.34	0.47
1:A:57:VAL:HG22	1:A:324:LEU:CD1	2.44	0.47
1:A:177:PHE:C	1:A:177:PHE:HD2	2.23	0.47
1:C:35:TYR:HA	1:C:38:LEU:HB2	1.97	0.47
1:C:245:ILE:O	1:C:248:ASN:OD1	2.32	0.47
1:D:77:ILE:CA	1:D:82:PHE:CE2	2.83	0.47
1:D:99:PHE:HD1	1:D:99:PHE:N	2.13	0.47
1:D:173:ASP:HB3	1:D:174:LEU:HG	1.96	0.47
1:A:92:ALA:CA	1:A:95:ARG:CG	2.87	0.47
1:A:174:LEU:HD13	1:A:204:LEU:HD21	1.96	0.47
1:A:364:HIS:HB2	3:A:601:HOH:O	2.14	0.47
1:B:170:PRO:HD2	1:B:174:LEU:HD12	1.97	0.47
1:D:257:MET:HE1	1:D:290:LEU:HA	1.97	0.47
1:D:301:LEU:C	1:D:302:ARG:HG3	2.39	0.47
1:A:78:ARG:HD3	1:A:97:ARG:HE	1.80	0.47
1:B:34:GLU:N	1:B:34:GLU:CD	2.72	0.47
1:B:290:LEU:HD13	1:B:353:PHE:CE2	2.50	0.47
1:C:76:ASP:O	1:C:82:PHE:CD2	2.67	0.47
1:C:190:THR:HG21	1:C:193:GLN:HB2	1.96	0.47
1:A:291:ARG:HG3	1:A:292:VAL:N	2.30	0.47
1:C:202:PHE:HD1	1:C:240:LEU:CD1	2.28	0.47
1:D:234:VAL:HA	1:D:238:GLN:NE2	2.29	0.47
1:D:384:LEU:HD13	1:D:385:ARG:N	2.30	0.47
1:A:112:ARG:HH12	1:C:308:ILE:HG23	1.80	0.47
1:A:201:LEU:HD23	1:A:201:LEU:C	2.39	0.47
1:C:347:ASP:OD1	1:C:347:ASP:N	2.45	0.47
1:D:21:PHE:HB2	1:D:47:VAL:CB	2.44	0.47
1:A:260:LEU:HD11	1:A:402:PHE:CE1	2.49	0.47
1:B:361:VAL:HG23	2:B:501:HEM:HBD2	1.97	0.47
1:D:64:VAL:HG13	1:D:323:ALA:HB1	1.96	0.47
1:A:42:ASP:CG	1:A:45:ALA:HB2	2.39	0.46
1:A:361:VAL:O	1:A:361:VAL:HG12	2.15	0.46
1:B:163:ILE:CG2	1:B:167:LEU:HD12	2.42	0.46
1:C:122:ARG:HG2	1:C:122:ARG:NH1	2.29	0.46
1:B:61:TYR:CD1	1:B:61:TYR:C	2.94	0.46
1:B:146:GLY:O	1:B:148:VAL:HG23	2.15	0.46
1:D:34:GLU:N	1:D:34:GLU:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:SER:C	1:D:190:THR:CG2	2.88	0.46
1:A:386:LEU:HD23	1:A:408:MET:O	2.15	0.46
1:B:77:ILE:HA	1:B:82:PHE:CD2	2.51	0.46
1:C:42:ASP:OD1	1:C:45:ALA:HA	2.14	0.46
1:C:57:VAL:HG22	1:C:324:LEU:CD2	2.45	0.46
1:C:414:HIS:ND1	1:C:414:HIS:N	2.62	0.46
1:D:97:ARG:HD2	1:D:97:ARG:HA	1.66	0.46
1:D:190:THR:OG1	1:D:193:GLN:HB2	2.15	0.46
1:D:251:ARG:HG2	1:D:251:ARG:HH11	1.80	0.46
1:A:149:ASP:OD2	1:A:407:LEU:O	2.34	0.46
1:A:302:ARG:NH1	1:A:302:ARG:CG	2.70	0.46
1:B:167:LEU:HD21	1:B:243:LEU:HD22	1.97	0.46
1:B:174:LEU:HD23	1:B:174:LEU:N	2.29	0.46
1:B:408:MET:HE3	1:B:408:MET:HB3	1.75	0.46
1:C:67:LEU:O	1:C:67:LEU:HD22	2.15	0.46
1:C:301:LEU:C	1:C:302:ARG:HG3	2.40	0.46
1:D:95:ARG:NE	1:D:95:ARG:C	2.74	0.46
1:A:77:ILE:O	1:A:77:ILE:HG13	2.15	0.46
1:B:84:ALA:HB1	1:B:89:GLU:HB2	1.97	0.46
1:D:353:PHE:HB3	1:D:360:CYS:HB3	1.97	0.46
1:A:382:PRO:CB	1:B:382:PRO:HB2	2.45	0.46
1:C:97:ARG:HB3	1:C:98:PRO:HD2	1.97	0.46
1:C:390:ARG:O	1:C:391:ASP:CB	2.62	0.46
1:D:82:PHE:CD1	1:D:83:PRO:N	2.81	0.46
1:D:164:CYS:SG	1:D:178:ARG:HD3	2.55	0.46
1:D:271:LEU:HB3	1:D:343:PHE:CE2	2.50	0.46
1:A:57:VAL:HG22	1:A:324:LEU:HD11	1.97	0.46
1:B:67:LEU:HD22	1:B:67:LEU:O	2.15	0.46
1:C:84:ALA:CB	1:C:89:GLU:HB2	2.46	0.46
1:C:411:TRP:C	1:C:412:HIS:ND1	2.74	0.46
1:A:114:LEU:C	1:A:114:LEU:HD12	2.41	0.46
1:A:368:LEU:CD1	1:A:372:VAL:CG2	2.94	0.46
1:B:149:ASP:O	1:B:153:ALA:CB	2.63	0.46
1:B:149:ASP:O	1:B:153:ALA:HB3	2.16	0.46
1:C:73:VAL:CG2	1:C:308:ILE:CD1	2.94	0.46
1:C:368:LEU:HD11	1:C:372:VAL:HG21	1.98	0.46
1:D:301:LEU:O	1:D:302:ARG:HG2	2.16	0.46
1:D:414:HIS:O	1:D:414:HIS:CD2	2.68	0.46
1:B:335:PHE:HB2	1:B:338:PRO:HB3	1.96	0.46
1:C:21:PHE:HB2	1:C:47:VAL:HG21	1.98	0.46
1:C:234:VAL:CB	1:C:238:GLN:HE21	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ALA:O	1:D:133:ARG:HG3	2.16	0.46
1:B:239:LEU:C	1:B:239:LEU:CD2	2.85	0.45
1:C:133:ARG:HH12	1:C:164:CYS:HB2	1.81	0.45
1:C:174:LEU:CD1	1:C:204:LEU:CD2	2.80	0.45
1:C:188:ASN:C	1:C:189:SER:HG	2.15	0.45
1:C:257:MET:CE	1:C:290:LEU:HD23	2.45	0.45
1:D:73:VAL:HG22	1:D:308:ILE:CD1	2.45	0.45
1:D:110:TYR:CD1	1:D:113:MET:CE	2.94	0.45
1:D:229:LEU:HD22	1:D:239:LEU:HD13	1.98	0.45
1:D:263:LEU:HD23	1:D:263:LEU:O	2.15	0.45
1:A:36:ALA:O	1:A:40:THR:HG23	2.16	0.45
1:B:21:PHE:HB2	1:B:47:VAL:HG21	1.97	0.45
1:C:100:ILE:O	1:C:100:ILE:HG22	2.15	0.45
1:C:137:ILE:HD13	1:C:157:ALA:HB1	1.99	0.45
1:B:390:ARG:O	1:B:391:ASP:CB	2.64	0.45
1:C:73:VAL:HG22	1:C:308:ILE:HD13	1.96	0.45
1:D:124:ARG:NH1	1:D:124:ARG:CG	2.75	0.45
1:B:175:GLU:O	1:B:179:ASP:HB2	2.16	0.45
1:D:74:SER:CA	1:D:103:ASP:OD2	2.65	0.45
1:D:234:VAL:HG12	1:D:238:GLN:CB	2.46	0.45
1:A:181:THR:HG21	1:A:201:LEU:HB2	1.97	0.45
1:B:96:PHE:CD1	1:B:96:PHE:O	2.70	0.45
1:B:182:ARG:HD3	1:B:247:ILE:HG21	1.98	0.45
1:D:77:ILE:CA	1:D:82:PHE:HD2	2.23	0.45
1:D:384:LEU:C	1:D:384:LEU:HD13	2.42	0.45
1:A:19:ARG:O	1:A:47:VAL:HA	2.16	0.45
1:B:95:ARG:O	1:B:96:PHE:CD2	2.69	0.45
1:B:198:LEU:O	1:B:202:PHE:HD2	2.00	0.45
1:B:73:VAL:CG1	1:B:302:ARG:HB3	2.47	0.45
1:B:174:LEU:CD1	1:B:204:LEU:HD21	2.47	0.45
1:C:353:PHE:CD1	1:C:363:GLN:HB3	2.52	0.45
1:D:21:PHE:O	1:D:23:ILE:HG13	2.16	0.45
1:D:36:ALA:O	1:D:40:THR:OG1	2.33	0.45
1:D:78:ARG:NH2	3:D:606:HOH:O	2.50	0.45
1:D:393:VAL:CG1	1:D:407:LEU:CD2	2.95	0.45
1:A:123:VAL:HG13	1:A:368:LEU:HD23	1.99	0.45
1:A:201:LEU:C	1:A:201:LEU:CD2	2.90	0.45
1:C:172:HIS:ND1	1:C:172:HIS:N	2.64	0.45
1:C:378:LEU:CD1	1:C:378:LEU:H	2.25	0.45
1:D:342:ASP:O	1:D:345:ARG:HG3	2.16	0.45
1:A:37:ALA:O	1:A:41:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLN:C	1:A:92:ALA:H	2.25	0.45
1:A:168:GLY:O	1:A:212:ARG:NH2	2.50	0.45
1:B:177:PHE:C	1:B:177:PHE:HD2	2.25	0.45
1:C:92:ALA:C	1:C:95:ARG:CD	2.86	0.45
1:C:282:MET:HB2	1:C:282:MET:HE2	1.86	0.45
1:C:411:TRP:C	1:C:412:HIS:CG	2.95	0.45
1:D:111:ARG:HD2	2:D:501:HEM:O2D	2.17	0.45
1:D:157:ALA:O	1:D:161:SER:HB2	2.17	0.45
1:A:396:LYS:HG3	1:A:405:GLU:HB2	1.99	0.45
1:C:300:PRO:HB3	2:C:501:HEM:O1A	2.17	0.45
1:C:411:TRP:O	1:C:412:HIS:CG	2.70	0.45
1:D:49:LEU:HB2	1:D:53:ARG:O	2.16	0.45
1:D:99:PHE:CD2	1:D:110:TYR:CB	2.99	0.45
1:C:110:TYR:CD1	1:C:113:MET:CE	2.97	0.44
1:D:225:VAL:O	1:D:230:VAL:HG23	2.17	0.44
1:D:299:ILE:HD11	1:D:401:THR:HG22	1.99	0.44
1:A:23:ILE:HG21	1:A:34:GLU:CG	2.48	0.44
1:C:25:ARG:HG3	1:C:402:PHE:CE2	2.52	0.44
1:D:95:ARG:NH2	1:D:96:PHE:O	2.50	0.44
1:D:375:GLU:C	1:D:375:GLU:CD	2.85	0.44
1:D:174:LEU:C	1:D:176:PHE:N	2.74	0.44
1:D:227:ASP:CB	1:D:228:HIS:HD2	2.29	0.44
1:B:95:ARG:O	1:B:96:PHE:CG	2.71	0.44
1:B:390:ARG:NH1	1:B:393:VAL:CG2	2.78	0.44
1:C:264:LEU:HD23	1:C:289:LEU:HD21	1.99	0.44
1:D:21:PHE:HB2	1:D:47:VAL:HG21	1.99	0.44
1:D:189:SER:O	1:D:190:THR:HG22	2.17	0.44
1:D:300:PRO:O	1:D:300:PRO:HG2	2.18	0.44
1:D:379:ARG:NH1	1:D:379:ARG:CG	2.75	0.44
1:D:395:VAL:CG1	1:D:396:LYS:N	2.72	0.44
1:A:21:PHE:O	1:A:23:ILE:HG13	2.17	0.44
1:A:177:PHE:O	1:A:177:PHE:HD2	2.01	0.44
1:C:256:SER:O	1:C:260:LEU:HB2	2.18	0.44
1:A:299:ILE:HD11	1:A:401:THR:HG22	1.98	0.44
1:C:82:PHE:CD1	1:C:83:PRO:CD	3.00	0.44
1:D:46:ARG:HH21	1:D:54:GLU:HB3	1.74	0.44
1:A:361:VAL:HG23	2:A:501:HEM:HBD2	2.00	0.44
1:B:25:ARG:HD2	1:B:32:PRO:HD3	2.00	0.44
1:B:60:ARG:O	1:B:64:VAL:HG23	2.18	0.44
1:D:220:LEU:HD22	1:D:224:LEU:HG	1.99	0.44
1:D:385:ARG:CG	1:D:386:LEU:H	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:MET:HE3	1:A:408:MET:HB3	1.75	0.44
1:B:90:GLN:NE2	1:B:90:GLN:C	2.75	0.44
1:B:107:HIS:CD2	1:B:358:HIS:CD2	3.06	0.44
1:C:271:LEU:O	1:C:274:GLU:HB2	2.18	0.44
1:D:154:TYR:CE1	1:D:377:LEU:HD22	2.53	0.44
1:D:281:LEU:HD23	1:D:281:LEU:HA	1.82	0.44
1:A:182:ARG:HD2	1:A:182:ARG:HA	1.76	0.44
1:A:220:LEU:HD23	1:A:224:LEU:HG	2.00	0.44
1:B:70:ASP:OD1	1:B:71:PRO:CD	2.66	0.44
1:B:169:ILE:CD1	1:B:178:ARG:CD	2.85	0.44
1:B:270:GLU:CD	1:B:270:GLU:H	2.26	0.44
1:C:149:ASP:OD2	1:C:407:LEU:O	2.36	0.44
1:C:28:PRO:HG2	1:C:29:PHE:CD1	2.53	0.43
1:C:65:ARG:CD	1:C:355:TYR:CE1	3.01	0.43
1:D:297:ASP:OD1	1:D:298:SER:N	2.51	0.43
1:D:407:LEU:HD22	1:D:407:LEU:HA	1.73	0.43
1:B:19:ARG:O	1:B:48:THR:N	2.41	0.43
1:C:70:ASP:OD1	1:C:71:PRO:CD	2.66	0.43
