



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:33 AM UTC

PDB ID : 3BCC / pdb_00003bcc
Title : STIGMATELLIN AND ANTIMYCIN BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.; Crofts, A.R.; Berry, E.A.; Kim, S.-H.
Deposited on : 1998-03-23
Resolution : 3.70 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:

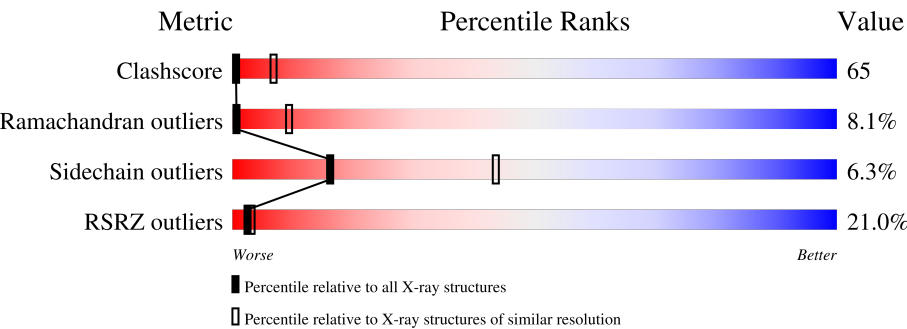
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	446	22% 26%61%12%..
2	B	422	31% 28%56%12%..
3	C	380	8% 15%66%17%.
4	D	241	14% 25%61%13%.
5	E	196	34% 24%60%15%.
6	F	109	9% 34%41%16%.8%

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Mol	Chain	Length	Quality of chain
7	G	81	
8	H	78	
9	I	33	
10	J	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	FES	E	197	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 15645 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 UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3423	2147	601	657	18			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	TYR	THR	conflict	UNP P31800
A	23	VAL	LEU	conflict	UNP P31800
A	59	LEU	VAL	conflict	UNP P31800
A	72	GLN	GLY	conflict	UNP P31800
A	91	SER	THR	conflict	UNP P31800
A	106	VAL	LEU	conflict	UNP P31800
A	135	VAL	LEU	conflict	UNP P31800
A	136	ARG	GLN	conflict	UNP P31800
A	147	GLU	ASP	conflict	UNP P31800
A	162	GLY	PRO	conflict	UNP P31800
A	174	ILE	VAL	conflict	UNP P31800
A	188	THR	ARG	conflict	UNP P31800
A	191	THR	LYS	conflict	UNP P31800
A	203	VAL	LEU	conflict	UNP P31800
A	206	GLN	ARG	conflict	UNP P31800
A	210	GLU	ASP	conflict	UNP P31800
A	217	GLY	SER	conflict	UNP P31800
A	219	VAL	LEU	conflict	UNP P31800
A	220	PRO	SER	conflict	UNP P31800
A	221	PHE	GLY	conflict	UNP P31800
A	225	ASP	GLU	conflict	UNP P31800
A	233	LYS	PRO	conflict	UNP P31800
A	242	ARG	CYS	conflict	UNP P31800
A	267	LEU	ASN	conflict	UNP P31800
A	282	ARG	CYS	conflict	UNP P31800
A	288	LEU	ALA	conflict	UNP P31800
A	290	SER	LEU	conflict	UNP P31800

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Chain	Residue	Modelled	Actual	Comment	Reference
A	299	VAL	ALA	conflict	UNP P31800
A	311	SER	ASN	conflict	UNP P31800
A	315	SER	ALA	conflict	UNP P31800
A	316	GLU	ASP	conflict	UNP P31800
A	320	PHE	LEU	conflict	UNP P31800
A	322	PHE	ALA	conflict	UNP P31800
A	323	TYR	HIS	conflict	UNP P31800
A	328	ARG	HIS	conflict	UNP P31800
A	349	ILE	ALA	conflict	UNP P31800
A	350	SER	THR	conflict	UNP P31800
A	360	PHE	LEU	conflict	UNP P31800
A	382	GLU	SER	conflict	UNP P31800
A	393	GLU	ALA	conflict	UNP P31800
A	397	GLU	SER	conflict	UNP P31800
A	399	LEU	ILE	conflict	UNP P31800
A	406	MET	VAL	conflict	UNP P31800
A	415	ILE	PHE	conflict	UNP P31800
A	425	PRO	PHE	conflict	UNP P31800

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			2994	1878	518	591	7			

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ILE	PHE	conflict	UNP P23004
B	28	LYS	ARG	conflict	UNP P23004
B	42	SER	ALA	conflict	UNP P23004
B	44	GLY	ALA	conflict	UNP P23004
B	46	THR	ARG	conflict	UNP P23004
B	49	VAL	LEU	conflict	UNP P23004
B	61	SER	ASN	conflict	UNP P23004
B	99	GLU	THR	conflict	UNP P23004
B	117	GLU	ASP	conflict	UNP P23004
B	134	PRO	ARG	conflict	UNP P23004
B	139	ASP	ALA	conflict	UNP P23004
B	145	LYS	ARG	conflict	UNP P23004
B	152	PHE	LEU	conflict	UNP P23004
B	157	THR	ALA	conflict	UNP P23004

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Chain	Residue	Modelled	Actual	Comment	Reference
B	174	ASP	ASN	conflict	UNP P23004
B	188	SER	PRO	conflict	UNP P23004
B	194	PHE	TYR	conflict	UNP P23004
B	207	VAL	ILE	conflict	UNP P23004
B	218	ASN	GLN	conflict	UNP P23004
B	223	LEU	PHE	conflict	UNP P23004
B	240	ARG	HIS	conflict	UNP P23004
B	257	ILE	LEU	conflict	UNP P23004
B	266	GLY	SER	conflict	UNP P23004
B	282	ASN	GLY	conflict	UNP P23004
B	304	LEU	SER	conflict	UNP P23004
B	332	TYR	SER	conflict	UNP P23004
B	335	GLN	ASP	conflict	UNP P23004
B	352	VAL	LEU	conflict	UNP P23004
B	355	GLU	PRO	conflict	UNP P23004
B	356	ASN	ASP	conflict	UNP P23004
B	367	LYS	GLY	conflict	UNP P23004
B	380	GLU	ASP	conflict	UNP P23004
B	393	ASN	THR	conflict	UNP P23004
B	412	LYS	ASN	conflict	UNP P23004
B	420	ARG	GLY	conflict	UNP P23004
B	421	GLN	ARG	conflict	UNP P23004
B	436	VAL	ILE	conflict	UNP P23004

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3002	2013	473	504	12			

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1899	1214	326	345	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PRO	LEU	conflict	UNP P00125
D	143	VAL	LEU	conflict	UNP P00125
D	167	ASP	GLU	conflict	UNP P00125

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Chain	Residue	Modelled	Actual	Comment	Reference
D	216	VAL	LEU	conflict	UNP P00125
D	221	TYR	ALA	conflict	UNP P00125

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1512	953	266	285	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ASN	ASP	conflict	UNP P13272
E	17	PRO	GLU	conflict	UNP P13272
E	18	ASP	VAL	conflict	UNP P13272
E	19	ASP	LEU	conflict	UNP P13272
E	20	TYR	ASP	conflict	UNP P13272
E	26	ARG	LYS	conflict	UNP P13272
E	29	ASP	SER	conflict	UNP P13272
E	30	PRO	GLU	conflict	UNP P13272
E	31	SER	ALA	conflict	UNP P13272
E	42	VAL	THR	conflict	UNP P13272
E	45	LEU	VAL	conflict	UNP P13272
E	56	THR	SER	conflict	UNP P13272

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			875	557	153	162	3			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	29	TYR	LEU	conflict	UNP P00129
F	38	TYR	HIS	conflict	UNP P00129
F	59	MET	VAL	conflict	UNP P00129
F	69	ASN	SER	conflict	UNP P00129
F	87	VAL	LYS	conflict	UNP P00129
F	88	PRO	SER	conflict	UNP P00129
F	108	ASP	ALA	conflict	UNP P00129

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	78	Total	C	N	O	S	0	0	0
			626	411	114	100	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	LEU	VAL	conflict	UNP P13271
G	25	PRO	ALA	conflict	UNP P13271
G	34	VAL	ILE	conflict	UNP P13271
G	38	TRP	LEU	conflict	UNP P13271
G	41	LEU	THR	conflict	UNP P13271
G	53	LEU	VAL	conflict	UNP P13271
G	58	LEU	VAL	conflict	UNP P13271
G	78	VAL	GLU	conflict	UNP P13271

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			490	301	88	96	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	59	PHE	LEU	conflict	UNP P00126

- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	0	0	0
			159	92	33	34			

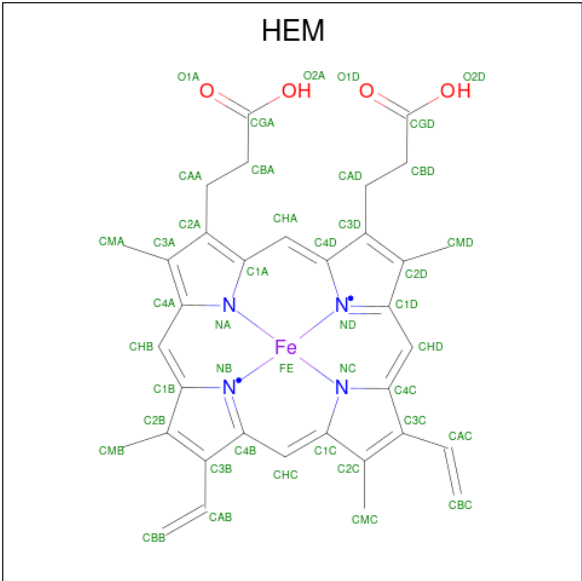
- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			459	299	78	82			

There is a discrepancy between the modelled and reference sequences:

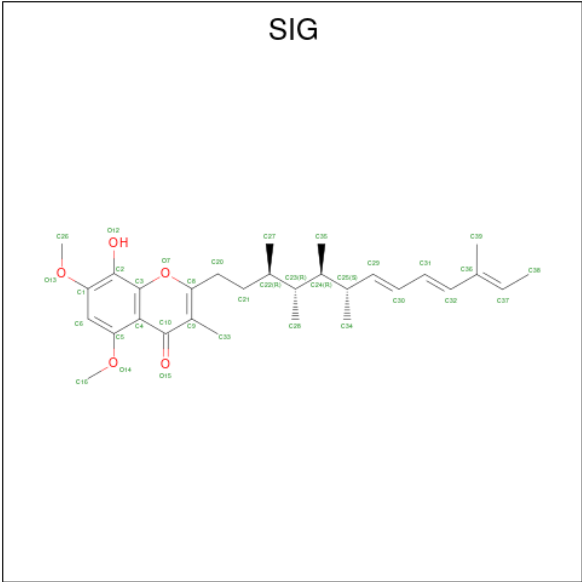
Chain	Residue	Modelled	Actual	Comment	Reference
J	30	LEU	PHE	conflict	UNP P00130

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



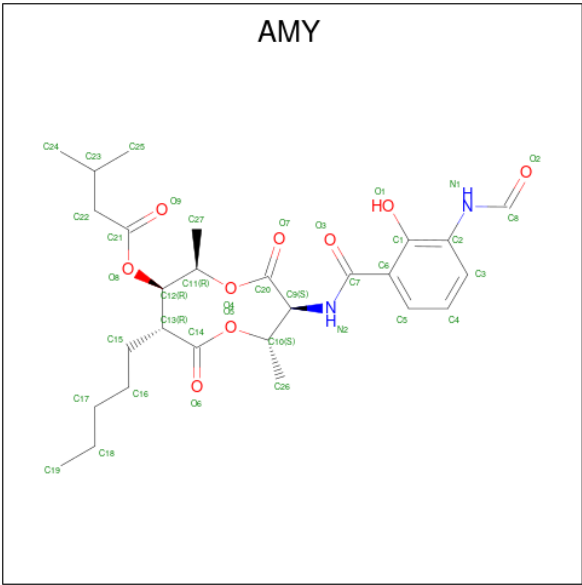
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 12 is STIGMATELLIN (CCD ID: SIG) (formula: $C_{30}H_{42}O_5$).



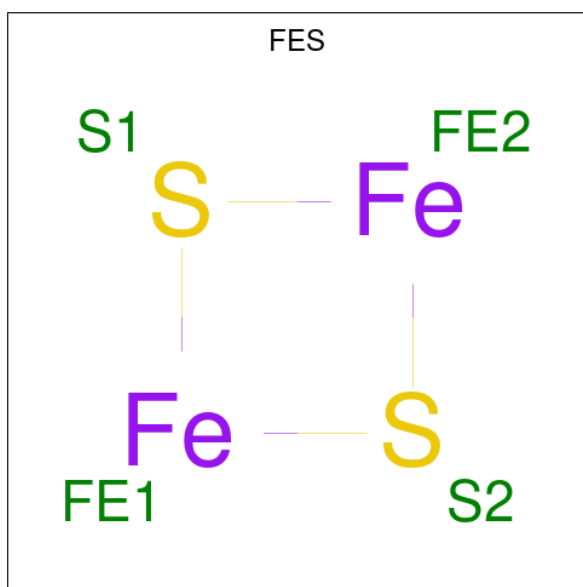
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			35	30	5		

- Molecule 13 is ANTIMYCIN (CCD ID: AMY) (formula: C₂₇H₃₈N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			38	27	2	9		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

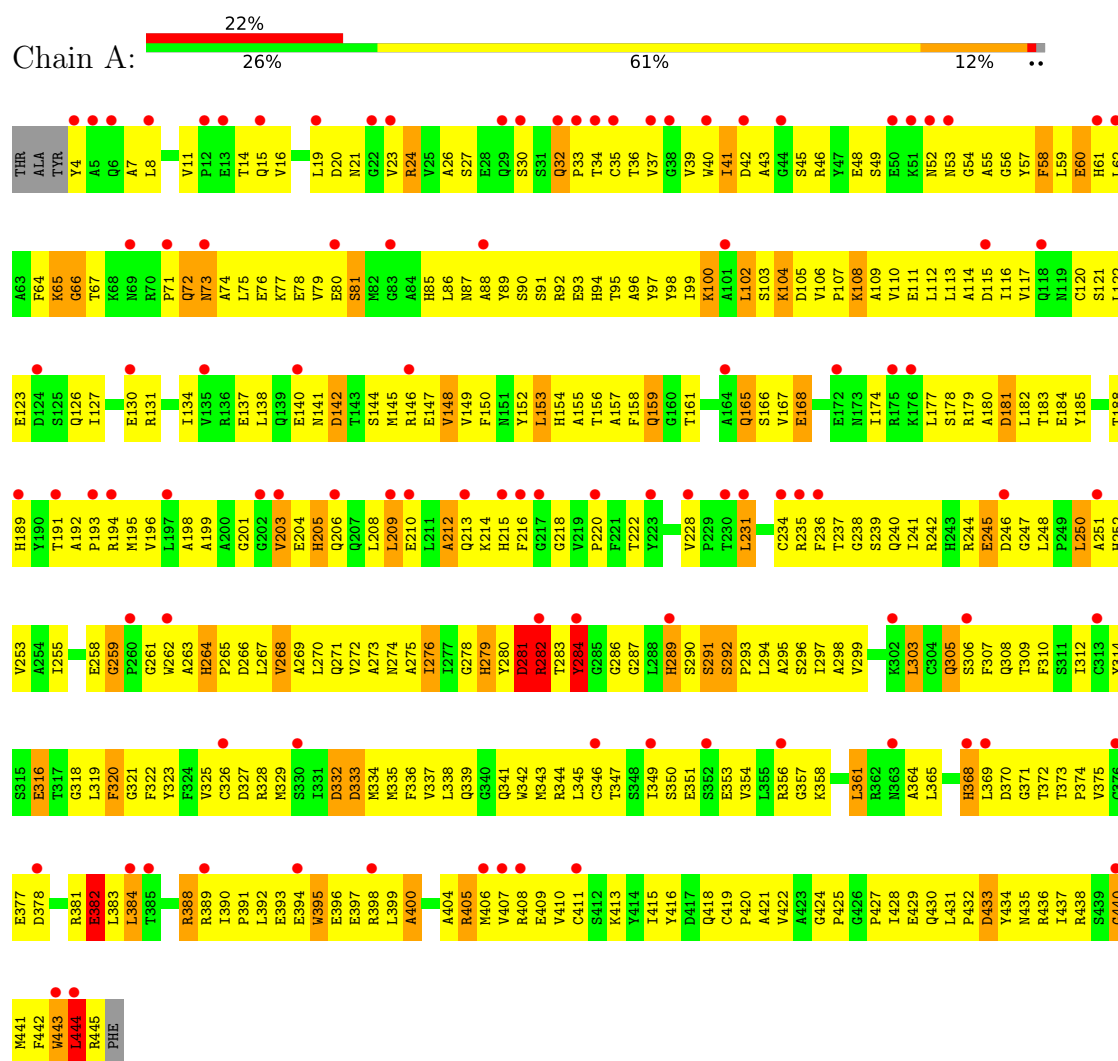


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	E	1	Total	Fe	S	0	0
			4	2	2		