1:C:269:PRO:C	1:C:272:PRO:HD2	2.43	0.43
1:D:299:ILE:H	1:D:300:PRO:CD	2.30	0.43
1:D:302:ARG:HH21	1:D:358:HIS:CB	2.31	0.43
1:A:70:ASP:OD1	1:A:71:PRO:CD	2.67	0.43
1:A:363:GLN:O	1:A:367:ARG:HG3	2.19	0.43
1:C:115:LEU:N	1:C:116:PRO:HD2	2.33	0.43
1:C:154:TYR:CE1	1:C:377:LEU:HD22	2.52	0.43
1:C:190:THR:HG21	1:C:193:GLN:CB	2.47	0.43
1:C:385:ARG:HG3	1:C:386:LEU:H	1.81	0.43
1:D:82:PHE:CD1	1:D:83:PRO:HD2	2.53	0.43
1:C:92:ALA:O	1:C:95:ARG:CG	2.64	0.43
1:A:46:ARG:HD3	1:A:56:TRP:CH2	2.53	0.43
1:A:313:ARG:H	1:A:313:ARG:HG2	1.66	0.43
1:B:151:VAL:HA	1:B:155:ALA:HB3	2.01	0.43
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.73	0.43
1:D:113:MET:SD	1:D:228:HIS:ND1	2.91	0.43
1:D:190:THR:O	1:D:191:ALA:CB	2.67	0.43
1:A:76:ASP:O	1:A:82:PHE:HD2	2.01	0.43
1:A:111:ARG:HD2	2:A:501:HEM:O2D	2.17	0.43
1:C:29:PHE:CD2	1:C:264:LEU:HD13	2.52	0.43
1:D:95:ARG:CD	1:D:95:ARG:C	2.91	0.43
1:D:115:LEU:N	1:D:116:PRO:HD2	2.33	0.43
1:B:264:LEU:HD12	1:B:264:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ASP:HB3	1:D:228:HIS:HD2	1.84	0.43
1:C:64:VAL:HG13	1:C:323:ALA:HB1	2.01	0.43
1:B:57:VAL:HG23	1:B:322:ILE:HB	2.00	0.43
1:C:269:PRO:O	1:C:272:PRO:HD2	2.19	0.43
1:C:412:HIS:ND1	1:C:412:HIS:N	2.64	0.43
1:D:70:ASP:OD1	1:D:71:PRO:CD	2.67	0.43
1:D:73:VAL:CG2	1:D:308:ILE:HD13	2.49	0.43
1:D:75:ALA:N	1:D:103:ASP:OD2	2.51	0.43
1:A:353:PHE:CE1	1:A:363:GLN:HA	2.54	0.43
1:B:32:PRO:HG2	1:B:35:TYR:CE1	2.54	0.43
1:B:148:VAL:HG12	1:B:149:ASP:H	1.84	0.43
1:D:61:TYR:CD1	1:D:334:GLN:HG3	2.53	0.43
1:D:414:HIS:C	1:D:415:HIS:CD2	2.97	0.43
1:C:108:THR:O	1:C:112:ARG:HB2	2.19	0.42
1:C:174:LEU:O	1:C:175:GLU:CB	2.66	0.42
1:C:407:LEU:HD22	1:C:407:LEU:HA	1.72	0.42
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.83	0.42
1:A:56:TRP:NE1	1:A:316:PRO:HD2	2.34	0.42
1:C:87:GLU:CD	1:C:87:GLU:H	2.27	0.42
1:C:227:ASP:HB3	1:C:228:HIS:CD2	2.53	0.42
1:C:310:LEU:O	1:C:311:SER:HB2	2.18	0.42
1:D:269:PRO:O	1:D:272:PRO:HD2	2.19	0.42
1:A:142:LEU:HD23	1:A:411:TRP:NE1	2.34	0.42
1:B:182:ARG:HE	1:B:251:ARG:HE	1.66	0.42
1:B:186:SER:O	1:B:187:ARG:HB2	2.18	0.42
1:D:282:MET:HE3	1:D:375:GLU:HB2	2.02	0.42
1:D:306:GLU:O	1:D:308:ILE:HG13	2.18	0.42
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.18	0.42
1:B:190:THR:HG22	1:B:193:GLN:HB3	1.97	0.42
1:A:19:ARG:O	1:A:48:THR:N	2.49	0.42
1:A:107:HIS:NE2	1:A:358:HIS:NE2	2.62	0.42
1:B:361:VAL:HG12	1:B:361:VAL:O	2.20	0.42
1:C:316:PRO:HG2	1:C:319:ASP:OD1	2.18	0.42
1:B:71:PRO:CB	1:D:71:PRO:HB3	2.49	0.42
1:B:296:ALA:HB1	1:B:299:ILE:HG12	2.00	0.42
1:B:368:LEU:HD12	1:B:372:VAL:CG2	2.50	0.42
1:C:169:ILE:HD13	1:C:178:ARG:CD	2.44	0.42
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.83	0.42
1:D:25:ARG:H	1:D:25:ARG:HG2	1.60	0.42
1:D:42:ASP:HB2	1:D:45:ALA:HB2	2.01	0.42
1:D:110:TYR:HA	1:D:113:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ARG:H	1:B:25:ARG:HG2	1.60	0.42
1:B:57:VAL:HG22	1:B:324:LEU:CD1	2.50	0.42
1:C:25:ARG:H	1:C:25:ARG:HG2	1.56	0.42
1:D:307:ASP:N	1:D:317:ALA:HB2	2.35	0.42
1:B:65:ARG:HA	1:B:355:TYR:HD1	1.84	0.42
1:C:113:MET:CG	1:C:228:HIS:CE1	3.03	0.42
1:D:380:ARG:HD2	1:D:415:HIS:CE1	2.54	0.42
1:D:413:HIS:O	1:D:414:HIS:CG	2.72	0.42
1:A:253:THR:CG2	1:A:401:THR:HG21	2.44	0.42
1:B:154:TYR:O	1:B:158:VAL:HG23	2.19	0.42
1:A:115:LEU:HD23	1:A:361:VAL:HG13	2.02	0.42
1:A:309:GLU:HG2	1:A:314:THR:HB	2.02	0.42
1:B:257:MET:HE3	1:B:290:LEU:HD23	2.02	0.42
1:D:174:LEU:HD12	1:D:204:LEU:HD21	2.00	0.42
1:D:230:VAL:N	1:D:231:PRO:CD	2.80	0.42
1:A:243:LEU:O	1:A:247:ILE:HG13	2.20	0.41
1:C:167:LEU:HD23	1:C:221:ILE:CG1	2.49	0.41
1:C:256:SER:OG	1:C:403:GLY:HA3	2.20	0.41
1:D:386:LEU:HD23	1:D:387:ALA:N	2.35	0.41
1:C:131:GLN:OE1	1:C:376:THR:CG2	2.63	0.41
1:D:44:VAL:CG1	1:D:315:VAL:HG12	2.46	0.41
1:D:254:THR:HA	2:D:501:HEM:HBB1	2.02	0.41
1:D:282:MET:HB2	1:D:282:MET:HE2	1.84	0.41
1:D:389:GLU:HG3	1:D:390:ARG:N	2.35	0.41
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.82	0.41
1:B:42:ASP:CG	1:B:45:ALA:HB2	2.45	0.41
1:C:51:THR:O	1:C:52:ARG:CB	2.68	0.41
1:C:193:GLN:O	1:C:194:VAL:C	2.63	0.41
1:D:46:ARG:HE	1:D:54:GLU:CD	2.27	0.41
1:D:92:ALA:O	1:D:95:ARG:CG	2.65	0.41
1:D:164:CYS:SG	1:D:178:ARG:NE	2.93	0.41
1:D:216:PRO:HB2	1:D:222:SER:OG	2.20	0.41
1:D:257:MET:HE2	1:D:295:VAL:HB	2.02	0.41
1:D:388:GLY:CA	1:D:408:MET:HE2	2.51	0.41
1:B:70:ASP:OD1	1:B:71:PRO:HD2	2.21	0.41
1:B:159:SER:HB3	1:B:255:THR:HG22	1.99	0.41
1:B:174:LEU:O	1:B:175:GLU:CB	2.69	0.41
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.76	0.41
1:B:202:PHE:CD1	1:B:240:LEU:HD12	2.53	0.41
1:C:42:ASP:OD1	1:C:45:ALA:CA	2.68	0.41
1:C:77:ILE:CA	1:C:82:PHE:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ARG:CG	1:C:345:ARG:HH11	2.34	0.41
1:D:175:GLU:O	1:D:179:ASP:CB	2.68	0.41
1:D:393:VAL:HG11	1:D:407:LEU:CD2	2.49	0.41
1:D:394:VAL:HG11	1:D:405:GLU:HB3	2.01	0.41
1:B:190:THR:HG22	1:B:193:GLN:H	1.85	0.41
1:C:115:LEU:HD23	1:C:361:VAL:HG13	2.01	0.41
1:D:256:SER:OG	1:D:403:GLY:HA3	2.20	0.41
1:B:174:LEU:HD13	1:B:204:LEU:HD21	2.02	0.41
1:B:190:THR:HG21	1:B:193:GLN:CB	2.51	0.41
1:C:92:ALA:HA	1:C:95:ARG:CG	2.50	0.41
1:C:95:ARG:NH1	1:C:97:ARG:HD3	2.35	0.41
1:C:137:ILE:HD13	1:C:157:ALA:HB3	2.01	0.41
1:C:384:LEU:HD13	1:C:384:LEU:C	2.44	0.41
1:D:56:TRP:NE1	1:D:316:PRO:HD2	2.36	0.41
1:D:335:PHE:O	1:D:338:PRO:HD3	2.21	0.41
1:A:86:GLY:CA	1:A:89:GLU:OE2	2.68	0.41
1:A:217:ARG:O	1:A:222:SER:CB	2.69	0.41
1:A:234:VAL:HG12	1:A:238:GLN:NE2	2.35	0.41
1:B:177:PHE:O	1:B:177:PHE:HD2	2.04	0.41
1:A:73:VAL:CG2	1:A:308:ILE:HD13	2.41	0.41
1:A:175:GLU:O	1:A:179:ASP:N	2.41	0.41
1:B:21:PHE:HB2	1:B:47:VAL:CG2	2.51	0.41
1:D:44:VAL:HG11	1:D:315:VAL:CG1	2.44	0.41
1:D:270:GLU:O	1:D:273:ALA:HB3	2.21	0.41
1:A:216:PRO:HG3	1:A:226:THR:HG21	2.03	0.41
1:A:220:LEU:HD22	1:A:224:LEU:HG	2.02	0.41
1:A:268:ARG:O	1:A:272:PRO:HD2	2.20	0.41
1:A:374:LEU:HD23	1:A:374:LEU:HA	1.85	0.41
1:B:234:VAL:HG13	1:B:238:GLN:HB3	2.03	0.41
1:C:45:ALA:HB3	1:C:57:VAL:HG12	1.98	0.41
1:C:95:ARG:H	1:C:95:ARG:HG3	1.52	0.41
1:C:243:LEU:O	1:C:247:ILE:HG13	2.21	0.41
1:D:46:ARG:CZ	1:D:54:GLU:HB3	2.51	0.41
1:D:133:ARG:O	1:D:137:ILE:HG13	2.20	0.41
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.91	0.41
1:D:390:ARG:O	1:D:391:ASP:CB	2.69	0.41
1:A:128:PRO:HG2	1:A:129:ALA:N	2.36	0.41
1:A:171:ARG:O	1:A:174:LEU:O	2.39	0.41
1:C:404:LEU:HD13	1:C:407:LEU:HG	2.02	0.41
1:D:187:ARG:CG	1:D:188:ASN:H	2.33	0.41
1:D:346:THR:OG1	1:D:347:ASP:OD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:HG22	1:A:163:ILE:O	2.21	0.40
1:A:290:LEU:HD13	1:A:353:PHE:HE2	1.85	0.40
1:A:384:LEU:HD13	1:A:385:ARG:N	2.36	0.40
1:C:408:MET:SD	1:C:408:MET:N	2.91	0.40
1:D:110:TYR:O	1:D:113:MET:CB	2.65	0.40
1:D:149:ASP:OD2	1:D:407:LEU:O	2.38	0.40
1:D:164:CYS:SG	1:D:178:ARG:CD	3.09	0.40
1:D:288:GLU:OE1	1:D:291:ARG:NH1	2.54	0.40
1:D:299:ILE:N	1:D:300:PRO:HD2	2.36	0.40
1:B:110:TYR:HD1	1:B:113:MET:HE1	1.86	0.40
1:B:260:LEU:HD22	1:B:293:LEU:HD22	2.02	0.40
1:C:375:GLU:C	1:C:375:GLU:CD	2.89	0.40
1:D:28:PRO:HG2	1:D:29:PHE:CD1	2.56	0.40
1:D:413:HIS:O	1:D:414:HIS:CB	2.69	0.40
1:A:20:ASP:HA	1:A:48:THR:O	2.21	0.40
1:A:190:THR:HG22	1:A:193:GLN:HB3	1.68	0.40
1:A:405:GLU:O	1:A:405:GLU:HG2	2.20	0.40
1:C:56:TRP:HE1	1:C:316:PRO:HD2	1.86	0.40
1:C:142:LEU:HA	1:C:142:LEU:HD23	1.94	0.40
1:D:189:SER:O	1:D:190:THR:CG2	2.69	0.40
1:A:103:ASP:O	1:A:104:ALA:CB	2.69	0.40
1:D:269:PRO:C	1:D:272:PRO:HD2	2.46	0.40
1:A:389:GLU:HB3	1:A:392:GLN:CG	2.52	0.40
1:B:119:THR:HG21	1:D:333:GLU:OE1	2.22	0.40
1:B:257:MET:HE2	1:B:295:VAL:HG23	2.03	0.40
1:C:186:SER:O	1:C:187:ARG:CB	2.69	0.40
1:D:336:ASP:O	1:D:337:ASP:C	2.64	0.40

All (31) 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:B:193:GLN:CD	1:C:95:ARG:CZ[3_444]	0.53	1.67
1:A:193:GLN:OE1	1:D:95:ARG:NH2[2_565]	0.57	1.63
1:A:193:GLN:NE2	1:D:95:ARG:NH1[2_565]	0.69	1.51
1:A:193:GLN:CD	1:D:95:ARG:CZ[2_565]	0.90	1.30
1:B:193:GLN:CD	1:C:95:ARG:NH2[3_444]	1.04	1.16
1:B:193:GLN:NE2	1:C:95:ARG:NH1[3_444]	1.12	1.08
1:A:193:GLN:CD	1:D:95:ARG:NH1[2_565]	1.14	1.06
1:A:193:GLN:OE1	1:D:95:ARG:CZ[2_565]	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:NE2	1:C:95:ARG:CZ[3_444]	1.14	1.06
1:B:193:GLN:OE1	1:C:95:ARG:NH2[3_444]	1.16	1.04
1:B:193:GLN:OE1	1:C:96:PHE:O[3_444]	1.38	0.82
1:A:193:GLN:CD	1:D:95:ARG:NH2[2_565]	1.44	0.76
1:A:193:GLN:NE2	1:D:95:ARG:CZ[2_565]	1.62	0.58
1:B:193:GLN:CG	1:C:95:ARG:NH2[3_444]	1.64	0.56
1:B:193:GLN:OE1	1:C:95:ARG:CZ[3_444]	1.65	0.55
1:B:193:GLN:NE2	1:C:95:ARG:NE[3_444]	1.66	0.54
1:B:193:GLN:CD	1:C:95:ARG:NH1[3_444]	1.70	0.50
1:C:172:HIS:NE2	1:D:171:ARG:NH1[6_555]	1.72	0.48
1:B:193:GLN:CD	1:C:95:ARG:NE[3_444]	1.74	0.46
1:C:172:HIS:NE2	1:D:171:ARG:CZ[6_555]	1.84	0.36
1:B:193:GLN:CG	1:C:95:ARG:CZ[3_444]	1.89	0.31
1:C:172:HIS:CE1	1:D:171:ARG:NH2[6_555]	1.91	0.29
1:B:193:GLN:CB	1:C:95:ARG:NH1[3_444]	1.99	0.21
1:A:193:GLN:OE1	1:D:95:ARG:NE[2_565]	2.01	0.19
1:A:193:GLN:CG	1:D:95:ARG:NH1[2_565]	2.03	0.17
1:B:193:GLN:OE1	1:C:95:ARG:NE[3_444]	2.06	0.14
1:B:193:GLN:NE2	1:C:95:ARG:CD[3_444]	2.08	0.12
1:A:193:GLN:OE1	1:D:96:PHE:O[2_565]	2.10	0.10
1:C:172:HIS:CD2	1:D:171:ARG:NH1[6_555]	2.13	0.07
1:A:193:GLN:CD	1:D:95:ARG:NE[2_565]	2.16	0.04
1:B:193:GLN:CG	1:C:95:ARG:NH1[3_444]	2.19	0.01