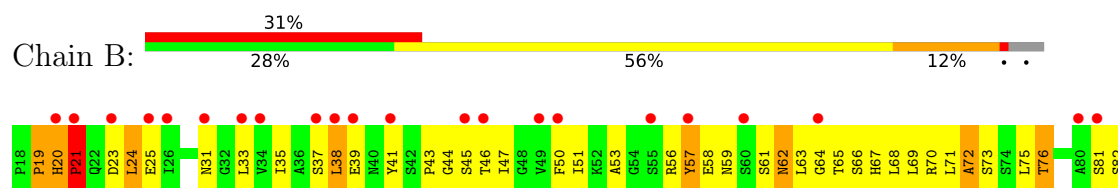
3 Residue-property plots

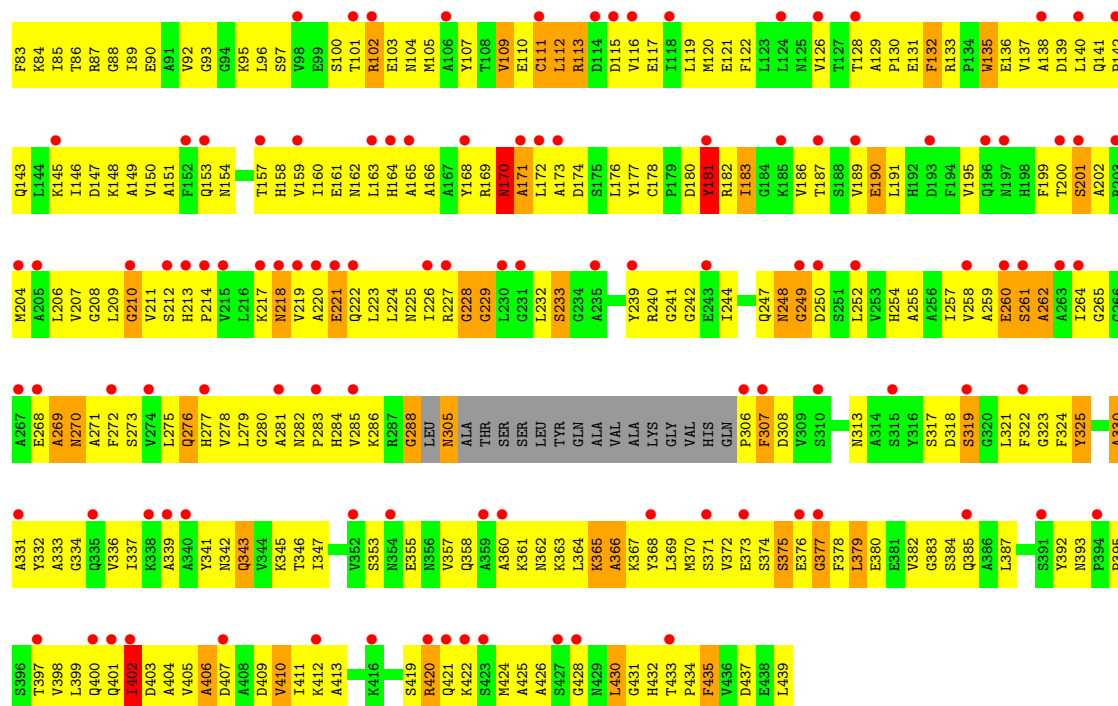
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

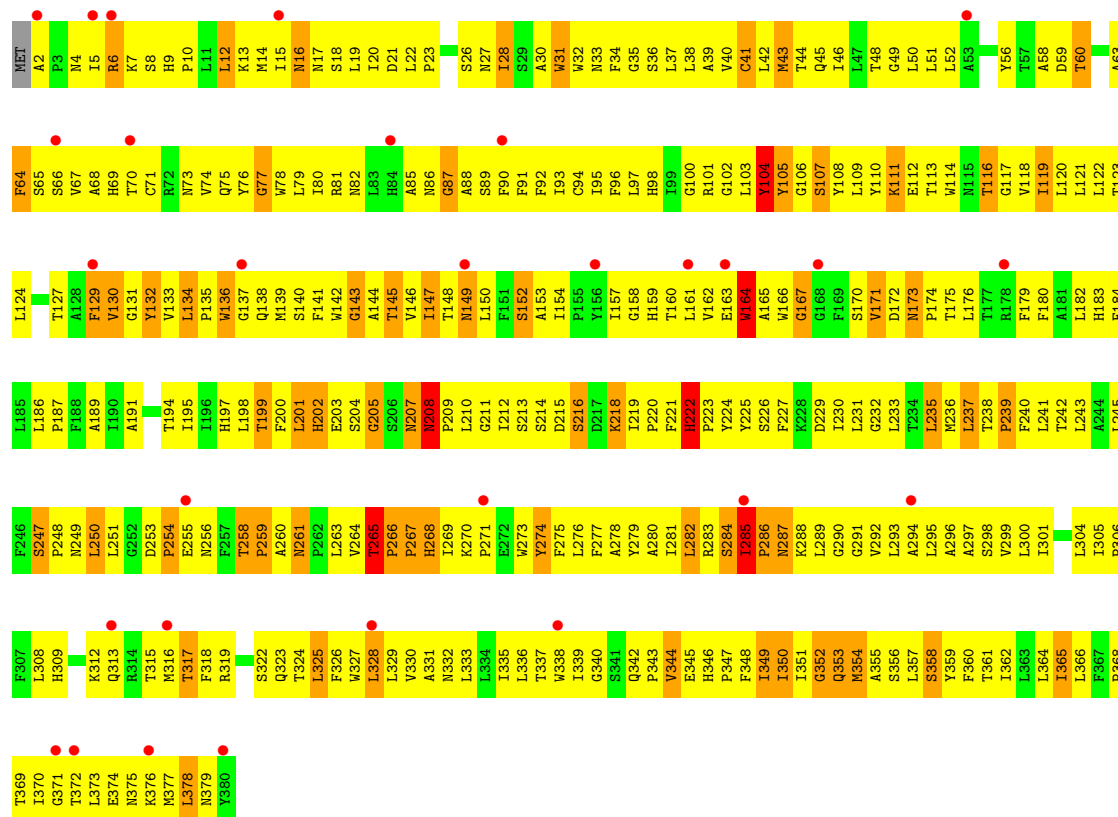


• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

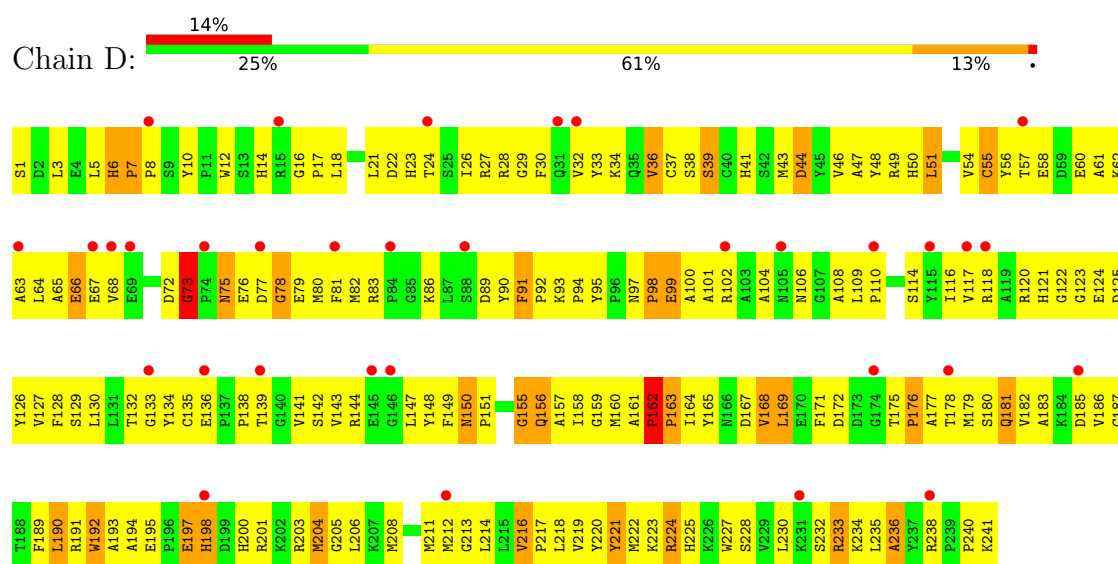




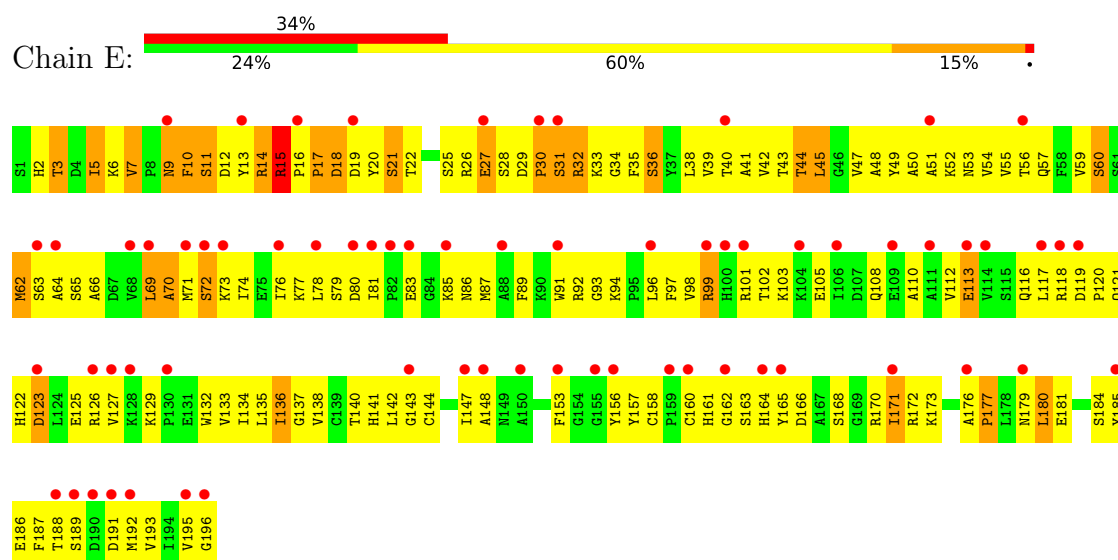
• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



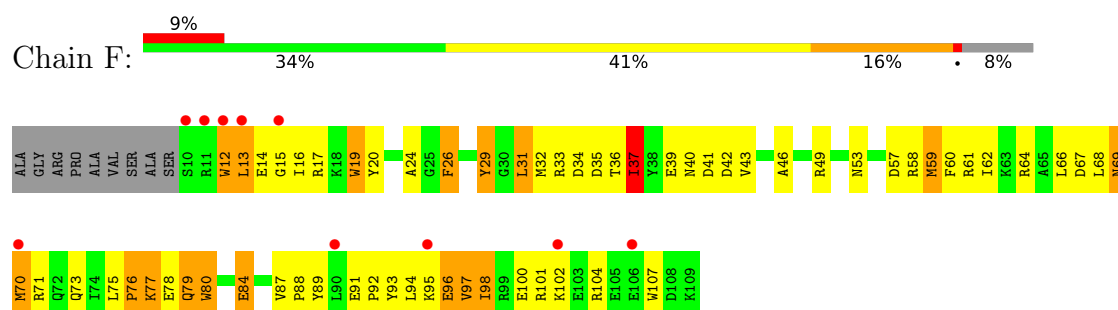
• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

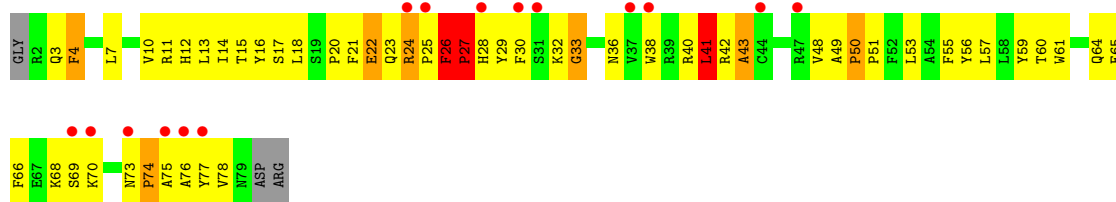


• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

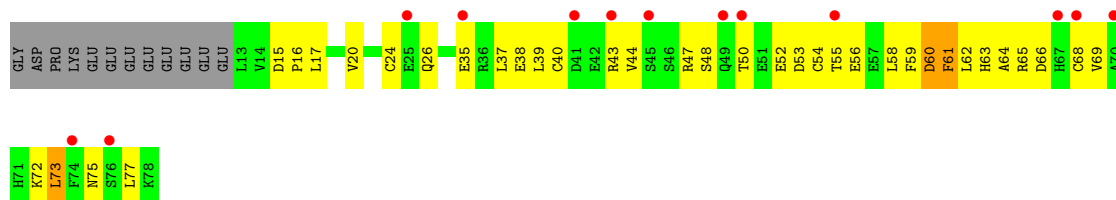


• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE





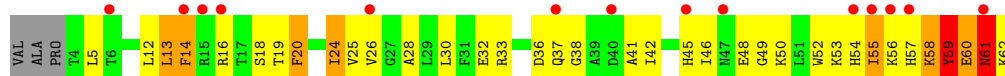
● Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



● Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



● Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.18Å 179.73Å 238.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.70 12.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	91.8 (12.00-3.70) 82.5 (12.00-3.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.71 (at 3.19Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.289 , 0.321 0.282 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.66	EDS
Total number of atoms	15645	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: AMY, FES, HEM, SIG

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	0.62	0/3495	1.18	32/4742 (0.7%)
2	B	0.60	1/3046 (0.0%)	1.08	13/4132 (0.3%)
3	C	0.80	0/3104	1.24	33/4252 (0.8%)
4	D	0.70	0/1960	1.29	30/2665 (1.1%)
5	E	0.69	1/1548 (0.1%)	1.15	16/2095 (0.8%)
6	F	0.64	0/896	1.11	7/1206 (0.6%)
7	G	0.68	0/648	2.54	10/882 (1.1%)
8	H	0.55	0/495	1.00	1/669 (0.1%)
10	J	0.77	0/470	1.20	6/635 (0.9%)
All	All	0.68	2/15662 (0.0%)	1.26	148/21278 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	288	GLY	CA-C	6.19	1.58	1.52
5	E	6	LYS	CD-CE	5.11	1.67	1.52