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	395/417 (95%)	374 (95%)	18 (5%)	3 (1%)	16	44
1	B	395/417 (95%)	378 (96%)	13 (3%)	4 (1%)	12	39
1	C	396/417 (95%)	375 (95%)	13 (3%)	8 (2%)	6	22
1	D	397/417 (95%)	371 (94%)	20 (5%)	6 (2%)	8	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1583/1668 (95%)	1498 (95%)	64 (4%)	21 (1%)	9	32

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ALA
1	B	104	ALA
1	C	104	ALA
1	C	391	ASP
1	C	412	HIS
1	D	104	ALA
1	D	391	ASP
1	D	413	HIS
1	D	414	HIS
1	A	187	ARG
1	B	187	ARG
1	C	175	GLU
1	C	395	VAL
1	D	187	ARG
1	D	191	ALA
1	B	96	PHE
1	C	187	ARG
1	A	297	ASP
1	B	297	ASP
1	C	190	THR
1	C	300	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/347 (95%)	241 (73%)	89 (27%)	0	1
1	B	330/347 (95%)	248 (75%)	82 (25%)	1	2
1	C	331/347 (95%)	240 (72%)	91 (28%)	0	1
1	D	332/347 (96%)	243 (73%)	89 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1323/1388 (95%)	972 (74%)	351 (26%)	0 2

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	20	ASP
1	A	23	ILE
1	A	34	GLU
1	A	48	THR
1	A	52	ARG
1	A	57	VAL
1	A	58	VAL
1	A	59	THR
1	A	67	LEU
1	A	77	ILE
1	A	78	ARG
1	A	91	GLU
1	A	95	ARG
1	A	97	ARG
1	A	113	MET
1	A	122	ARG
1	A	124	ARG
1	A	127	ARG
1	A	141	MET
1	A	148	VAL
1	A	152	SER
1	A	160	THR
1	A	167	LEU
1	A	174	LEU
1	A	175	GLU
1	A	177	PHE
1	A	178	ARG
1	A	179	ASP
1	A	180	VAL
1	A	186	SER
1	A	187	ARG
1	A	195	SER
1	A	201	LEU
1	A	211	GLU
1	A	217	ARG
1	A	219	ASP

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	222	SER
1	A	223	LYS
1	A	226	THR
1	A	227	ASP
1	A	231	PRO
1	A	234	VAL
1	A	240	LEU
1	A	251	ARG
1	A	252	GLU
1	A	253	THR
1	A	254	THR
1	A	260	LEU
1	A	261	SER
1	A	263	LEU
1	A	267	ASP
1	A	269	PRO
1	A	277	LYS
1	A	278	ASP
1	A	291	ARG
1	A	292	VAL
1	A	298	SER
1	A	300	PRO
1	A	302	ARG
1	A	306	GLU
1	A	307	ASP
1	A	309	GLU
1	A	314	THR
1	A	319	ASP
1	A	321	VAL
1	A	324	LEU
1	A	334	GLN
1	A	345	ARG
1	A	346	THR
1	A	348	ASN
1	A	357	VAL
1	A	365	LEU
1	A	368	LEU
1	A	369	GLU
1	A	376	THR
1	A	380	ARG
1	A	384	LEU

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Mol	Chain	Res	Type
1	A	385	ARG
1	A	386	LEU
1	A	389	GLU
1	A	391	ASP
1	A	394	VAL
1	A	396	LYS
1	A	397	HIS
1	A	399	SER
1	A	407	LEU
1	A	412	HIS
1	B	19	ARG
1	B	20	ASP
1	B	23	ILE
1	B	25	ARG
1	B	34	GLU
1	B	48	THR
1	B	52	ARG
1	B	57	VAL
1	B	59	THR
1	B	67	LEU
1	B	69	SER
1	B	77	ILE
1	B	78	ARG
1	B	91	GLU
1	B	95	ARG
1	B	96	PHE
1	B	97	ARG
1	B	106	GLU
1	B	141	MET
1	B	148	VAL
1	B	150	LEU
1	B	152	SER
1	B	160	THR
1	B	167	LEU
1	B	175	GLU
1	B	178	ARG
1	B	179	ASP
1	B	180	VAL
1	B	184	SER
1	B	186	SER
1	B	187	ARG
1	B	193	GLN