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	26	PHE	CA-C-N	44.92	175.99	119.84
7	G	26	PHE	C-N-CA	44.92	175.99	119.84
4	D	76	GLU	N-CA-C	-15.69	94.27	113.41
1	A	66	GLY	N-CA-C	12.83	125.12	112.04
7	G	26	PHE	C-N-CD	-11.89	76.25	125.00
1	A	287	GLY	N-CA-C	-11.20	96.12	115.61
1	A	20	ASP	N-CA-C	-10.07	100.92	113.01
7	G	76	ALA	N-CA-C	-10.04	101.03	113.38
7	G	24	ARG	CA-C-N	10.02	129.77	118.85
7	G	24	ARG	C-N-CA	10.02	129.77	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	13	LEU	N-CA-C	-10.01	100.37	111.28
3	C	267	PRO	N-CA-C	-9.78	96.04	110.80
1	A	329	MET	N-CA-C	9.65	124.39	112.23
3	C	237	LEU	N-CA-C	-9.22	100.92	113.18
3	C	344	VAL	N-CA-C	9.21	119.91	106.55
3	C	328	LEU	N-CA-C	-9.15	101.31	111.28
10	J	59	TYR	N-CA-C	-8.77	100.94	113.21
3	C	36	SER	N-CA-C	-8.68	101.89	111.36
4	D	44	ASP	N-CA-C	8.49	123.38	112.34
5	E	31	SER	N-CA-C	-8.38	101.99	112.72
7	G	41	LEU	N-CA-C	-8.28	101.31	111.33
7	G	27	PRO	CA-N-CD	-8.24	100.47	112.00
4	D	6	HIS	CA-C-N	7.99	128.61	120.38
4	D	6	HIS	C-N-CA	7.99	128.61	120.38
5	E	7	VAL	N-CA-C	-7.95	99.73	107.76
10	J	61	ASN	N-CA-C	7.94	127.72	110.80
4	D	155	GLY	N-CA-C	-7.89	104.42	114.37
4	D	7	PRO	CA-C-N	7.75	127.67	119.85
4	D	7	PRO	C-N-CA	7.75	127.67	119.85
5	E	3	THR	N-CA-C	-7.70	103.68	113.23
1	A	368	HIS	N-CA-C	-7.68	102.92	111.82
3	C	317	THR	N-CA-C	-7.60	103.84	113.72
3	C	87	GLY	N-CA-C	-7.44	103.75	112.83
3	C	325	LEU	N-CA-C	-7.43	103.18	111.28
5	E	25	SER	N-CA-C	-7.42	103.21	111.82
5	E	60	SER	N-CA-C	-7.27	104.01	113.17
7	G	32	LYS	N-CA-C	-7.13	105.19	114.04
1	A	231	LEU	N-CA-C	7.11	121.00	110.48
1	A	142	ASP	N-CA-C	7.03	118.59	111.07
1	A	276	ILE	N-CA-C	7.01	117.81	110.72
3	C	145	THR	N-CA-C	6.91	119.66	111.71
2	B	377	GLY	N-CA-C	-6.82	106.39	115.32
2	B	183	ILE	N-CA-C	6.81	118.39	110.62
4	D	216	VAL	CA-C-N	-6.73	111.43	119.84
4	D	216	VAL	C-N-CA	-6.73	111.43	119.84
2	B	153	GLN	N-CA-C	-6.72	104.55	112.89
3	C	132	TYR	N-CA-C	-6.58	104.51	112.54
4	D	66	GLU	N-CA-C	-6.55	104.14	111.28
4	D	150	ASN	CA-C-N	6.42	126.64	119.32
4	D	150	ASN	C-N-CA	6.42	126.64	119.32
3	C	104	TYR	N-CA-C	6.34	120.94	111.81
5	E	118	ARG	N-CA-C	-6.34	104.30	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	99	ARG	N-CA-C	6.30	119.77	109.24
1	A	400	ALA	N-CA-C	-6.30	105.17	112.92
3	C	77	GLY	N-CA-C	-6.22	105.26	112.73
4	D	221	TYR	N-CA-C	-6.19	103.47	111.02
3	C	143	GLY	N-CA-C	-6.17	105.02	112.49
1	A	303	LEU	N-CA-C	6.16	117.79	111.14
5	E	18	ASP	N-CA-C	-6.14	104.40	113.61
1	A	104	LYS	N-CA-C	-6.13	105.85	113.15
3	C	261	ASN	CA-C-N	6.04	125.74	119.82
3	C	261	ASN	C-N-CA	6.04	125.74	119.82
1	A	282	ARG	N-CA-C	6.04	123.67	110.80
2	B	93	GLY	N-CA-C	-6.04	103.53	114.46
1	A	212	ALA	N-CA-C	-6.01	104.36	111.03
10	J	24	ILE	N-CA-C	-6.00	104.66	110.42
2	B	276	GLN	N-CA-C	-5.99	104.66	111.07
4	D	110	PRO	CA-C-N	5.95	125.89	119.76
4	D	110	PRO	C-N-CA	5.95	125.89	119.76
10	J	13	LEU	N-CA-C	5.93	120.56	112.68
1	A	264	HIS	CA-C-N	5.92	125.60	119.56
1	A	264	HIS	C-N-CA	5.92	125.60	119.56
4	D	77	ASP	N-CA-C	-5.92	105.82	113.16
1	A	259	GLY	CA-C-N	5.90	125.11	118.97
1	A	259	GLY	C-N-CA	5.90	125.11	118.97
6	F	24	ALA	N-CA-C	-5.86	104.89	111.28
2	B	403	ASP	N-CA-C	-5.84	104.92	111.28
3	C	129	PHE	N-CA-C	-5.83	104.85	111.14
6	F	80	TRP	N-CA-C	-5.82	102.80	110.43
5	E	143	GLY	N-CA-C	5.78	123.87	115.32
1	A	203	VAL	N-CA-C	5.78	117.95	109.63
3	C	285	ILE	CA-C-N	5.77	127.06	119.84
3	C	285	ILE	C-N-CA	5.77	127.06	119.84
2	B	212	SER	N-CA-C	-5.77	99.89	109.46
10	J	55	ILE	N-CA-C	-5.76	107.65	113.47
1	A	248	LEU	CA-C-N	5.75	125.22	119.24
1	A	248	LEU	C-N-CA	5.75	125.22	119.24
1	A	305	GLN	N-CA-C	-5.74	105.16	111.82
4	D	41	HIS	N-CA-C	5.74	118.01	108.20
7	G	78	VAL	N-CA-C	-5.73	105.28	113.07
1	A	440	GLY	N-CA-C	-5.72	105.65	115.61
3	C	265	THR	N-CA-C	-5.71	102.59	109.72
3	C	358	SER	N-CA-C	-5.71	105.06	111.28
3	C	41	CYS	N-CA-C	-5.69	103.90	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	185	TYR	N-CA-C	5.67	116.88	108.60
6	F	96	GLU	N-CA-C	-5.67	104.10	111.02
2	B	365	LYS	N-CA-C	-5.66	104.48	111.33
4	D	73	GLY	CA-C-N	5.65	125.60	119.78
4	D	73	GLY	C-N-CA	5.65	125.60	119.78
2	B	402	ILE	N-CA-C	-5.65	104.84	111.00
1	A	320	PHE	CA-C-N	-5.63	117.83	122.16
1	A	320	PHE	C-N-CA	-5.63	117.83	122.16
1	A	32	GLN	N-CA-C	5.62	122.23	109.81
1	A	284	TYR	N-CA-C	5.61	122.74	110.80
4	D	142	SER	N-CA-C	5.59	117.97	108.02
8	H	43	ARG	N-CA-C	-5.59	106.63	113.50
4	D	93	LYS	N-CA-C	-5.56	103.06	110.07
4	D	204	MET	N-CA-C	-5.55	104.25	111.02
1	A	153	LEU	N-CA-C	-5.52	104.96	110.97
2	B	379	LEU	N-CA-C	-5.51	106.26	112.87
3	C	226	SER	N-CA-C	-5.48	105.00	110.97
5	E	14	ARG	N-CA-C	-5.39	99.31	110.80
3	C	152	SER	N-CA-C	-5.38	105.42	111.28
6	F	29	TYR	N-CA-C	-5.38	106.22	112.89
6	F	79	GLN	N-CA-C	5.35	119.29	112.87
4	D	162	PRO	CA-C-N	5.33	127.19	121.00
4	D	162	PRO	C-N-CA	5.33	127.19	121.00
2	B	307	PHE	CB-CA-C	-5.27	106.91	114.87
10	J	53	LYS	N-CA-C	-5.27	105.65	111.71
3	C	365	ILE	N-CA-C	5.27	120.30	109.34
3	C	222	HIS	N-CA-C	5.25	121.41	109.81
1	A	32	GLN	CA-C-N	5.25	124.43	118.97
1	A	32	GLN	C-N-CA	5.25	124.43	118.97
3	C	116	THR	N-CA-C	-5.25	104.81	111.11
1	A	424	GLY	CA-C-N	5.25	126.40	119.84
1	A	424	GLY	C-N-CA	5.25	126.40	119.84
5	E	10	PHE	N-CA-C	-5.24	106.28	113.30
6	F	26	PHE	N-CA-C	-5.23	106.90	113.28
1	A	24	ARG	N-CA-C	-5.20	100.42	108.90
5	E	103	LYS	N-CA-C	-5.19	105.31	110.97
5	E	5	ILE	N-CA-C	5.18	116.43	108.71
2	B	265	GLY	N-CA-C	-5.15	108.95	115.08
3	C	266	PRO	N-CA-C	5.15	116.99	110.70
4	D	114	SER	N-CA-C	-5.12	104.63	111.24
5	E	44	THR	N-CA-C	-5.12	104.97	111.11
4	D	7	PRO	N-CA-C	5.11	116.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	426	ALA	N-CA-C	5.10	116.82	108.55
3	C	6	ARG	N-CA-C	-5.09	106.77	112.87
3	C	107	SER	N-CA-C	-5.08	106.19	112.38
4	D	39	SER	N-CA-C	-5.06	106.25	114.09
3	C	247	SER	CA-C-N	5.05	126.16	119.84
3	C	247	SER	C-N-CA	5.05	126.16	119.84
3	C	134	LEU	N-CA-C	5.03	120.93	109.81
4	D	91	PHE	CA-C-N	5.02	125.02	119.90
4	D	91	PHE	C-N-CA	5.02	125.02	119.90
4	D	24	THR	N-CA-C	-5.02	105.70	111.07
5	E	15	ARG	N-CA-C	5.01	120.88	109.81
3	C	378	LEU	N-CA-C	-5.00	106.76	114.16

There are no chirality outliers.

There are no planarity outliers.

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	3423	0	3286	473	0
2	B	2994	0	2906	350	0
3	C	3002	0	3036	540	0
4	D	1899	0	1822	274	1
5	E	1512	0	1483	194	0
6	F	875	0	839	101	1
7	G	626	0	591	70	0
8	H	490	0	445	48	0
9	I	159	0	43	21	0
10	J	459	0	424	61	0
11	C	86	0	60	23	0
11	D	43	0	30	6	0
12	C	35	0	42	15	0
13	C	38	0	36	15	0
14	E	4	0	0	2	0
All	All	15645	0	15043	2004	1

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 65.

All (2004) 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)
3:C:107:SER:HB3	11:C:382:HEM:HBD1	1.22	1.17
3:C:43:MET:HA	3:C:43:MET:HE2	1.27	1.16
3:C:316:MET:SD	3:C:319:ARG:HG3	1.90	1.11
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.31	1.11
3:C:146:VAL:HG23	3:C:147:ILE:H	1.15	1.08
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.14	1.07
3:C:327:TRP:HA	3:C:330:VAL:HG12	1.33	1.07
2:B:76:THR:HG22	2:B:82:SER:H	1.18	1.07
1:A:361:LEU:HD13	1:A:399:LEU:HD22	1.38	1.06
4:D:158:ILE:HG22	4:D:160:MET:H	1.05	1.05
1:A:159:GLN:HE21	5:E:7:VAL:HG11	1.21	1.01
3:C:325:LEU:HD11	3:C:366:LEU:HB3	1.36	1.01
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.27	1.00
2:B:62:ASN:C	2:B:62:ASN:HD22	1.67	0.99
2:B:280:GLY:H	2:B:283:PRO:HD2	1.28	0.98
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.43	0.98
3:C:167:GLY:N	3:C:175:THR:HG22	1.78	0.98
4:D:102:ARG:HH11	4:D:109:LEU:HB2	1.29	0.97
1:A:382:GLU:HG2	1:A:389:ARG:HA	1.46	0.97
4:D:54:VAL:HG21	4:D:192:TRP:CZ3	2.00	0.96
3:C:138:GLN:NE2	3:C:261:ASN:H	1.65	0.95
1:A:159:GLN:NE2	5:E:7:VAL:HG11	1.81	0.95
2:B:241:GLY:HA3	2:B:421:GLN:HE21	1.30	0.94
1:A:436:ARG:HD3	3:C:223:PRO:HD3	1.50	0.93
2:B:337:ILE:HD11	2:B:434:PRO:HD2	1.49	0.93
2:B:168:TYR:CB	2:B:173:ALA:HB2	1.98	0.93
1:A:281:ASP:HB3	1:A:284:TYR:HE1	1.34	0.93
4:D:158:ILE:CG2	4:D:160:MET:H	1.83	0.92
3:C:107:SER:CB	11:C:382:HEM:HBD1	2.00	0.92
3:C:120:LEU:HG	11:C:382:HEM:HBB2	1.52	0.90
1:A:297:ILE:HG21	1:A:337:VAL:HG11	1.49	0.90
2:B:258:VAL:HG13	2:B:322:PHE:H	1.34	0.90
4:D:158:ILE:HG22	4:D:160:MET:N	1.87	0.89
5:E:29:ASP:C	5:E:31:SER:H	1.79	0.89
3:C:43:MET:HA	3:C:43:MET:CE	2.02	0.89
2:B:250:ASP:O	2:B:252:LEU:HD23	1.73	0.89
1:A:49:SER:H	1:A:52:ASN:HB3	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:ARG:CZ	3:C:374:GLU:HB2	2.03	0.88
3:C:147:ILE:O	3:C:150:LEU:HB3	1.73	0.88
5:E:45:LEU:HD11	10:J:28:ALA:HA	1.54	0.88
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.56	0.87
1:A:166:SER:OG	5:E:3:THR:HG23	1.74	0.87
1:A:349:ILE:HG22	1:A:408:ARG:HG3	1.56	0.86
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.58	0.86
4:D:164:ILE:HD11	4:D:182:VAL:HG13	1.55	0.85
2:B:101:THR:HB	2:B:104:ASN:OD1	1.76	0.85
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.11	0.85
3:C:167:GLY:H	3:C:175:THR:HG22	1.39	0.85
5:E:13:TYR:O	5:E:14:ARG:HD3	1.75	0.85
3:C:283:ARG:HG3	3:C:283:ARG:O	1.76	0.85
3:C:242:THR:HA	4:D:208:MET:HE1	1.59	0.85
10:J:57:HIS:HB2	10:J:61:ASN:C	2.02	0.84
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.59	0.84
1:A:346:CYS:HB3	1:A:411:CYS:HB2	1.57	0.84
10:J:57:HIS:O	10:J:61:ASN:N	2.11	0.84
1:A:343:MET:HE2	1:A:343:MET:HA	1.60	0.83
3:C:207:ASN:O	3:C:208:ASN:HB3	1.76	0.83
1:A:210:GLU:O	1:A:214:LYS:HB2	1.78	0.83
1:A:345:LEU:HD12	1:A:349:ILE:HD12	1.60	0.83
2:B:69:LEU:HD12	2:B:105:MET:HE1	1.61	0.82
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.60	0.82
1:A:406:MET:O	1:A:410:VAL:HG23	1.80	0.82
3:C:166:TRP:HB2	3:C:175:THR:CG2	2.08	0.82
4:D:28:ARG:HD2	4:D:171:PHE:CD2	2.14	0.82
3:C:146:VAL:HG23	3:C:147:ILE:N	1.90	0.81
2:B:128:THR:C	2:B:130:PRO:HD3	2.04	0.81
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.60	0.81
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.10	0.81
4:D:165:TYR:O	4:D:168:VAL:HG23	1.79	0.81
1:A:250:LEU:HD21	1:A:325:VAL:HG13	1.61	0.81
3:C:342:GLN:HB3	3:C:348:PHE:CE2	2.16	0.81
2:B:96:LEU:HD23	2:B:97:SER:N	1.95	0.81
9:I:107:UNK:HA	9:I:115:UNK:O	1.80	0.81
3:C:372:THR:HA	3:C:375:ASN:HD22	1.45	0.81
8:H:69:VAL:O	8:H:73:LEU:HB2	1.80	0.81
2:B:146:ILE:HG13	2:B:147:ASP:N	1.96	0.80
2:B:168:TYR:CE2	2:B:172:LEU:HD23	2.16	0.80
3:C:92:PHE:O	3:C:95:ILE:HG22	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB1	1:A:96:ALA:O	1.82	0.80
5:E:72:SER:O	5:E:196:GLY:HA3	1.82	0.80
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.45	0.80
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.06	0.80
1:A:333:ASP:O	1:A:337:VAL:HG23	1.82	0.79
2:B:357:VAL:HG11	2:B:406:ALA:HB1	1.62	0.79
3:C:27:ASN:HD22	6:F:69:ASN:ND2	1.79	0.79
4:D:214:LEU:O	4:D:218:LEU:HG	1.80	0.79
1:A:61:HIS:HE2	1:A:137:GLU:CD	1.89	0.79
2:B:280:GLY:H	2:B:283:PRO:CD	1.95	0.79
3:C:370:ILE:O	3:C:374:GLU:HG3	1.83	0.79
4:D:233:ARG:HB3	6:F:71:ARG:HH21	1.47	0.79
1:A:36:THR:HG22	1:A:100:LYS:CB	2.11	0.79
3:C:327:TRP:HA	3:C:330:VAL:CG1	2.12	0.79
2:B:143:GLN:OE1	2:B:146:ILE:HD11	1.81	0.79
3:C:316:MET:HE3	3:C:322:SER:OG	1.82	0.79
3:C:27:ASN:HB2	6:F:69:ASN:ND2	1.97	0.78
1:A:189:HIS:HD2	1:A:194:ARG:HH12	1.31	0.78
1:A:276:ILE:HD13	1:A:349:ILE:HD11	1.66	0.78
3:C:130:VAL:HG12	3:C:131:GLY:H	1.46	0.78
10:J:57:HIS:C	10:J:59:TYR:H	1.88	0.78
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.66	0.78
5:E:11:SER:HA	5:E:15:ARG:HD2	1.63	0.78
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.64	0.78
3:C:285:ILE:HG23	3:C:291:GLY:HA2	1.63	0.77
2:B:132:PHE:CE2	2:B:191:LEU:HB3	2.20	0.77
1:A:291:SER:O	1:A:293:PRO:N	2.17	0.77
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.00	0.77
1:A:252:HIS:HB3	1:A:323:TYR:HE1	1.50	0.77
4:D:46:VAL:HG12	4:D:47:ALA:H	1.50	0.77
3:C:275:PHE:CG	12:C:383:SIG:H332	2.20	0.77
1:A:391:PRO:HG2	1:A:394:GLU:HB2	1.65	0.77
1:A:276:ILE:CD1	1:A:349:ILE:HD11	2.15	0.77
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.19	0.76
1:A:88:ALA:HB2	1:A:97:TYR:HA	1.66	0.76
2:B:24:LEU:HD23	2:B:24:LEU:H	1.48	0.76
1:A:328:ARG:HG3	1:A:427:PRO:HB2	1.68	0.76
2:B:199:PHE:C	2:B:204:MET:HE3	2.09	0.76
12:C:383:SIG:H333	12:C:383:SIG:H282	1.68	0.76
1:A:4:TYR:CG	2:B:113:ARG:HB3	2.21	0.76
2:B:62:ASN:C	2:B:62:ASN:ND2	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:ASP:O	5:E:31:SER:N	2.19	0.76
1:A:205:HIS:NE2	1:A:209:LEU:HD21	2.00	0.75
4:D:54:VAL:HG11	4:D:192:TRP:CH2	2.22	0.75
1:A:250:LEU:C	1:A:250:LEU:HD22	2.11	0.75
5:E:15:ARG:NH1	5:E:19:ASP:HB3	2.01	0.75
1:A:53:ASN:HD22	1:A:54:GLY:N	1.83	0.75
3:C:6:ARG:HA	3:C:12:LEU:HD22	1.67	0.75
1:A:279:HIS:HA	1:A:307:PHE:CE1	2.22	0.75
1:A:342:TRP:O	1:A:345:LEU:HB3	1.86	0.75
3:C:145:THR:O	3:C:149:ASN:HB2	1.87	0.75
4:D:167:ASP:O	4:D:169:LEU:N	2.20	0.75
4:D:233:ARG:HB3	6:F:71:ARG:NH2	2.00	0.75
5:E:76:ILE:HB	5:E:193:VAL:HG13	1.69	0.75
3:C:138:GLN:HE22	3:C:261:ASN:H	1.33	0.75
1:A:85:HIS:CB	9:I:314:UNK:HG1	2.16	0.75
1:A:46:ARG:NH1	1:A:316:GLU:OE2	2.18	0.75
2:B:272:PHE:O	2:B:276:GLN:N	2.20	0.75
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.16	0.75
1:A:242:ARG:O	7:G:14:ILE:HA	1.87	0.75
1:A:145:MET:HA	1:A:148:VAL:CG1	2.17	0.74
3:C:131:GLY:HA2	3:C:134:LEU:HD22	1.69	0.74
4:D:32:VAL:HG21	4:D:186:VAL:HG22	1.68	0.74
1:A:56:GLY:HA2	1:A:185:TYR:CE2	2.23	0.74
1:A:189:HIS:CD2	1:A:194:ARG:HH12	2.04	0.74
2:B:76:THR:CG2	2:B:82:SER:H	1.99	0.74
1:A:178:SER:HB2	1:A:181:ASP:OD1	1.88	0.74
2:B:132:PHE:CD2	2:B:191:LEU:HB3	2.22	0.74
2:B:258:VAL:CG1	2:B:322:PHE:H	2.01	0.74
1:A:102:LEU:HD12	1:A:102:LEU:H	1.53	0.74
3:C:76:TYR:HE1	4:D:200:HIS:HE1	1.36	0.74
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.23	0.74
2:B:154:ASN:O	2:B:157:THR:HG22	1.88	0.74
4:D:32:VAL:O	4:D:36:VAL:HG13	1.88	0.74
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.53	0.74
4:D:230:LEU:HB3	6:F:70:MET:HE3	1.70	0.74
10:J:57:HIS:HB2	10:J:61:ASN:O	1.87	0.73
2:B:379:LEU:O	2:B:379:LEU:HD13	1.88	0.73
2:B:76:THR:HG22	2:B:82:SER:N	2.01	0.73
4:D:224:ARG:HB3	4:D:224:ARG:HH11	1.53	0.73
3:C:12:LEU:HD23	3:C:12:LEU:O	1.89	0.73
3:C:138:GLN:NE2	3:C:261:ASN:N	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:ARG:NH1	4:D:109:LEU:HB2	2.03	0.72
4:D:212:MET:O	4:D:216:VAL:HG22	1.89	0.72
3:C:354:MET:HE2	3:C:354:MET:HA	1.70	0.72
2:B:248:ASN:C	2:B:248:ASN:HD22	1.97	0.72
3:C:101:ARG:HD2	3:C:101:ARG:C	2.14	0.72
3:C:253:ASP:OD1	3:C:255:GLU:N	2.21	0.72
5:E:5:ILE:HD13	7:G:14:ILE:HD13	1.70	0.72
2:B:341:TYR:OH	2:B:422:LYS:HE3	1.88	0.72
2:B:241:GLY:HA3	2:B:421:GLN:NE2	2.04	0.72
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.23	0.72
4:D:180:SER:HB2	8:H:17:LEU:HB2	1.71	0.72
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.71	0.72
1:A:382:GLU:HG2	1:A:389:ARG:HD2	1.71	0.72
3:C:327:TRP:CA	3:C:330:VAL:HG12	2.17	0.72
3:C:127:THR:HG22	3:C:186:LEU:HB3	1.71	0.72
3:C:325:LEU:HD12	3:C:370:ILE:HG13	1.70	0.72
1:A:283:THR:HG21	9:I:114:UNK:CB	2.20	0.72
2:B:209:LEU:HG	2:B:379:LEU:HD23	1.72	0.71
3:C:127:THR:HG22	3:C:186:LEU:HD13	1.70	0.71
5:E:26:ARG:O	5:E:28:SER:N	2.20	0.71
4:D:75:ASN:HB2	4:D:78:GLY:N	2.04	0.71
3:C:282:LEU:HD22	3:C:291:GLY:O	1.90	0.71
3:C:271:PRO:HG2	3:C:276:LEU:HD23	1.73	0.71
1:A:108:LYS:O	1:A:112:LEU:HG	1.90	0.71
1:A:161:THR:HG21	1:A:234:CYS:HA	1.72	0.71
2:B:122:PHE:O	2:B:126:VAL:HG23	1.90	0.71
3:C:319:ARG:NH2	3:C:371:GLY:HA2	2.05	0.71
3:C:347:PRO:HG3	7:G:66:PHE:HD1	1.56	0.71
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.26	0.70
3:C:378:LEU:O	6:F:33:ARG:NH1	2.24	0.70
7:G:50:PRO:HG2	7:G:51:PRO:HD2	1.73	0.70
2:B:92:VAL:HG11	2:B:115:ASP:HB3	1.73	0.70
1:A:33:PRO:HG3	2:B:369:LEU:HD22	1.72	0.70
3:C:46:ILE:HA	11:C:381:HEM:HMC2	1.72	0.70
1:A:23:VAL:HG23	1:A:192:ALA:HB1	1.72	0.70
1:A:250:LEU:CD2	1:A:325:VAL:HG13	2.21	0.70
3:C:107:SER:HB3	11:C:382:HEM:CBD	2.13	0.70
3:C:120:LEU:CG	11:C:382:HEM:HBB2	2.22	0.70
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.56	0.70
7:G:26:PHE:HD1	7:G:26:PHE:H	1.37	0.70
4:D:46:VAL:HG12	4:D:47:ALA:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:188:THR:OG1	5:E:192:MET:HB3	1.92	0.70
2:B:207:VAL:HG12	2:B:208:GLY:N	2.07	0.70
1:A:281:ASP:O	1:A:283:THR:N	2.24	0.70
1:A:282:ARG:HB2	9:I:203:UNK:CB	2.22	0.70
3:C:276:LEU:O	3:C:279:TYR:HB3	1.92	0.70
2:B:405:VAL:HG12	2:B:406:ALA:N	2.04	0.69