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Mol	Chain	Res	Type
1	B	195	SER
1	B	204	LEU
1	B	211	GLU
1	B	216	PRO
1	B	217	ARG
1	B	219	ASP
1	B	220	LEU
1	B	222	SER
1	B	226	THR
1	B	227	ASP
1	B	248	ASN
1	B	252	GLU
1	B	253	THR
1	B	254	THR
1	B	255	THR
1	B	260	LEU
1	B	261	SER
1	B	263	LEU
1	B	267	ASP
1	B	278	ASP
1	B	291	ARG
1	B	292	VAL
1	B	298	SER
1	B	302	ARG
1	B	306	GLU
1	B	307	ASP
1	B	313	ARG
1	B	314	THR
1	B	319	ASP
1	B	321	VAL
1	B	324	LEU
1	B	334	GLN
1	B	340	ARG
1	B	345	ARG
1	B	351	VAL
1	B	357	VAL
1	B	365	LEU
1	B	368	LEU
1	B	370	LEU
1	B	376	THR
1	B	380	ARG
1	B	382	PRO

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Mol	Chain	Res	Type
1	B	384	LEU
1	B	385	ARG
1	B	386	LEU
1	B	389	GLU
1	B	391	ASP
1	B	397	HIS
1	B	399	SER
1	B	407	LEU
1	C	19	ARG
1	C	25	ARG
1	C	34	GLU
1	C	39	ARG
1	C	40	THR
1	C	46	ARG
1	C	49	LEU
1	C	52	ARG
1	C	58	VAL
1	C	59	THR
1	C	65	ARG
1	C	67	LEU
1	C	69	SER
1	C	80	PRO
1	C	83	PRO
1	C	87	GLU
1	C	95	ARG
1	C	97	ARG
1	C	98	PRO
1	C	99	PHE
1	C	103	ASP
1	C	111	ARG
1	C	114	LEU
1	C	122	ARG
1	C	141	MET
1	C	160	THR
1	C	167	LEU
1	C	172	HIS
1	C	175	GLU
1	C	178	ARG
1	C	179	ASP
1	C	180	VAL
1	C	187	ARG
1	C	188	ASN

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Mol	Chain	Res	Type
1	C	195	SER
1	C	196	GLU
1	C	204	LEU
1	C	211	GLU
1	C	213	ARG
1	C	214	GLU
1	C	215	GLU
1	C	219	ASP
1	C	220	LEU
1	C	223	LYS
1	C	226	THR
1	C	231	PRO
1	C	234	VAL
1	C	240	LEU
1	C	242	THR
1	C	246	THR
1	C	251	ARG
1	C	252	GLU
1	C	253	THR
1	C	255	THR
1	C	256	SER
1	C	260	LEU
1	C	261	SER
1	C	263	LEU
1	C	270	GLU
1	C	277	LYS
1	C	278	ASP
1	C	281	LEU
1	C	291	ARG
1	C	295	VAL
1	C	303	VAL
1	C	307	ASP
1	C	313	ARG
1	C	314	THR
1	C	315	VAL
1	C	321	VAL
1	C	322	ILE
1	C	324	LEU
1	C	334	GLN
1	C	340	ARG
1	C	345	ARG
1	C	357	VAL

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Mol	Chain	Res	Type
1	C	368	LEU
1	C	376	THR
1	C	383	THR
1	C	384	LEU
1	C	385	ARG
1	C	386	LEU
1	C	390	ARG
1	C	393	VAL
1	C	396	LYS
1	C	398	ASP
1	C	405	GLU
1	C	407	LEU
1	C	408	MET
1	C	412	HIS
1	C	414	HIS
1	D	19	ARG
1	D	25	ARG
1	D	28	PRO
1	D	34	GLU
1	D	40	THR
1	D	42	ASP
1	D	49	LEU
1	D	52	ARG
1	D	53	ARG
1	D	58	VAL
1	D	59	THR
1	D	65	ARG
1	D	67	LEU
1	D	74	SER
1	D	78	ARG
1	D	87	GLU
1	D	95	ARG
1	D	97	ARG
1	D	99	PHE
1	D	103	ASP
1	D	114	LEU
1	D	121	ARG
1	D	122	ARG
1	D	124	ARG
1	D	141	MET
1	D	148	VAL
1	D	160	THR

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Mol	Chain	Res	Type
1	D	161	SER
1	D	166	LEU
1	D	167	LEU
1	D	169	ILE
1	D	175	GLU
1	D	176	PHE
1	D	180	VAL
1	D	187	ARG
1	D	192	GLU
1	D	195	SER
1	D	201	LEU
1	D	204	LEU
1	D	211	GLU
1	D	213	ARG
1	D	214	GLU
1	D	215	GLU
1	D	217	ARG
1	D	220	LEU
1	D	223	LYS
1	D	226	THR
1	D	238	GLN
1	D	240	LEU
1	D	242	THR
1	D	246	THR
1	D	251	ARG
1	D	252	GLU
1	D	253	THR
1	D	255	THR
1	D	256	SER
1	D	260	LEU
1	D	261	SER
1	D	263	LEU
1	D	270	GLU
1	D	277	LYS
1	D	291	ARG
1	D	295	VAL
1	D	300	PRO
1	D	302	ARG
1	D	303	VAL
1	D	307	ASP
1	D	310	LEU
1	D	313	ARG

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Mol	Chain	Res	Type
1	D	314	THR
1	D	315	VAL
1	D	316	PRO
1	D	321	VAL
1	D	322	ILE
1	D	324	LEU
1	D	347	ASP
1	D	348	ASN
1	D	357	VAL
1	D	376	THR
1	D	383	THR
1	D	384	LEU
1	D	385	ARG
1	D	386	LEU
1	D	389	GLU
1	D	390	ARG
1	D	393	VAL
1	D	406	GLU
1	D	407	LEU
1	D	408	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	A	238	GLN
1	A	248	ASN
1	A	344	HIS
1	A	358	HIS
1	A	359	GLN
1	A	364	HIS
1	B	24	GLN
1	B	131	GLN
1	B	228	HIS
1	B	238	GLN
1	B	330	HIS
1	B	344	HIS
1	B	358	HIS
1	B	359	GLN
1	B	363	GLN
1	B	412	HIS
1	C	238	GLN

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Mol	Chain	Res	Type
1	C	330	HIS
1	C	344	HIS
1	C	359	GLN
1	C	392	GLN
1	C	413	HIS
1	D	24	GLN
1	D	193	GLN
1	D	228	HIS
1	D	238	GLN
1	D	348	ASN
1	D	358	HIS
1	D	359	GLN
1	D	412	HIS
1	D	415	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	501	1	50,50,50	1.60	7 (14%)	67,82,82	0.87	3 (4%)
2	HEM	B	501	1	50,50,50	1.65	8 (16%)	67,82,82	0.85	3 (4%)
2	HEM	D	501	1	50,50,50	1.59	7 (14%)	67,82,82	0.87	3 (4%)
2	HEM	A	501	1	50,50,50	1.62	10 (20%)	67,82,82	0.85	3 (4%)

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	HEM	C	501	1	-	8/14/54/54	-
2	HEM	B	501	1	-	8/14/54/54	-
2	HEM	D	501	1	-	8/14/54/54	-
2	HEM	A	501	1	-	8/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CBB-CAB	5.04	1.54	1.30
2	C	501	HEM	CBC-CAC	4.98	1.54	1.30
2	B	501	HEM	CBC-CAC	4.93	1.54	1.30
2	A	501	HEM	CBC-CAC	4.92	1.54	1.30
2	D	501	HEM	CBC-CAC	4.91	1.54	1.30
2	A	501	HEM	CBB-CAB	4.85	1.53	1.30
2	C	501	HEM	CBB-CAB	4.75	1.53	1.30
2	D	501	HEM	CBB-CAB	4.68	1.52	1.30
2	D	501	HEM	FE-NA	3.16	2.05	1.95
2	B	501	HEM	CAC-C3C	2.92	1.55	1.47
2	C	501	HEM	FE-NA	2.82	2.04	1.95
2	A	501	HEM	CAC-C3C	2.67	1.54	1.47
2	A	501	HEM	FE-NA	2.61	2.03	1.95
2	C	501	HEM	CAC-C3C	2.56	1.54	1.47
2	B	501	HEM	FE-NA	2.49	2.03	1.95
2	C	501	HEM	CAB-C3B	2.45	1.53	1.47
2	D	501	HEM	CAC-C3C	2.41	1.53	1.47
2	D	501	HEM	CAB-C3B	2.39	1.53	1.47
2	A	501	HEM	FE-NB	2.32	2.02	1.94
2	B	501	HEM	CAB-C3B	2.29	1.53	1.47
2	A	501	HEM	CAB-C3B	2.26	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C2A-C3A	-2.22	1.33	1.38
2	D	501	HEM	CMC-C2C	2.17	1.55	1.50
2	D	501	HEM	CMB-C2B	2.14	1.55	1.50
2	C	501	HEM	CMC-C2C	2.13	1.55	1.50
2	A	501	HEM	CMC-C2C	2.13	1.55	1.50
2	C	501	HEM	FE-NC	2.07	2.02	1.95
2	A	501	HEM	O2A-CGA	-2.06	1.24	1.30
2	B	501	HEM	FE-NC	2.04	2.01	1.95
2	B	501	HEM	FE-NB	2.04	2.01	1.94
2	B	501	HEM	C2A-C3A	-2.03	1.33	1.38
2	A	501	HEM	CMD-C2D	2.02	1.54	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBB-CAB-C3B	-2.83	113.36	127.53
2	C	501	HEM	CBB-CAB-C3B	-2.83	113.38	127.53
2	D	501	HEM	O1A-CGA-CBA	-2.82	114.15	123.09
2	D	501	HEM	CBB-CAB-C3B	-2.81	113.47	127.53
2	D	501	HEM	CBC-CAC-C3C	-2.77	113.69	127.53
2	B	501	HEM	CBB-CAB-C3B	-2.75	113.76	127.53
2	C	501	HEM	O1A-CGA-CBA	-2.75	114.38	123.09
2	C	501	HEM	CBC-CAC-C3C	-2.74	113.83	127.53
2	B	501	HEM	O1A-CGA-CBA	-2.71	114.51	123.09
2	A	501	HEM	O1A-CGA-CBA	-2.65	114.70	123.09
2	A	501	HEM	CBC-CAC-C3C	-2.56	114.73	127.53
2	B	501	HEM	CBC-CAC-C3C	-2.48	115.14	127.53