1:A:102:LEU:HD12	1:A:102:LEU:N	2.06	0.69
1:A:382:GLU:CG	1:A:389:ARG:HA	2.22	0.69
1:A:85:HIS:CG	9:I:314:UNK:HG1	2.27	0.69
3:C:90:PHE:CZ	3:C:236:MET:O	2.45	0.69
3:C:325:LEU:CD2	3:C:362:ILE:HG23	2.23	0.69
3:C:347:PRO:HG3	7:G:66:PHE:CD1	2.27	0.69
1:A:343:MET:O	1:A:347:THR:HG22	1.91	0.69
2:B:162:ASN:O	2:B:244:ILE:HD11	1.93	0.69
3:C:9:HIS:HB3	3:C:12:LEU:HB3	1.74	0.69
4:D:83:ARG:NH1	4:D:86:LYS:HG3	2.08	0.69
2:B:213:HIS:N	2:B:214:PRO:HD2	2.08	0.69
2:B:273:SER:O	2:B:276:GLN:HB3	1.92	0.69
3:C:18:SER:C	3:C:19:LEU:HD12	2.17	0.69
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.73	0.69
1:A:191:THR:O	1:A:195:MET:HG3	1.92	0.69
1:A:297:ILE:HG22	1:A:303:LEU:HD11	1.74	0.69
3:C:150:LEU:HD12	3:C:292:VAL:HG22	1.74	0.69
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.75	0.69
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.27	0.69
5:E:136:ILE:HB	5:E:181:GLU:HB3	1.74	0.69
5:E:13:TYR:C	5:E:14:ARG:HD3	2.17	0.68
1:A:388:ARG:HH11	1:A:388:ARG:HG3	1.57	0.68
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.28	0.68
5:E:171:ILE:HG12	5:E:176:ALA:HB3	1.75	0.68
4:D:75:ASN:ND2	4:D:79:GLU:O	2.25	0.68
5:E:62:MET:HG3	5:E:63:SER:H	1.58	0.68
1:A:61:HIS:HD2	1:A:134:ILE:HG12	1.57	0.68
1:A:106:VAL:O	1:A:110:VAL:HG23	1.93	0.68
3:C:138:GLN:HE21	3:C:260:ALA:HA	1.59	0.68
6:F:32:MET:HE3	6:F:87:VAL:HG22	1.76	0.68
3:C:289:LEU:O	3:C:293:LEU:HD23	1.94	0.68
4:D:138:PRO:HG3	8:H:55:THR:HA	1.75	0.68
1:A:159:GLN:OE1	1:A:237:THR:HG21	1.92	0.68
1:A:286:GLY:HA3	1:A:289:HIS:CD2	2.28	0.68
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:161:HIS:HB2	14:E:197:FES:S1	2.34	0.68
3:C:27:ASN:ND2	3:C:208:ASN:OD1	2.26	0.68
3:C:90:PHE:CE1	3:C:236:MET:O	2.47	0.68
3:C:131:GLY:N	3:C:134:LEU:HD13	2.09	0.68
2:B:62:ASN:HD22	2:B:63:LEU:N	1.91	0.68
2:B:111:CYS:HB3	2:B:119:LEU:HD22	1.75	0.68
2:B:273:SER:HB3	2:B:364:LEU:HD11	1.74	0.68
3:C:323:GLN:O	3:C:326:PHE:HB3	1.94	0.68
6:F:64:ARG:O	6:F:68:LEU:HD13	1.94	0.68
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.74	0.68
12:C:383:SIG:H333	12:C:383:SIG:H353	1.75	0.68
1:A:245:GLU:HG3	7:G:11:ARG:HG2	1.75	0.67
3:C:372:THR:HA	3:C:375:ASN:ND2	2.07	0.67
5:E:119:ASP:HB3	5:E:179:ASN:CG	2.19	0.67
5:E:101:ARG:NH2	5:E:127:VAL:HG21	2.05	0.67
2:B:71:LEU:C	2:B:73:SER:H	1.99	0.67
3:C:271:PRO:HG2	3:C:276:LEU:CD2	2.24	0.67
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.25	0.67
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.75	0.67
3:C:146:VAL:CG2	3:C:147:ILE:H	1.98	0.67
1:A:16:VAL:HG13	1:A:26:ALA:HB2	1.76	0.67
3:C:348:PHE:O	3:C:350:ILE:N	2.28	0.67
1:A:307:PHE:CD1	1:A:307:PHE:C	2.73	0.67
2:B:332:TYR:O	2:B:336:VAL:HG23	1.95	0.67
5:E:10:PHE:O	5:E:11:SER:O	2.12	0.67
5:E:60:SER:C	5:E:62:MET:H	2.00	0.67
1:A:36:THR:HG23	1:A:372:THR:OG1	1.94	0.67
3:C:130:VAL:HG13	3:C:179:PHE:HB3	1.76	0.67
1:A:145:MET:HA	1:A:148:VAL:HG13	1.76	0.67
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.25	0.67
5:E:44:THR:HB	10:J:24:ILE:HD12	1.77	0.67
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.77	0.67
2:B:428:GLY:O	2:B:430:LEU:HG	1.95	0.67
3:C:282:LEU:HD13	3:C:282:LEU:O	1.94	0.67
4:D:132:THR:HA	4:D:179:MET:CE	2.25	0.67
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.25	0.66
1:A:264:HIS:HD2	1:A:266:ASP:HB2	1.60	0.66
2:B:397:THR:O	2:B:401:GLN:HG2	1.94	0.66
3:C:148:THR:HG21	3:C:166:TRP:CE3	2.30	0.66
2:B:258:VAL:HG13	2:B:322:PHE:N	2.08	0.66
4:D:164:ILE:HD11	4:D:182:VAL:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:16:ILE:O	6:F:19:TRP:HB3	1.95	0.66
10:J:59:TYR:O	10:J:60:GLU:HG3	1.95	0.66
1:A:253:VAL:HG11	1:A:335:MET:HE1	1.77	0.66
1:A:343:MET:HE2	1:A:343:MET:CA	2.24	0.66
2:B:113:ARG:O	2:B:116:VAL:HG23	1.95	0.66
1:A:19:LEU:HB2	1:A:21:ASN:HB3	1.77	0.66
1:A:57:TYR:C	1:A:59:LEU:N	2.51	0.66
3:C:233:LEU:O	3:C:237:LEU:HB2	1.95	0.66
4:D:141:VAL:HG21	8:H:55:THR:HG23	1.77	0.66
3:C:282:LEU:HD22	3:C:291:GLY:C	2.20	0.66
3:C:327:TRP:CE3	3:C:330:VAL:HG11	2.31	0.66
4:D:116:ILE:HG23	4:D:117:VAL:N	2.11	0.66
1:A:291:SER:O	1:A:292:SER:C	2.38	0.66
3:C:131:GLY:H	3:C:134:LEU:HD13	1.61	0.66
3:C:319:ARG:NH2	3:C:374:GLU:HB2	2.11	0.66
5:E:26:ARG:C	5:E:28:SER:H	2.04	0.66
5:E:113:GLU:OE2	5:E:116:GLN:HG3	1.95	0.66
3:C:41:CYS:HB3	3:C:91:PHE:CD2	2.31	0.66
3:C:166:TRP:HB2	3:C:175:THR:HB	1.78	0.66
1:A:156:THR:HA	5:E:7:VAL:HG21	1.76	0.66
3:C:131:GLY:CA	3:C:134:LEU:HD13	2.26	0.66
3:C:162:VAL:O	3:C:164:TRP:N	2.26	0.66
3:C:183:HIS:O	3:C:187:PRO:HD3	1.95	0.66
4:D:192:TRP:CD1	4:D:193:ALA:N	2.64	0.65
7:G:25:PRO:HG2	7:G:26:PHE:HD1	1.60	0.65
1:A:246:ASP:HA	1:A:427:PRO:HB3	1.77	0.65
1:A:416:TYR:CE1	1:A:442:PHE:HA	2.30	0.65
2:B:209:LEU:O	2:B:211:VAL:HG22	1.96	0.65
2:B:280:GLY:N	2:B:283:PRO:HD2	2.08	0.65
3:C:313:GLN:HE21	6:F:36:THR:CB	2.08	0.65
4:D:178:THR:OG1	4:D:181:GLN:HB2	1.95	0.65
1:A:281:ASP:O	1:A:284:TYR:HD1	1.77	0.65
1:A:431:LEU:HD23	1:A:432:PRO:CD	2.26	0.65
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.30	0.65
7:G:12:HIS:O	7:G:13:LEU:HD23	1.96	0.65
1:A:320:PHE:HE2	1:A:415:ILE:HD11	1.61	0.65
3:C:332:ASN:HD21	3:C:359:TYR:HA	1.61	0.65
5:E:52:LYS:C	5:E:52:LYS:HD3	2.22	0.65
1:A:26:ALA:O	1:A:198:ALA:HA	1.96	0.65
1:A:57:TYR:O	1:A:59:LEU:N	2.30	0.65
2:B:19:PRO:C	2:B:21:PRO:HD3	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:CYS:SG	2:B:116:VAL:HA	2.37	0.65
3:C:32:TRP:O	13:C:384:AMY:H8	1.96	0.65
4:D:132:THR:HA	4:D:179:MET:HE2	1.77	0.65
4:D:230:LEU:HB3	6:F:70:MET:CE	2.26	0.65
1:A:291:SER:HB2	1:A:356:ARG:HH22	1.61	0.65
5:E:32:ARG:HH22	7:G:25:PRO:HD2	1.61	0.65
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.32	0.65
2:B:150:VAL:HG23	2:B:151:ALA:N	2.11	0.65
2:B:337:ILE:HD11	2:B:434:PRO:CD	2.25	0.65
1:A:349:ILE:HG22	1:A:408:ARG:CG	2.26	0.65
3:C:166:TRP:HB2	3:C:175:THR:CB	2.27	0.65
3:C:332:ASN:HD21	3:C:359:TYR:CA	2.10	0.65
7:G:25:PRO:O	7:G:26:PHE:C	2.40	0.65
3:C:142:TRP:CZ3	3:C:265:THR:HG22	2.31	0.65
3:C:365:ILE:HG23	3:C:366:LEU:HD22	1.78	0.65
1:A:42:ASP:HB2	1:A:384:LEU:HD21	1.79	0.64
1:A:264:HIS:CD2	1:A:266:ASP:HB2	2.31	0.64
3:C:5:ILE:HA	3:C:8:SER:OG	1.97	0.64
3:C:76:TYR:HE1	4:D:200:HIS:CE1	2.14	0.64
3:C:133:VAL:O	3:C:140:SER:HB3	1.97	0.64
4:D:75:ASN:H	4:D:79:GLU:H	1.42	0.64
4:D:75:ASN:OD1	4:D:79:GLU:HB2	1.97	0.64
1:A:93:GLU:OE1	1:A:314:TYR:HB3	1.97	0.64
1:A:293:PRO:O	1:A:294:LEU:C	2.40	0.64
1:A:378:ASP:O	1:A:382:GLU:N	2.29	0.64
3:C:35:GLY:HA2	3:C:38:LEU:HD12	1.79	0.64
4:D:233:ARG:C	6:F:71:ARG:HH22	2.05	0.64
1:A:268:VAL:O	1:A:271:GLN:N	2.30	0.64
1:A:294:LEU:HD13	1:A:338:LEU:HA	1.78	0.64
2:B:260:GLU:O	2:B:261:SER:HB3	1.97	0.64
2:B:368:TYR:O	2:B:372:VAL:HG23	1.97	0.64
3:C:109:LEU:C	3:C:111:LYS:H	2.04	0.64
5:E:70:ALA:C	5:E:72:SER:H	2.05	0.64
1:A:444:LEU:H	1:A:444:LEU:HD12	1.63	0.64
2:B:401:GLN:O	2:B:404:ALA:HB3	1.97	0.64
3:C:242:THR:HA	4:D:208:MET:CE	2.27	0.64
3:C:261:ASN:HD22	3:C:264:VAL:HB	1.61	0.64
3:C:267:PRO:O	3:C:268:HIS:HB2	1.97	0.64
2:B:207:VAL:HG12	2:B:208:GLY:H	1.62	0.64
1:A:65:LYS:N	1:A:65:LYS:HD2	2.13	0.64
2:B:20:HIS:N	2:B:21:PRO:HD3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:O	2:B:323:GLY:HA3	1.98	0.64
3:C:174:PRO:O	3:C:175:THR:C	2.41	0.64
3:C:183:HIS:O	3:C:187:PRO:CD	2.46	0.64
8:H:50:THR:HG22	8:H:52:GLU:H	1.62	0.64
1:A:19:LEU:C	1:A:21:ASN:H	2.06	0.64
1:A:374:PRO:O	1:A:377:GLU:HB3	1.97	0.64
3:C:31:TRP:O	3:C:101:ARG:HG3	1.98	0.64
5:E:5:ILE:HD13	7:G:14:ILE:CD1	2.26	0.64
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.62	0.63
2:B:342:ASN:O	2:B:345:LYS:HB3	1.97	0.63
3:C:106:GLY:HA2	3:C:108:TYR:CD2	2.33	0.63
3:C:373:LEU:HD23	3:C:373:LEU:C	2.24	0.63
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.33	0.63
1:A:85:HIS:HB3	9:I:314:UNK:HG1	1.80	0.63
1:A:102:LEU:C	1:A:104:LYS:H	2.07	0.63
2:B:131:GLU:O	2:B:132:PHE:C	2.41	0.63
3:C:51:LEU:HG	3:C:80:ILE:HD13	1.80	0.63
3:C:355:ALA:C	3:C:357:LEU:H	2.07	0.63
6:F:59:MET:HA	6:F:59:MET:CE	2.28	0.63
1:A:42:ASP:HB3	1:A:194:ARG:HB3	1.79	0.63
5:E:72:SER:HA	5:E:92:ARG:HD3	1.80	0.63
3:C:232:GLY:HA2	3:C:235:LEU:HD12	1.79	0.63
3:C:245:LEU:O	4:D:201:ARG:HD2	1.98	0.63
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.34	0.63
3:C:130:VAL:HG12	3:C:131:GLY:N	2.12	0.63
4:D:227:TRP:O	4:D:230:LEU:N	2.29	0.63
1:A:130:GLU:O	1:A:134:ILE:HG13	1.98	0.63
1:A:161:THR:HG21	1:A:235:ARG:H	1.62	0.63
2:B:84:LYS:O	2:B:88:GLY:N	2.28	0.63
3:C:289:LEU:HG	3:C:293:LEU:HD23	1.81	0.63
7:G:68:LYS:C	7:G:70:LYS:H	2.07	0.63
2:B:402:ILE:O	2:B:402:ILE:HD13	1.99	0.63
3:C:113:THR:HG21	3:C:201:LEU:HA	1.79	0.63
6:F:12:TRP:HB3	6:F:15:GLY:H	1.64	0.63
6:F:57:ASP:HB3	6:F:61:ARG:HH12	1.64	0.63
2:B:56:ARG:NH2	2:B:318:ASP:OD2	2.32	0.62
3:C:45:GLN:HG3	11:C:381:HEM:HAB	1.80	0.62
5:E:32:ARG:C	5:E:32:ARG:HD3	2.23	0.62
1:A:64:PHE:CE1	1:A:86:LEU:HG	2.34	0.62
1:A:381:ARG:O	1:A:382:GLU:C	2.42	0.62
3:C:204:SER:O	3:C:205:GLY:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:HD13	3:C:80:ILE:HG22	1.81	0.62
5:E:38:LEU:HA	10:J:14:PHE:CE2	2.34	0.62
5:E:45:LEU:CD1	10:J:28:ALA:HA	2.26	0.62
8:H:66:ASP:HA	8:H:69:VAL:HB	1.81	0.62
1:A:438:ARG:C	1:A:440:GLY:H	2.07	0.62
4:D:12:TRP:CH2	4:D:124:GLU:HB2	2.34	0.62
1:A:16:VAL:HG22	1:A:26:ALA:CB	2.30	0.62
2:B:272:PHE:HB3	2:B:322:PHE:CE2	2.34	0.62
2:B:405:VAL:CG1	2:B:406:ALA:N	2.63	0.62
4:D:141:VAL:HG23	8:H:53:ASP:HB3	1.80	0.62
1:A:106:VAL:HB	1:A:107:PRO:CD	2.29	0.62
2:B:258:VAL:HG12	2:B:259:ALA:N	2.13	0.62
6:F:59:MET:HA	6:F:59:MET:HE3	1.80	0.62
8:H:47:ARG:HD3	8:H:48:SER:H	1.63	0.62
2:B:92:VAL:O	2:B:92:VAL:HG12	1.99	0.62
2:B:146:ILE:HG13	2:B:147:ASP:H	1.63	0.62
3:C:365:ILE:O	3:C:368:PRO:HG2	1.99	0.62
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.34	0.62