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2B-C3B-CAB-CBB
2	A	501	HEM	C4B-C3B-CAB-CBB
2	A	501	HEM	C2C-C3C-CAC-CBC
2	A	501	HEM	C4C-C3C-CAC-CBC
2	B	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	C4C-C3C-CAC-CBC
2	C	501	HEM	C2B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C2C-C3C-CAC-CBC
2	C	501	HEM	C4C-C3C-CAC-CBC
2	D	501	HEM	C2B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C2C-C3C-CAC-CBC
2	D	501	HEM	C4C-C3C-CAC-CBC
2	A	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O1D

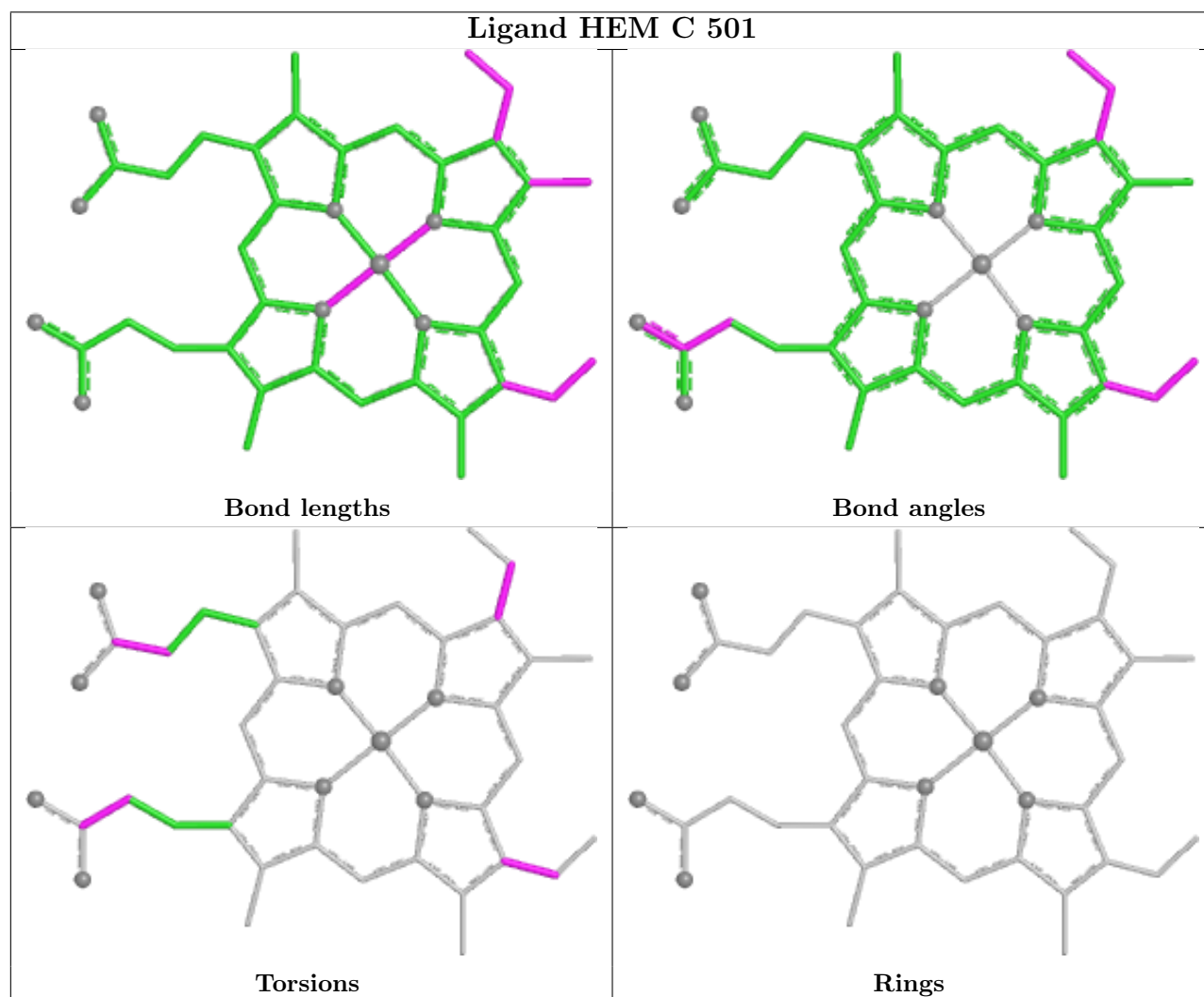
There are no ring outliers.

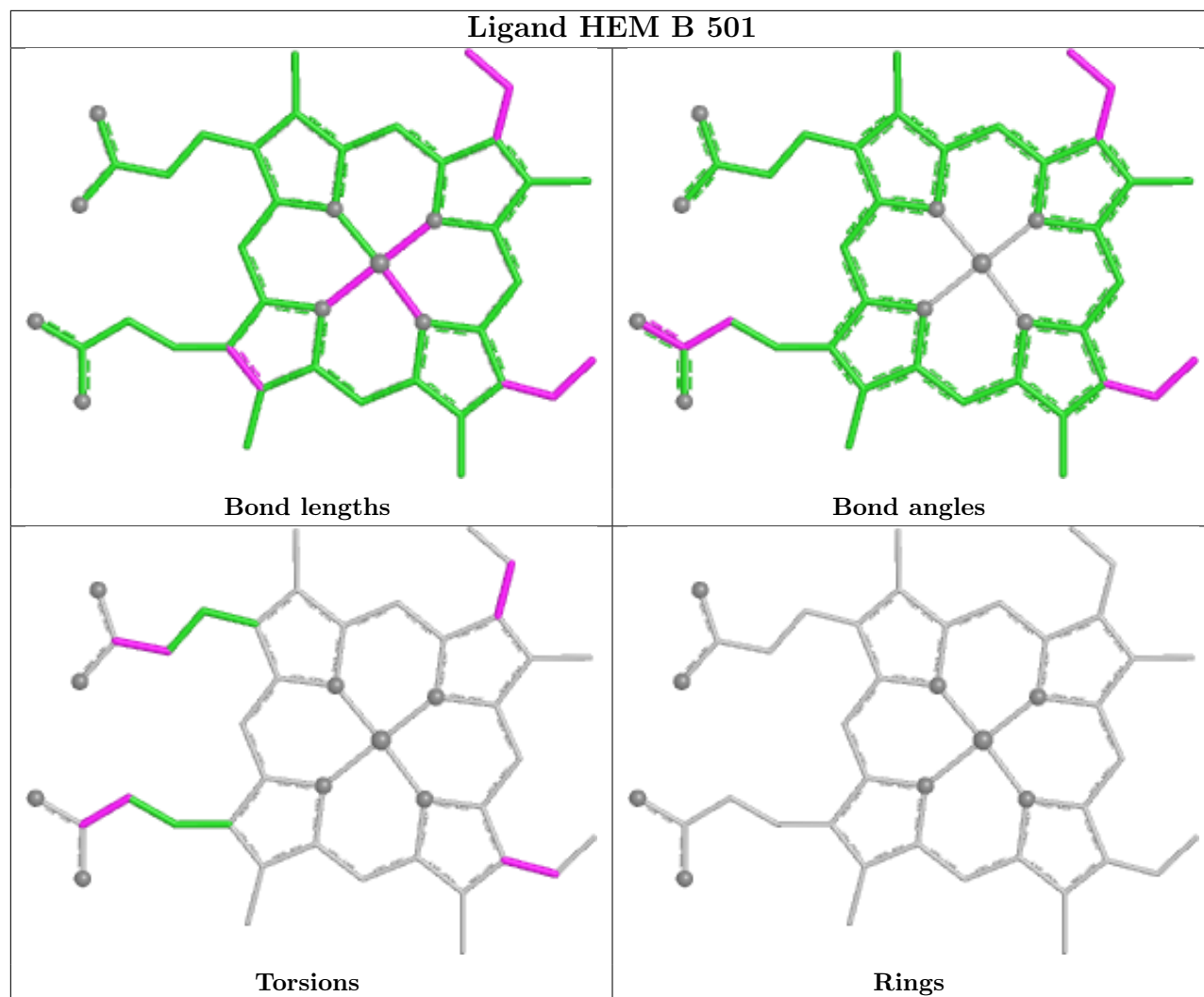
4 monomers are involved in 19 short contacts:

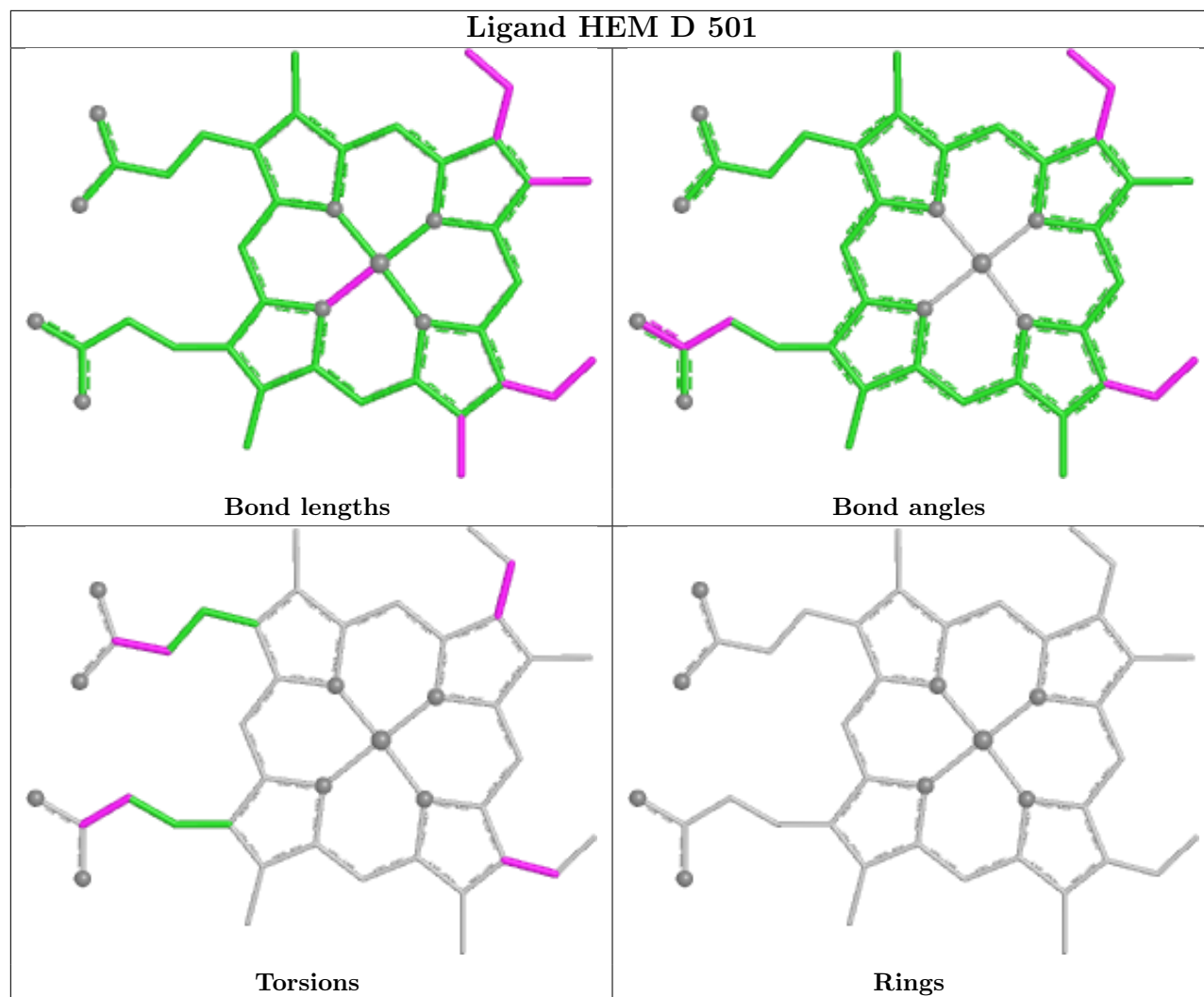
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	4	0
2	B	501	HEM	4	0
2	D	501	HEM	6	0
2	A	501	HEM	5	0

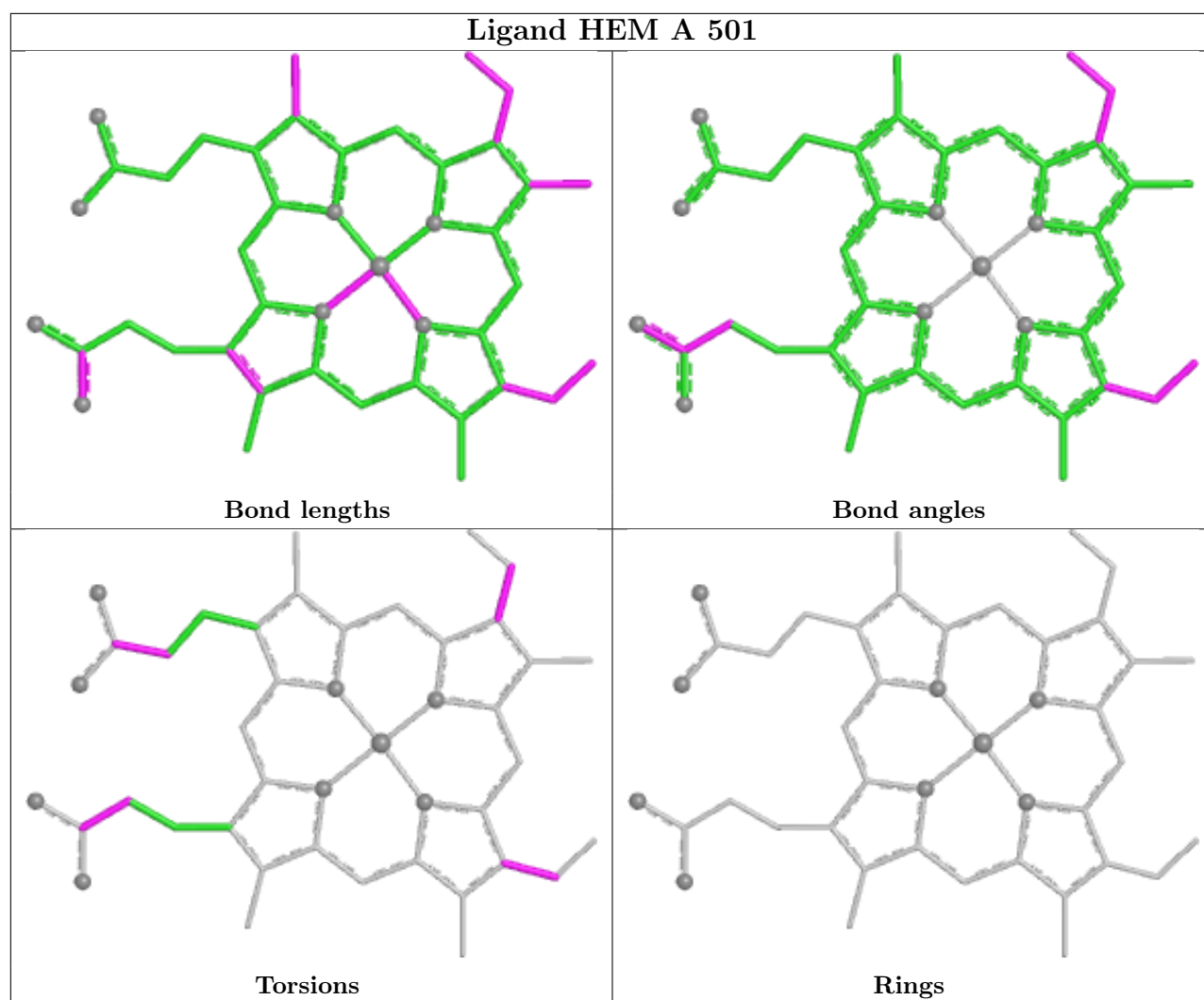
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	397/417 (95%)	-1.52	0 100 100	28, 64, 93, 102	2 (0%)
1	B	397/417 (95%)	-1.54	0 100 100	30, 63, 92, 103	2 (0%)
1	C	398/417 (95%)	-1.47	0 100 100	34, 74, 100, 127	2 (0%)
1	D	399/417 (95%)	-1.49	0 100 100	32, 74, 99, 130	2 (0%)
All	All	1591/1668 (95%)	-1.51	0 100 100	28, 68, 96, 130	8 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