4:D:225:HIS:HA	7:G:25:PRO:HB3	1.81	0.62
7:G:29:TYR:O	7:G:30:PHE:HB2	2.00	0.62
3:C:28:ILE:HG23	3:C:32:TRP:HB2	1.82	0.62
3:C:164:TRP:O	3:C:165:ALA:C	2.42	0.62
4:D:55:CYS:SG	4:D:56:TYR:HD1	2.23	0.62
1:A:100:LYS:HE3	2:B:370:MET:CE	2.30	0.62
1:A:382:GLU:HG2	1:A:390:ILE:H	1.65	0.62
1:A:431:LEU:HD23	1:A:432:PRO:HD2	1.81	0.62
2:B:66:SER:O	2:B:69:LEU:HB3	2.00	0.62
3:C:101:ARG:HE	3:C:102:GLY:N	1.98	0.62
3:C:148:THR:HG22	3:C:162:VAL:HG13	1.79	0.62
5:E:29:ASP:C	5:E:31:SER:N	2.49	0.62
5:E:113:GLU:CD	5:E:116:GLN:HG3	2.25	0.62
1:A:306:SER:HB2	9:I:206:UNK:CB	2.29	0.61
3:C:104:TYR:CZ	3:C:316:MET:HB2	2.35	0.61
1:A:49:SER:N	1:A:52:ASN:HB3	2.13	0.61
1:A:116:ILE:O	1:A:120:CYS:SG	2.57	0.61
1:A:153:LEU:HD23	1:A:153:LEU:C	2.25	0.61
2:B:112:LEU:N	2:B:112:LEU:HD23	2.16	0.61
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.35	0.61
3:C:210:LEU:HD12	6:F:66:LEU:HD23	1.81	0.61
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.82	0.61
3:C:91:PHE:CE1	3:C:124:LEU:HG	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:VAL:HA	3:C:175:THR:HG21	1.82	0.61
3:C:365:ILE:HG23	3:C:366:LEU:H	1.65	0.61
4:D:232:SER:HB2	7:G:23:GLN:OE1	2.01	0.61
1:A:100:LYS:HE3	2:B:370:MET:HE3	1.82	0.61
1:A:429:GLU:OE2	7:G:7:LEU:HB2	2.00	0.61
3:C:15:ILE:C	3:C:17:ASN:H	2.08	0.61
8:H:17:LEU:HD13	8:H:73:LEU:HD11	1.81	0.61
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.32	0.61
1:A:159:GLN:NE2	5:E:7:VAL:CG1	2.61	0.61
1:A:191:THR:C	1:A:195:MET:HG3	2.26	0.61
2:B:272:PHE:O	2:B:275:LEU:N	2.34	0.61
3:C:27:ASN:ND2	6:F:69:ASN:HD22	1.98	0.61
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.82	0.61
2:B:357:VAL:O	2:B:361:LYS:HG3	2.01	0.61
4:D:221:TYR:CE2	5:E:36:SER:HA	2.35	0.61
4:D:134:TYR:CD2	4:D:162:PRO:HG3	2.36	0.61
4:D:216:VAL:HG23	4:D:217:PRO:CD	2.31	0.61
5:E:55:VAL:O	5:E:56:THR:C	2.43	0.61
1:A:15:GLN:O	1:A:26:ALA:HA	2.01	0.61
1:A:40:TRP:CH2	1:A:377:GLU:HA	2.36	0.61
5:E:45:LEU:HD21	10:J:28:ALA:N	2.15	0.61
5:E:71:MET:O	5:E:73:LYS:N	2.34	0.61
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.15	0.61
10:J:14:PHE:CD1	10:J:14:PHE:N	2.66	0.61
1:A:291:SER:HB2	1:A:356:ARG:NH2	2.16	0.61
1:A:332:ASP:O	1:A:333:ASP:C	2.42	0.61
1:A:399:LEU:C	1:A:399:LEU:HD12	2.25	0.61
2:B:130:PRO:HB3	2:B:132:PHE:CE1	2.36	0.61
3:C:46:ILE:HA	11:C:381:HEM:CMC	2.31	0.61
6:F:93:TYR:O	6:F:97:VAL:HG23	2.00	0.61
1:A:7:ALA:O	1:A:11:VAL:HG23	2.01	0.60
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.83	0.60
3:C:27:ASN:ND2	6:F:69:ASN:ND2	2.48	0.60
3:C:222:HIS:HB3	3:C:223:PRO:HD2	1.83	0.60
3:C:361:THR:HA	3:C:365:ILE:HG22	1.83	0.60
4:D:118:ARG:HD3	4:D:191:ARG:HH12	1.65	0.60
4:D:144:ARG:CZ	4:D:147:LEU:HD21	2.31	0.60
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.16	0.60
2:B:45:SER:HB3	2:B:210:GLY:HA3	1.82	0.60
1:A:349:ILE:CG2	1:A:408:ARG:HG3	2.29	0.60
2:B:385:GLN:C	2:B:387:LEU:H	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.83	0.60
5:E:11:SER:O	5:E:15:ARG:HB2	2.00	0.60
3:C:9:HIS:HD2	3:C:10:PRO:HG2	1.65	0.60
1:A:239:SER:HB2	7:G:17:SER:O	2.01	0.60
1:A:270:LEU:O	1:A:273:ALA:HB3	2.01	0.60
5:E:43:THR:O	5:E:47:VAL:HG23	2.00	0.60
2:B:399:LEU:HA	2:B:402:ILE:HG22	1.83	0.60
3:C:32:TRP:HZ2	3:C:207:ASN:HB3	1.67	0.60
8:H:66:ASP:O	8:H:69:VAL:HB	2.02	0.60
2:B:92:VAL:CG1	2:B:115:ASP:HB3	2.31	0.60
1:A:279:HIS:HB3	1:A:308:GLN:HA	1.84	0.60
1:A:371:GLY:O	1:A:375:VAL:HG23	2.01	0.60
9:I:313:UNK:CB	9:I:314:UNK:CD	2.80	0.60
1:A:4:TYR:O	1:A:7:ALA:N	2.34	0.60
1:A:120:CYS:O	1:A:122:LEU:HG	2.02	0.60
1:A:147:GLU:O	1:A:150:PHE:N	2.30	0.60
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.84	0.60
2:B:180:ASP:O	2:B:183:ILE:HG12	2.02	0.60
3:C:278:ALA:HB1	3:C:295:LEU:HD12	1.84	0.60
10:J:57:HIS:C	10:J:59:TYR:N	2.57	0.60
1:A:235:ARG:NH1	5:E:15:ARG:CZ	2.65	0.59
1:A:265:PRO:O	1:A:268:VAL:HG23	2.02	0.59
2:B:31:ASN:HB3	2:B:201:SER:CB	2.31	0.59
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.16	0.59
2:B:109:VAL:HG13	2:B:119:LEU:CD2	2.32	0.59
3:C:30:ALA:C	3:C:32:TRP:H	2.08	0.59
3:C:92:PHE:CZ	3:C:124:LEU:HD13	2.38	0.59
3:C:316:MET:SD	3:C:319:ARG:CG	2.80	0.59
4:D:27:ARG:NH2	4:D:60:GLU:OE2	2.25	0.59
4:D:169:LEU:N	4:D:169:LEU:HD23	2.17	0.59
5:E:136:ILE:HG22	5:E:136:ILE:O	2.01	0.59
2:B:374:SER:O	2:B:376:GLU:N	2.35	0.59
6:F:101:ARG:HG3	6:F:104:ARG:HH21	1.67	0.59
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.31	0.59
2:B:357:VAL:HG12	2:B:361:LYS:CD	2.31	0.59
3:C:20:ILE:HA	3:C:222:HIS:HB2	1.83	0.59
3:C:319:ARG:NH1	3:C:374:GLU:HB2	2.16	0.59
6:F:71:ARG:O	6:F:73:GLN:HG2	2.02	0.59
2:B:120:MET:HE2	2:B:219:VAL:HG11	1.84	0.59
3:C:235:LEU:O	3:C:239:PRO:HD3	2.01	0.59
3:C:247:SER:O	3:C:250:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:LEU:HD22	3:C:362:ILE:HG23	1.84	0.59
6:F:36:THR:O	6:F:37:ILE:C	2.46	0.59
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.31	0.59
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.85	0.59
2:B:286:LYS:CB	2:B:343:GLN:HG3	2.33	0.59
2:B:400:GLN:O	2:B:404:ALA:HB2	2.02	0.59
3:C:222:HIS:HB3	3:C:223:PRO:CD	2.32	0.59
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.38	0.59
2:B:406:ALA:O	2:B:407:ASP:C	2.45	0.59
3:C:332:ASN:ND2	3:C:359:TYR:HA	2.17	0.59
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.59
1:A:364:ALA:O	1:A:368:HIS:HB2	2.03	0.59
6:F:68:LEU:O	6:F:71:ARG:N	2.24	0.59
7:G:24:ARG:HH21	7:G:28:HIS:CE1	2.21	0.59
1:A:332:ASP:O	1:A:334:MET:N	2.35	0.59
3:C:20:ILE:O	3:C:21:ASP:HB2	2.02	0.59
3:C:127:THR:CG2	3:C:186:LEU:HB3	2.33	0.59
4:D:218:LEU:O	4:D:222:MET:HG3	2.02	0.59
4:D:232:SER:O	4:D:233:ARG:O	2.21	0.59
6:F:57:ASP:HB3	6:F:61:ARG:NH1	2.16	0.59
1:A:110:VAL:HA	1:A:113:LEU:HD12	1.85	0.58
4:D:235:LEU:HD12	6:F:64:ARG:HA	1.85	0.58
5:E:69:LEU:HD12	5:E:69:LEU:N	2.18	0.58
2:B:277:HIS:HB2	2:B:360:ALA:HB1	1.84	0.58
3:C:219:ILE:HD11	3:C:225:TYR:HE1	1.68	0.58
4:D:191:ARG:O	4:D:192:TRP:C	2.45	0.58
10:J:52:TRP:O	10:J:56:LYS:HB2	2.03	0.58
1:A:36:THR:CG2	1:A:100:LYS:HB3	2.20	0.58
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.04	0.58
2:B:39:GLU:HG3	2:B:41:TYR:CE1	2.39	0.58
3:C:376:LYS:C	3:C:378:LEU:H	2.11	0.58
1:A:75:LEU:O	1:A:79:VAL:HG23	2.03	0.58
3:C:362:ILE:HA	3:C:366:LEU:HB2	1.86	0.58
3:C:292:VAL:O	3:C:295:LEU:HB3	2.03	0.58
7:G:73:ASN:O	7:G:75:ALA:N	2.36	0.58
1:A:64:PHE:C	1:A:66:GLY:H	2.11	0.58
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.18	0.58
2:B:187:THR:OG1	2:B:190:GLU:HG3	2.02	0.58
3:C:211:GLY:HA3	3:C:315:THR:HG23	1.85	0.58
3:C:346:HIS:N	3:C:347:PRO:HD2	2.18	0.58
4:D:149:PHE:CE1	4:D:156:GLN:HB3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ALA:HA	1:A:112:LEU:HD12	1.85	0.58
2:B:58:GLU:HB3	2:B:62:ASN:HD21	1.68	0.58
2:B:159:VAL:HG21	2:B:254:HIS:HB3	1.84	0.58
3:C:277:PHE:CG	3:C:278:ALA:N	2.69	0.58
4:D:34:LYS:O	4:D:38:SER:OG	2.21	0.58
1:A:250:LEU:C	1:A:250:LEU:CD2	2.77	0.58
1:A:394:GLU:O	1:A:395:TRP:C	2.47	0.58
3:C:342:GLN:HB3	3:C:348:PHE:CD2	2.38	0.58
3:C:350:ILE:O	3:C:351:ILE:C	2.44	0.58
1:A:250:LEU:HD13	1:A:250:LEU:N	2.19	0.58
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.43	0.58
1:A:253:VAL:HG11	1:A:335:MET:CE	2.34	0.58
1:A:292:SER:O	1:A:295:ALA:HB3	2.04	0.58
3:C:101:ARG:NH1	11:C:382:HEM:O2A	2.31	0.58
4:D:181:GLN:HE21	4:D:181:GLN:C	2.12	0.58
1:A:85:HIS:HB2	1:A:100:LYS:HG3	1.85	0.57
13:C:384:AMY:O6	13:C:384:AMY:H262	2.03	0.57
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.39	0.57
5:E:164:HIS:O	5:E:171:ILE:HD12	2.03	0.57
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.38	0.57
1:A:46:ARG:HD3	1:A:231:LEU:HD13	1.84	0.57
2:B:31:ASN:HB3	2:B:201:SER:HB2	1.87	0.57
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.86	0.57
1:A:85:HIS:HB2	1:A:100:LYS:CG	2.35	0.57
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.38	0.57
1:A:297:ILE:CG2	1:A:337:VAL:HG11	2.29	0.57
4:D:197:GLU:O	4:D:198:HIS:C	2.47	0.57
2:B:272:PHE:HA	2:B:275:LEU:HB3	1.85	0.57
3:C:43:MET:CE	3:C:43:MET:CA	2.80	0.57
3:C:261:ASN:HD21	3:C:264:VAL:HG23	1.69	0.57
4:D:216:VAL:HG23	4:D:217:PRO:HD3	1.86	0.57
5:E:136:ILE:O	5:E:138:VAL:N	2.35	0.57
5:E:171:ILE:HD11	5:E:173:LYS:O	2.04	0.57
1:A:16:VAL:HG22	1:A:26:ALA:HB1	1.87	0.57
1:A:290:SER:O	1:A:291:SER:C	2.46	0.57
2:B:46:THR:HG22	2:B:110:GLU:HB2	1.87	0.57
3:C:149:ASN:O	3:C:152:SER:HB2	2.03	0.57
4:D:180:SER:OG	8:H:73:LEU:HD21	2.04	0.57
1:A:86:LEU:HD13	1:A:99:ILE:HG13	1.86	0.57
1:A:272:VAL:O	1:A:275:ALA:HB3	2.05	0.57
5:E:11:SER:OG	5:E:12:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:CE1	2:B:87:ARG:HD2	2.40	0.57
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.40	0.57
1:A:90:SER:O	1:A:167:VAL:HG11	2.05	0.57
1:A:178:SER:O	1:A:179:ARG:C	2.47	0.57
1:A:343:MET:O	1:A:344:ARG:C	2.48	0.57
2:B:133:ARG:HD3	2:B:135:TRP:CH2	2.39	0.57
8:H:16:PRO:O	8:H:20:VAL:HG23	2.05	0.57
1:A:33:PRO:HG2	1:A:34:THR:H	1.70	0.57
1:A:391:PRO:HG2	1:A:394:GLU:CB	2.34	0.57
2:B:85:ILE:HA	2:B:122:PHE:CD1	2.39	0.57
2:B:170:ASN:C	2:B:170:ASN:HD22	2.12	0.57
3:C:32:TRP:C	13:C:384:AMY:H8	2.30	0.57
3:C:219:ILE:HD11	3:C:225:TYR:CE1	2.40	0.57
8:H:66:ASP:HA	8:H:69:VAL:CB	2.35	0.57
2:B:109:VAL:HG13	2:B:119:LEU:HD21	1.86	0.57
2:B:146:ILE:O	2:B:149:ALA:N	2.38	0.57
3:C:201:LEU:O	3:C:203:GLU:N	2.37	0.57
4:D:32:VAL:HG21	4:D:186:VAL:CG2	2.35	0.57
4:D:62:LYS:O	4:D:66:GLU:HG2	2.05	0.57
4:D:203:ARG:O	4:D:206:LEU:HB3	2.05	0.57
7:G:4:PHE:HA	7:G:7:LEU:HD21	1.87	0.57
1:A:39:VAL:HG13	1:A:39:VAL:O	2.04	0.56
3:C:101:ARG:C	3:C:101:ARG:CD	2.78	0.56
4:D:63:ALA:HA	4:D:66:GLU:CG	2.34	0.56
8:H:59:PHE:O	8:H:60:ASP:C	2.48	0.56
2:B:20:HIS:N	2:B:21:PRO:CD	2.68	0.56
2:B:358:GLN:O	2:B:362:ASN:ND2	2.38	0.56
5:E:16:PRO:O	5:E:18:ASP:N	2.37	0.56
5:E:93:GLY:O	5:E:94:LYS:HE3	2.05	0.56
7:G:68:LYS:O	7:G:70:LYS:N	2.38	0.56
1:A:339:GLN:OE1	1:A:437:ILE:O	2.24	0.56
2:B:130:PRO:CB	2:B:132:PHE:CE1	2.88	0.56
3:C:137:GLY:H	3:C:140:SER:HB2	1.70	0.56
5:E:140:THR:OG1	5:E:177:PRO:HD2	2.05	0.56
6:F:87:VAL:HG23	6:F:87:VAL:O	2.04	0.56
3:C:95:ILE:CG2	3:C:96:PHE:N	2.68	0.56
3:C:95:ILE:HD13	3:C:121:LEU:HD12	1.86	0.56
3:C:123:THR:O	3:C:127:THR:HG23	2.05	0.56
3:C:283:ARG:NH2	3:C:342:GLN:O	2.32	0.56
4:D:72:ASP:O	4:D:73:GLY:O	2.23	0.56
1:A:77:LYS:O	1:A:81:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TYR:CD1	2:B:57:TYR:N	2.73	0.56
4:D:222:MET:HE3	5:E:40:THR:OG1	2.05	0.56
1:A:15:GLN:HB3	1:A:205:HIS:ND1	2.20	0.56
1:A:393:GLU:O	1:A:396:GLU:HB3	2.06	0.56
3:C:142:TRP:CH2	3:C:265:THR:HG22	2.41	0.56
3:C:335:ILE:O	3:C:336:LEU:C	2.48	0.56
1:A:4:TYR:CB	2:B:113:ARG:HB3	2.35	0.56
1:A:49:SER:HB2	1:A:52:ASN:HB3	1.87	0.56
1:A:345:LEU:CD1	1:A:349:ILE:HD12	2.32	0.56
1:A:356:ARG:O	1:A:357:GLY:C	2.49	0.56
2:B:402:ILE:HD13	2:B:402:ILE:C	2.30	0.56
3:C:41:CYS:O	3:C:42:LEU:C	2.46	0.56
3:C:150:LEU:CD1	3:C:292:VAL:HG22	2.35	0.56
3:C:295:LEU:O	3:C:296:ALA:C	2.47	0.56
4:D:240:PRO:O	4:D:241:LYS:CB	2.53	0.56
5:E:71:MET:C	5:E:73:LYS:H	2.14	0.56
1:A:250:LEU:HD21	1:A:325:VAL:CG1	2.33	0.56
3:C:27:ASN:CB	6:F:69:ASN:HD22	2.19	0.56
3:C:30:ALA:C	3:C:32:TRP:N	2.64	0.56
13:C:384:AMY:H272	13:C:384:AMY:C21	2.36	0.56
5:E:19:ASP:C	5:E:20:TYR:CD1	2.84	0.56
2:B:162:ASN:HB3	2:B:244:ILE:CD1	2.36	0.56
2:B:282:ASN:HB3	2:B:343:GLN:NE2	2.21	0.56
4:D:109:LEU:HG	4:D:109:LEU:O	2.05	0.56
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.38	0.56
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.34	0.56
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.88	0.56
7:G:55:PHE:O	7:G:56:TYR:C	2.49	0.56
10:J:13:LEU:HA	10:J:19:THR:HG21	1.88	0.55
1:A:100:LYS:CB	1:A:100:LYS:HZ2	2.18	0.55
1:A:274:ASN:ND2	1:A:320:PHE:CE1	2.75	0.55
1:A:280:TYR:CG	1:A:281:ASP:N	2.73	0.55
3:C:365:ILE:HG23	3:C:366:LEU:CD2	2.36	0.55
5:E:160:CYS:HB2	14:E:197:FES:S2	2.46	0.55
1:A:57:TYR:C	1:A:59:LEU:H	2.13	0.55
1:A:153:LEU:HD23	1:A:157:ALA:HB2	1.88	0.55
1:A:345:LEU:O	1:A:349:ILE:HB	2.06	0.55
3:C:26:SER:HA	3:C:219:ILE:CD1	2.36	0.55
3:C:344:VAL:HG23	3:C:344:VAL:O	2.06	0.55
13:C:384:AMY:H253	13:C:384:AMY:O9	2.06	0.55
6:F:12:TRP:HA	6:F:12:TRP:HE3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:HIS:O	10:J:59:TYR:N	2.39	0.55
1:A:40:TRP:HE3	1:A:94:HIS:HE1	1.54	0.55
1:A:53:ASN:HD22	1:A:53:ASN:C	2.11	0.55
1:A:244:ARG:NH2	1:A:429:GLU:HB2	2.20	0.55
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.41	0.55
4:D:61:ALA:O	4:D:64:LEU:HB3	2.07	0.55
7:G:25:PRO:HG2	7:G:26:PHE:CD1	2.41	0.55
8:H:40:CYS:C	8:H:54:CYS:SG	2.89	0.55
1:A:297:ILE:HG22	1:A:303:LEU:CD1	2.37	0.55
1:A:429:GLU:CD	7:G:7:LEU:HB2	2.31	0.55
2:B:58:GLU:CB	2:B:62:ASN:HD21	2.19	0.55
2:B:170:ASN:C	2:B:170:ASN:ND2	2.65	0.55
3:C:13:LYS:O	3:C:14:MET:C	2.49	0.55
3:C:78:TRP:CG	4:D:197:GLU:HG2	2.41	0.55
4:D:186:VAL:HG11	11:D:242:HEM:CBB	2.36	0.55
5:E:129:LYS:HB2	5:E:187:PHE:CZ	2.42	0.55
6:F:97:VAL:O	6:F:100:GLU:HB2	2.07	0.55
6:F:100:GLU:O	6:F:104:ARG:HG3	2.07	0.55
4:D:230:LEU:C	6:F:70:MET:HE1	2.32	0.55
2:B:68:LEU:HD23	2:B:186:VAL:HG11	1.89	0.55
3:C:319:ARG:HA	6:F:20:TYR:OH	2.07	0.55
5:E:126:ARG:NH2	5:E:168:SER:O	2.39	0.55
10:J:61:ASN:O	10:J:62:LYS:CB	2.55	0.55
2:B:38:LEU:HD23	2:B:378:PHE:HZ	1.72	0.55
2:B:200:THR:HG22	2:B:226:ILE:HG21	1.89	0.55
3:C:184:PHE:HD1	3:C:184:PHE:O	1.89	0.55
3:C:209:PRO:HG2	6:F:69:ASN:HD21	1.72	0.55
4:D:217:PRO:O	4:D:220:TYR:N	2.40	0.55
10:J:42:ILE:O	10:J:46:ILE:HG13	2.07	0.55
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.89	0.55
3:C:378:LEU:O	3:C:379:ASN:HB2	2.07	0.55
4:D:102:ARG:NH1	4:D:109:LEU:CB	2.69	0.55
7:G:68:LYS:C	7:G:70:LYS:N	2.65	0.55
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.88	0.54
2:B:71:LEU:C	2:B:73:SER:N	2.63	0.54
3:C:19:LEU:HD12	3:C:19:LEU:N	2.22	0.54
4:D:169:LEU:HD23	4:D:169:LEU:H	1.72	0.54
1:A:246:ASP:OD2	7:G:10:VAL:N	2.34	0.54
1:A:251:ALA:HB1	1:A:428:ILE:CG2	2.37	0.54
2:B:372:VAL:O	2:B:378:PHE:HB2	2.06	0.54
3:C:222:HIS:CB	3:C:223:PRO:CD	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:PHE:O	3:C:329:LEU:HB3	2.08	0.54
4:D:43:MET:CE	4:D:46:VAL:HG21	2.37	0.54
5:E:122:HIS:O	5:E:125:GLU:HG2	2.06	0.54
10:J:54:HIS:O	10:J:57:HIS:CD2	2.60	0.54
1:A:19:LEU:C	1:A:21:ASN:N	2.59	0.54
1:A:45:SER:HA	1:A:48:GLU:HG3	1.88	0.54
1:A:212:ALA:C	1:A:214:LYS:N	2.64	0.54
3:C:95:ILE:HG23	3:C:96:PHE:N	2.22	0.54
3:C:308:LEU:CD1	3:C:364:LEU:HA	2.38	0.54
7:G:26:PHE:HD1	7:G:26:PHE:N	2.03	0.54
10:J:57:HIS:HA	10:J:60:GLU:C	2.32	0.54
2:B:141:GLN:N	2:B:142:PRO:HD2	2.22	0.54
3:C:167:GLY:H	3:C:175:THR:CG2	2.16	0.54
5:E:85:LYS:HE2	5:E:86:ASN:O	2.07	0.54
1:A:36:THR:HA	1:A:100:LYS:HA	1.90	0.54
1:A:212:ALA:C	1:A:214:LYS:H	2.16	0.54
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.41	0.54
2:B:405:VAL:HG11	2:B:409:ASP:OD1	2.06	0.54
3:C:60:THR:HG23	3:C:136:TRP:CZ3	2.42	0.54
3:C:113:THR:O	3:C:197:HIS:CE1	2.59	0.54
3:C:131:GLY:O	3:C:134:LEU:HB2	2.08	0.54
3:C:289:LEU:HG	3:C:293:LEU:CD2	2.38	0.54
13:C:384:AMY:O7	13:C:384:AMY:H271	2.08	0.54
4:D:66:GLU:O	4:D:68:VAL:N	2.40	0.54
4:D:117:VAL:CG2	4:D:190:LEU:HB3	2.37	0.54
4:D:164:ILE:HG23	4:D:179:MET:HE3	1.89	0.54
7:G:60:THR:O	7:G:61:TRP:C	2.49	0.54
7:G:73:ASN:C	7:G:75:ALA:N	2.65	0.54
3:C:222:HIS:O	3:C:223:PRO:C	2.49	0.54
1:A:208:LEU:O	1:A:209:LEU:C	2.50	0.54
2:B:81:SER:O	2:B:85:ILE:HG22	2.08	0.54
3:C:213:SER:HB2	6:F:39:GLU:OE2	2.08	0.54
4:D:123:GLY:O	4:D:126:TYR:N	2.41	0.54
5:E:34:GLY:O	5:E:38:LEU:N	2.33	0.54
5:E:69:LEU:N	5:E:69:LEU:CD1	2.71	0.54
6:F:31:LEU:HD23	6:F:31:LEU:H	1.73	0.54
10:J:55:ILE:C	10:J:57:HIS:N	2.64	0.54
1:A:45:SER:HB3	1:A:167:VAL:HA	1.88	0.54
2:B:250:ASP:C	2:B:252:LEU:H	2.16	0.54
3:C:92:PHE:CZ	3:C:124:LEU:CD1	2.91	0.54
3:C:343:PRO:O	3:C:348:PHE:HD2	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.08	0.54
7:G:24:ARG:NH2	7:G:28:HIS:CE1	2.76	0.54
1:A:114:ALA:HA	1:A:216:PHE:HE1	1.73	0.54
1:A:255:ILE:HA	1:A:421:ALA:O	2.08	0.54
1:A:294:LEU:O	1:A:298:ALA:HB2	2.08	0.54
1:A:443:TRP:O	1:A:445:ARG:N	2.37	0.54
2:B:100:SER:O	9:I:106:UNK:HA	2.08	0.54
2:B:169:ARG:O	2:B:170:ASN:CB	2.56	0.54
3:C:201:LEU:O	3:C:204:SER:N	2.33	0.54
3:C:295:LEU:HD11	12:C:383:SIG:H273	1.88	0.54
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.89	0.54
3:C:273:TRP:C	3:C:275:PHE:H	2.16	0.54
6:F:31:LEU:HD23	6:F:31:LEU:N	2.22	0.54
1:A:27:SER:HB2	1:A:199:ALA:O	2.08	0.53
1:A:204:GLU:O	1:A:205:HIS:C	2.50	0.53
1:A:266:ASP:C	1:A:268:VAL:N	2.66	0.53
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.43	0.53
2:B:345:LYS:C	2:B:347:ILE:H	2.15	0.53
3:C:282:LEU:HD13	3:C:282:LEU:C	2.33	0.53
4:D:102:ARG:HA	4:D:108:ALA:O	2.08	0.53
4:D:195:GLU:HG3	4:D:195:GLU:O	2.07	0.53
1:A:241:ILE:HG23	1:A:241:ILE:O	2.07	0.53
3:C:231:LEU:HD12	4:D:219:VAL:HG23	1.90	0.53
3:C:354:MET:O	3:C:357:LEU:N	2.41	0.53
4:D:47:ALA:O	4:D:50:HIS:ND1	2.30	0.53
4:D:181:GLN:C	4:D:181:GLN:NE2	2.67	0.53
5:E:33:LYS:HG2	7:G:21:PHE:CD1	2.43	0.53
1:A:65:LYS:NZ	9:I:311:UNK:N	2.57	0.53
1:A:123:GLU:HB3	1:A:126:GLN:HB2	1.89	0.53
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.37	0.53
10:J:46:ILE:O	10:J:46:ILE:HG22	2.08	0.53
1:A:388:ARG:HG3	1:A:388:ARG:NH1	2.23	0.53
2:B:163:LEU:HD21	2:B:258:VAL:HG21	1.89	0.53
3:C:130:VAL:O	3:C:132:TYR:N	2.40	0.53
3:C:338:TRP:CE3	3:C:339:ILE:HG12	2.44	0.53
4:D:149:PHE:HA	4:D:156:GLN:O	2.08	0.53
10:J:56:LYS:O	10:J:60:GLU:HB2	2.08	0.53
1:A:45:SER:OG	1:A:92:ARG:HA	2.09	0.53
1:A:79:VAL:O	1:A:80:GLU:C	2.51	0.53
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.22	0.53
4:D:75:ASN:HB2	4:D:78:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:61:PHE:O	8:H:62:LEU:C	2.50	0.53
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.73	0.53
2:B:435:PHE:N	2:B:435:PHE:CD1	2.77	0.53
1:A:23:VAL:HG23	1:A:192:ALA:CB	2.38	0.53
1:A:100:LYS:HZ2	1:A:100:LYS:HB2	1.72	0.53
1:A:184:GLU:O	1:A:188:THR:OG1	2.22	0.53
2:B:85:ILE:HG23	2:B:86:THR:N	2.23	0.53
4:D:48:TYR:CE2	4:D:65:ALA:HA	2.43	0.53
4:D:155:GLY:C	4:D:156:GLN:NE2	2.66	0.53
1:A:356:ARG:HG3	2:B:90:GLU:O	2.09	0.53
2:B:278:VAL:O	2:B:282:ASN:ND2	2.42	0.53
2:B:339:ALA:HA	2:B:342:ASN:HD22	1.74	0.53
3:C:95:ILE:HD11	3:C:121:LEU:HA	1.90	0.53
3:C:312:LYS:HB3	6:F:37:ILE:HG22	1.90	0.53
4:D:30:PHE:CE2	4:D:64:LEU:HD21	2.44	0.53
4:D:57:THR:HB	4:D:60:GLU:HB2	1.91	0.53
5:E:51:ALA:O	5:E:52:LYS:C	2.52	0.53
5:E:91:TRP:O	5:E:94:LYS:O	2.27	0.53
6:F:49:ARG:NH1	6:F:97:VAL:HG22	2.24	0.53
8:H:50:THR:HG22	8:H:52:GLU:N	2.23	0.53
2:B:129:ALA:N	2:B:130:PRO:HD3	2.24	0.53
4:D:61:ALA:HA	4:D:64:LEU:HB3	1.91	0.53
1:A:373:THR:N	1:A:374:PRO:HD2	2.23	0.53
2:B:146:ILE:O	2:B:147:ASP:C	2.52	0.53
2:B:405:VAL:HG11	2:B:409:ASP:CG	2.34	0.53
3:C:162:VAL:O	3:C:165:ALA:N	2.42	0.53
4:D:117:VAL:HG23	4:D:190:LEU:HB3	1.91	0.53
4:D:158:ILE:CG2	4:D:159:GLY:N	2.71	0.53
5:E:85:LYS:HG2	5:E:86:ASN:H	1.74	0.53
6:F:70:MET:HG2	6:F:70:MET:O	2.08	0.53
10:J:19:THR:O	10:J:20:PHE:C	2.51	0.53
2:B:258:VAL:HG11	2:B:321:LEU:HD22	1.90	0.52
2:B:333:ALA:O	2:B:337:ILE:HG12	2.10	0.52
4:D:122:GLY:O	4:D:123:GLY:C	2.51	0.52
10:J:59:TYR:N	10:J:59:TYR:CD1	2.78	0.52
1:A:383:LEU:HD23	1:A:388:ARG:HA	1.91	0.52
1:A:418:GLN:O	1:A:420:PRO:HD3	2.10	0.52
2:B:217:LYS:C	2:B:219:VAL:H	2.17	0.52
2:B:221:GLU:HG3	2:B:222:GLN:N	2.24	0.52
2:B:255:ALA:O	2:B:325:TYR:HA	2.09	0.52
3:C:342:GLN:HE21	3:C:342:GLN:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:ILE:N	3:C:350:ILE:HD13	2.25	0.52
3:C:365:ILE:HG23	3:C:366:LEU:N	2.23	0.52
4:D:81:PHE:CD1	4:D:81:PHE:C	2.88	0.52