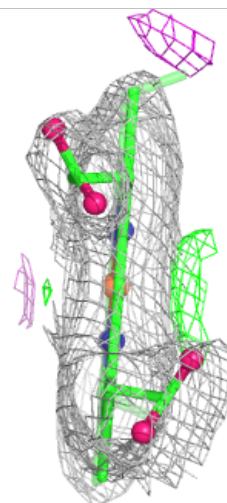
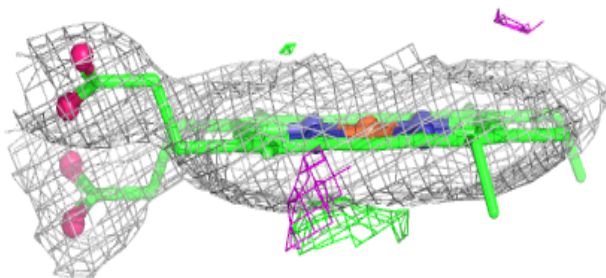
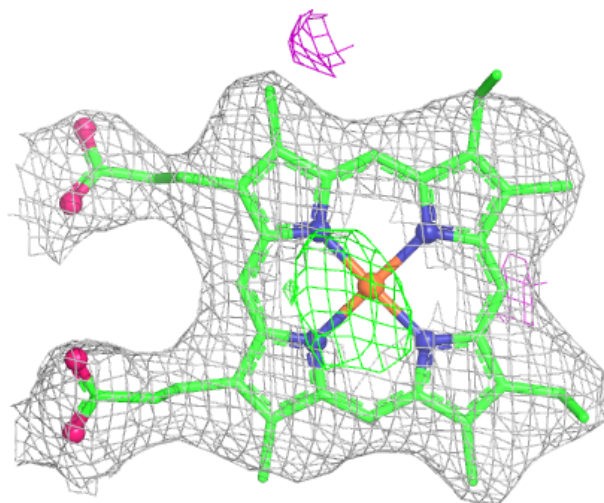
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	501	43/43	1.00	0.04	31,40,50,55	0
2	HEM	B	501	43/43	1.00	0.04	30,38,51,55	0
2	HEM	C	501	43/43	1.00	0.03	47,50,56,59	0
2	HEM	D	501	43/43	1.00	0.03	48,50,56,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

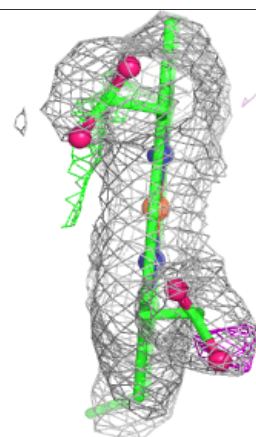
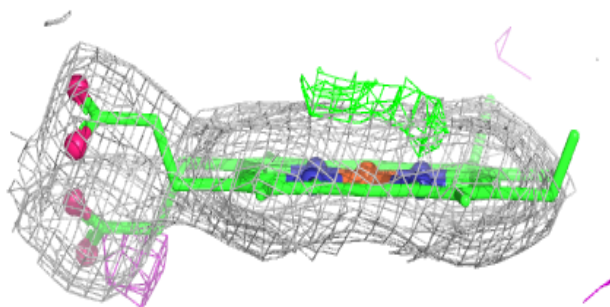
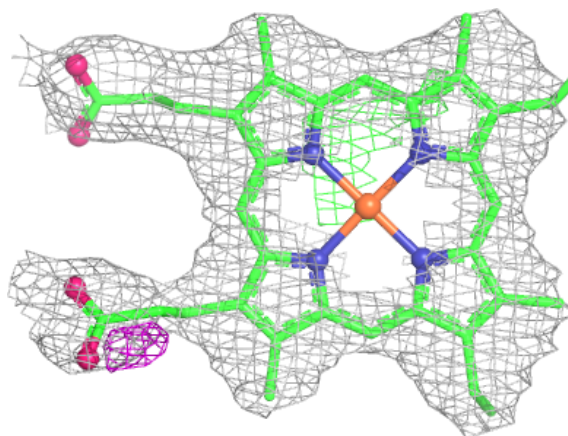
Electron density around HEM A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



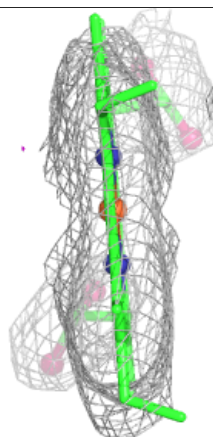
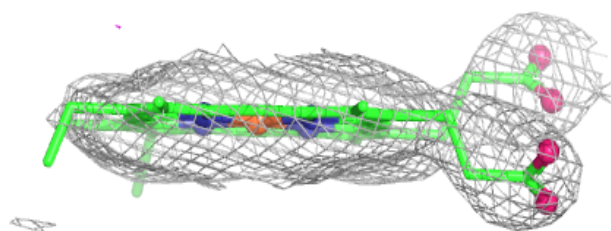
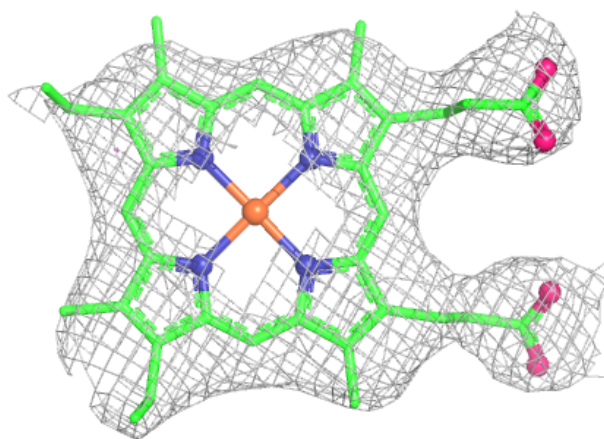
Electron density around HEM B 501:

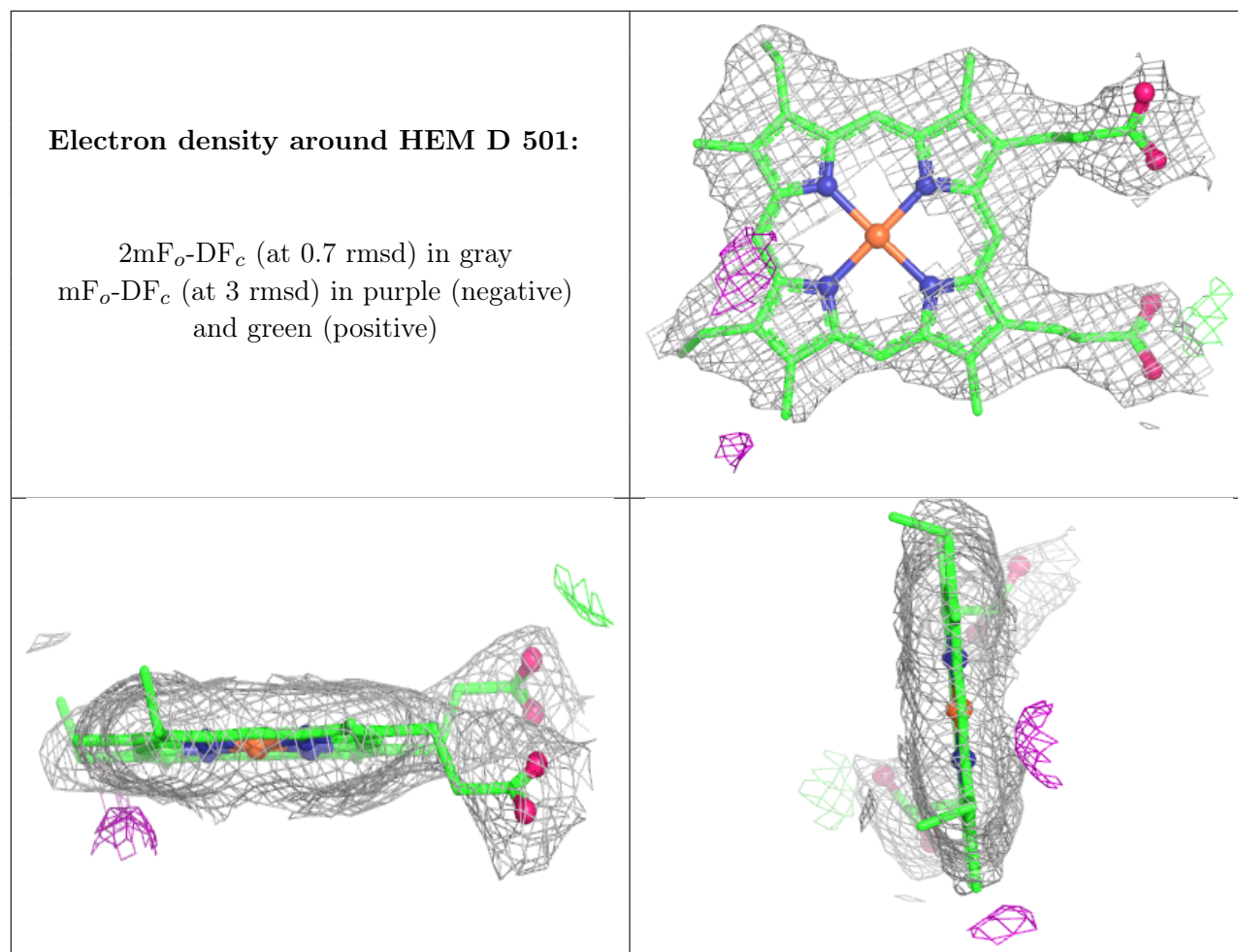
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.