4:D:117:VAL:HG21	4:D:190:LEU:C	2.34	0.52
4:D:118:ARG:HD3	4:D:191:ARG:NH1	2.25	0.52
5:E:60:SER:C	5:E:62:MET:N	2.67	0.52
6:F:75:LEU:HG	6:F:79:GLN:HB2	1.90	0.52
7:G:29:TYR:HA	7:G:33:GLY:HA3	1.92	0.52
1:A:53:ASN:C	1:A:53:ASN:ND2	2.64	0.52
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.91	0.52
2:B:132:PHE:CD2	2:B:191:LEU:CB	2.93	0.52
2:B:170:ASN:O	2:B:171:ALA:O	2.27	0.52
3:C:103:LEU:HD13	3:C:103:LEU:C	2.34	0.52
3:C:199:THR:HG22	3:C:200:PHE:N	2.24	0.52
3:C:299:VAL:C	3:C:301:ILE:H	2.18	0.52
4:D:165:TYR:CZ	4:D:168:VAL:HG22	2.43	0.52
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.74	0.52
1:A:341:GLN:O	1:A:342:TRP:C	2.51	0.52
2:B:85:ILE:HG23	2:B:86:THR:H	1.75	0.52
2:B:324:PHE:O	2:B:324:PHE:CD1	2.62	0.52
3:C:15:ILE:O	3:C:17:ASN:N	2.39	0.52
4:D:21:LEU:HD13	4:D:26:ILE:HD11	1.91	0.52
4:D:217:PRO:O	4:D:218:LEU:C	2.52	0.52
4:D:223:LYS:HD2	4:D:223:LYS:O	2.09	0.52
1:A:4:TYR:HB2	2:B:113:ARG:HB3	1.92	0.52
1:A:123:GLU:O	1:A:126:GLN:N	2.40	0.52
3:C:45:GLN:OE1	3:C:45:GLN:HA	2.10	0.52
3:C:59:ASP:O	3:C:60:THR:C	2.53	0.52
3:C:104:TYR:CE2	3:C:316:MET:HB2	2.45	0.52
3:C:118:VAL:O	3:C:119:ILE:C	2.53	0.52
3:C:137:GLY:H	3:C:140:SER:CB	2.22	0.52
3:C:293:LEU:O	3:C:296:ALA:HB3	2.10	0.52
4:D:167:ASP:C	4:D:169:LEU:N	2.67	0.52
8:H:66:ASP:HA	8:H:69:VAL:HG21	1.91	0.52
1:A:86:LEU:HB2	1:A:99:ILE:HG12	1.91	0.52
4:D:117:VAL:O	4:D:123:GLY:HA2	2.10	0.52
4:D:221:TYR:HE2	5:E:36:SER:HA	1.74	0.52
4:D:224:ARG:HH22	7:G:27:PRO:HG3	1.75	0.52
5:E:13:TYR:O	7:G:28:HIS:HD2	1.93	0.52
5:E:39:VAL:O	5:E:42:VAL:HB	2.10	0.52
8:H:58:LEU:HD12	8:H:58:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:HD13	1:A:399:LEU:CD2	2.27	0.52
2:B:405:VAL:CG1	2:B:409:ASP:OD1	2.58	0.52
3:C:111:LYS:O	3:C:114:TRP:N	2.42	0.52
3:C:352:GLY:O	3:C:354:MET:N	2.43	0.52
4:D:155:GLY:C	4:D:157:ALA:H	2.18	0.52
1:A:64:PHE:O	1:A:75:LEU:HD23	2.10	0.52
1:A:87:ASN:HB3	1:A:98:TYR:CE1	2.45	0.52
1:A:91:SER:O	1:A:167:VAL:HG22	2.10	0.52
2:B:137:VAL:HG23	2:B:138:ALA:N	2.24	0.52
2:B:378:PHE:C	2:B:380:GLU:N	2.68	0.52
3:C:4:ASN:O	3:C:5:ILE:HB	2.09	0.52
3:C:107:SER:C	3:C:109:LEU:H	2.17	0.52
3:C:219:ILE:CD1	3:C:225:TYR:HE1	2.22	0.52
3:C:275:PHE:CD2	12:C:383:SIG:H332	2.45	0.52
4:D:165:TYR:CE2	4:D:168:VAL:HG22	2.45	0.52
1:A:239:SER:O	1:A:421:ALA:HA	2.09	0.52
2:B:209:LEU:O	2:B:211:VAL:HG13	2.10	0.52
3:C:101:ARG:NE	3:C:102:GLY:N	2.58	0.52
5:E:22:THR:O	5:E:22:THR:HG22	2.10	0.52
5:E:112:VAL:HG21	5:E:170:ARG:HH22	1.75	0.52
10:J:14:PHE:N	10:J:14:PHE:HD1	2.06	0.52
1:A:4:TYR:HB2	2:B:113:ARG:CB	2.40	0.52
1:A:335:MET:O	1:A:336:PHE:C	2.53	0.52
1:A:338:LEU:O	1:A:341:GLN:N	2.43	0.52
2:B:260:GLU:O	2:B:261:SER:CB	2.58	0.52
2:B:284:HIS:C	2:B:286:LYS:H	2.17	0.52
2:B:385:GLN:C	2:B:387:LEU:N	2.68	0.52
3:C:38:LEU:HD21	3:C:95:ILE:N	2.25	0.52
3:C:131:GLY:HA2	3:C:134:LEU:HD13	1.90	0.52
3:C:245:LEU:O	4:D:201:ARG:CD	2.58	0.52
2:B:96:LEU:HD23	2:B:96:LEU:C	2.35	0.51
2:B:182:ARG:NH2	2:B:190:GLU:OE1	2.42	0.51
2:B:361:LYS:O	2:B:365:LYS:HG3	2.10	0.51
3:C:238:THR:OG1	4:D:212:MET:HG3	2.09	0.51
10:J:13:LEU:HD12	10:J:13:LEU:N	2.25	0.51
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.51
1:A:39:VAL:HA	1:A:196:VAL:O	2.10	0.51
2:B:150:VAL:CG2	2:B:151:ALA:N	2.72	0.51
3:C:85:ALA:O	3:C:88:ALA:HB3	2.11	0.51
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.45	0.51
3:C:191:ALA:HB1	13:C:384:AMY:H251	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:382:HEM:HBA1	11:C:382:HEM:O2D	2.10	0.51
4:D:29:GLY:O	4:D:32:VAL:CG1	2.58	0.51
1:A:41:ILE:C	1:A:43:ALA:H	2.18	0.51
1:A:294:LEU:HG	1:A:307:PHE:CE2	2.46	0.51
1:A:416:TYR:HE1	1:A:443:TRP:H	1.58	0.51
3:C:157:ILE:O	3:C:161:LEU:HB2	2.10	0.51
3:C:287:ASN:O	3:C:288:LYS:C	2.51	0.51
4:D:182:VAL:HG13	4:D:183:ALA:H	1.75	0.51
6:F:84:GLU:CD	6:F:84:GLU:H	2.18	0.51
1:A:87:ASN:O	1:A:88:ALA:HB2	2.10	0.51
1:A:438:ARG:O	1:A:438:ARG:HD3	2.11	0.51
2:B:170:ASN:O	2:B:171:ALA:C	2.54	0.51
2:B:189:VAL:O	2:B:191:LEU:N	2.43	0.51
3:C:18:SER:HB2	3:C:19:LEU:HD12	1.92	0.51
3:C:166:TRP:HB2	3:C:175:THR:HG22	1.91	0.51
3:C:215:ASP:HB3	7:G:7:LEU:HB3	1.91	0.51
3:C:274:TYR:HE1	3:C:275:PHE:CE2	2.28	0.51
3:C:377:MET:HE3	6:F:16:ILE:CG2	2.40	0.51
4:D:57:THR:H	4:D:60:GLU:HB3	1.75	0.51
4:D:63:ALA:HA	4:D:66:GLU:HG2	1.93	0.51
4:D:169:LEU:HD11	4:D:171:PHE:HE1	1.75	0.51
1:A:58:PHE:CE1	1:A:127:ILE:HG23	2.45	0.51
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.09	0.51
1:A:228:VAL:HG13	1:A:228:VAL:O	2.10	0.51
3:C:162:VAL:C	3:C:164:TRP:N	2.68	0.51
3:C:280:ALA:O	3:C:281:ILE:C	2.54	0.51
4:D:186:VAL:O	4:D:190:LEU:HG	2.10	0.51
3:C:281:ILE:O	3:C:285:ILE:HG22	2.11	0.51
4:D:47:ALA:N	4:D:50:HIS:CE1	2.78	0.51
4:D:56:TYR:HD2	4:D:60:GLU:HG2	1.74	0.51
4:D:134:TYR:O	4:D:135:CYS:HB3	2.10	0.51
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.93	0.51
6:F:67:ASP:OD1	6:F:71:ARG:CZ	2.59	0.51
7:G:73:ASN:C	7:G:75:ALA:H	2.19	0.51
1:A:65:LYS:N	1:A:65:LYS:CD	2.73	0.51
1:A:88:ALA:CB	1:A:97:TYR:HA	2.38	0.51
1:A:282:ARG:NH2	2:B:146:ILE:HG21	2.25	0.51
2:B:202:ALA:HB3	2:B:229:GLY:O	2.11	0.51
2:B:353:SER:C	2:B:355:GLU:H	2.19	0.51
3:C:172:ASP:O	3:C:173:ASN:C	2.54	0.51
3:C:275:PHE:HB3	12:C:383:SIG:H332	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:383:SIG:H282	12:C:383:SIG:C33	2.38	0.51
4:D:32:VAL:CG2	4:D:186:VAL:HG22	2.37	0.51
4:D:46:VAL:CG1	4:D:47:ALA:N	2.74	0.51
4:D:189:PHE:O	4:D:191:ARG:N	2.44	0.51
1:A:105:ASP:O	1:A:106:VAL:C	2.54	0.51
1:A:310:PHE:CE1	1:A:322:PHE:N	2.79	0.51
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.73	0.51
2:B:146:ILE:CG1	2:B:147:ASP:N	2.72	0.51
2:B:209:LEU:O	2:B:210:GLY:C	2.53	0.51
4:D:124:GLU:OE1	4:D:124:GLU:N	2.37	0.51
5:E:11:SER:HA	5:E:15:ARG:CD	2.36	0.51
5:E:163:SER:OG	5:E:176:ALA:HB2	2.11	0.51
2:B:345:LYS:O	2:B:347:ILE:N	2.43	0.51
6:F:75:LEU:O	6:F:80:TRP:NE1	2.41	0.51
6:F:96:GLU:O	6:F:97:VAL:C	2.54	0.51
1:A:295:ALA:O	1:A:298:ALA:HB3	2.11	0.50
1:A:351:GLU:O	1:A:354:VAL:HG22	2.11	0.50
3:C:253:ASP:OD1	3:C:253:ASP:C	2.53	0.50
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.46	0.50
4:D:98:PRO:O	4:D:101:ALA:N	2.44	0.50
4:D:182:VAL:HG13	4:D:183:ALA:N	2.25	0.50
4:D:213:GLY:O	4:D:217:PRO:CD	2.59	0.50
5:E:29:ASP:O	5:E:32:ARG:N	2.44	0.50
6:F:94:LEU:O	6:F:97:VAL:HB	2.11	0.50
7:G:40:ARG:O	7:G:41:LEU:C	2.53	0.50
1:A:46:ARG:CD	1:A:231:LEU:HD13	2.41	0.50
1:A:57:TYR:O	1:A:60:GLU:N	2.45	0.50
1:A:59:LEU:O	1:A:60:GLU:C	2.54	0.50
1:A:180:ALA:O	1:A:183:THR:N	2.45	0.50
1:A:343:MET:SD	1:A:441:MET:O	2.69	0.50
2:B:288:GLY:O	2:B:305:ASN:CB	2.59	0.50
3:C:166:TRP:O	3:C:167:GLY:O	2.29	0.50
3:C:273:TRP:CD2	3:C:274:TYR:N	2.79	0.50
1:A:24:ARG:HH11	1:A:24:ARG:HG3	1.76	0.50
1:A:410:VAL:O	1:A:413:LYS:HB3	2.12	0.50
3:C:113:THR:HG22	3:C:200:PHE:C	2.36	0.50
3:C:138:GLN:HE21	3:C:261:ASN:H	1.55	0.50
3:C:273:TRP:HA	3:C:276:LEU:HG	1.93	0.50
3:C:293:LEU:O	3:C:294:ALA:C	2.55	0.50
6:F:16:ILE:O	6:F:19:TRP:N	2.45	0.50
6:F:29:TYR:HB2	6:F:31:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:HG2	1:A:389:ARG:CA	2.30	0.50
3:C:282:LEU:C	3:C:282:LEU:CD1	2.85	0.50
4:D:123:GLY:O	4:D:124:GLU:C	2.54	0.50
5:E:32:ARG:NH2	7:G:25:PRO:HD2	2.26	0.50
2:B:141:GLN:C	2:B:143:GLN:H	2.19	0.50
2:B:363:LYS:O	2:B:366:ALA:HB3	2.11	0.50
2:B:430:LEU:O	2:B:432:HIS:N	2.45	0.50
3:C:31:TRP:CD1	3:C:31:TRP:H	2.29	0.50
3:C:34:PHE:CD1	3:C:37:LEU:HD12	2.47	0.50
3:C:101:ARG:HE	3:C:102:GLY:CA	2.24	0.50
3:C:184:PHE:C	3:C:184:PHE:CD1	2.90	0.50
10:J:26:VAL:O	10:J:30:LEU:HG	2.11	0.50
1:A:444:LEU:O	1:A:445:ARG:O	2.29	0.50
2:B:92:VAL:O	2:B:92:VAL:CG1	2.60	0.50
3:C:230:ILE:O	3:C:233:LEU:HB3	2.12	0.50
4:D:54:VAL:HG21	4:D:192:TRP:CE3	2.43	0.50
1:A:250:LEU:HD22	1:A:250:LEU:O	2.10	0.50
3:C:116:THR:O	3:C:117:GLY:C	2.55	0.50
3:C:285:ILE:CG2	3:C:291:GLY:HA2	2.37	0.50
1:A:103:SER:C	1:A:105:ASP:H	2.18	0.50
2:B:177:TYR:O	2:B:178:CYS:C	2.54	0.50
4:D:47:ALA:HB1	4:D:89:ASP:O	2.11	0.50
5:E:123:ASP:O	5:E:127:VAL:HG22	2.12	0.50
6:F:97:VAL:O	6:F:98:ILE:C	2.54	0.50
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.80	0.50
2:B:250:ASP:O	2:B:252:LEU:CD2	2.54	0.50
2:B:272:PHE:O	2:B:273:SER:C	2.55	0.50
3:C:27:ASN:O	3:C:209:PRO:HD2	2.12	0.50
5:E:16:PRO:C	5:E:18:ASP:H	2.19	0.50
7:G:49:ALA:O	7:G:50:PRO:C	2.52	0.50
7:G:60:THR:HG22	7:G:64:GLN:HE21	1.77	0.50
3:C:273:TRP:CG	3:C:274:TYR:N	2.80	0.49
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.93	0.49
6:F:26:PHE:O	6:F:31:LEU:HD23	2.12	0.49
6:F:32:MET:CE	6:F:87:VAL:HG22	2.41	0.49
9:I:314:UNK:O	9:I:314:UNK:HG2	2.12	0.49
1:A:153:LEU:HD23	1:A:153:LEU:O	2.12	0.49
1:A:267:LEU:O	1:A:271:GLN:HB2	2.12	0.49
2:B:285:VAL:O	2:B:285:VAL:HG12	2.12	0.49
3:C:81:ARG:O	3:C:82:ASN:C	2.55	0.49
3:C:120:LEU:O	3:C:121:LEU:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ASN:ND2	3:C:264:VAL:HB	2.26	0.49
3:C:353:GLN:HA	3:C:356:SER:HB3	1.94	0.49
4:D:141:VAL:HG21	8:H:55:THR:CG2	2.42	0.49
5:E:134:ILE:O	5:E:135:LEU:HD23	2.13	0.49
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.49
9:I:310:UNK:O	9:I:311:UNK:C	2.59	0.49
1:A:443:TRP:C	1:A:445:ARG:H	2.19	0.49
2:B:218:ASN:O	2:B:221:GLU:HG2	2.12	0.49
3:C:108:TYR:HE1	3:C:309:HIS:HB2	1.77	0.49
3:C:138:GLN:OE1	3:C:266:PRO:HD3	2.11	0.49
3:C:222:HIS:CG	3:C:223:PRO:N	2.80	0.49
4:D:116:ILE:CG2	4:D:117:VAL:N	2.75	0.49
4:D:138:PRO:HD3	8:H:58:LEU:CD2	2.42	0.49
4:D:189:PHE:O	4:D:190:LEU:C	2.55	0.49
10:J:57:HIS:HB2	10:J:61:ASN:CA	2.42	0.49
1:A:430:GLN:O	1:A:430:GLN:HG2	2.13	0.49
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.78	0.49
2:B:232:LEU:O	2:B:233:SER:O	2.30	0.49
3:C:30:ALA:HA	3:C:33:ASN:OD1	2.12	0.49
3:C:339:ILE:HG22	3:C:339:ILE:O	2.11	0.49
5:E:15:ARG:O	7:G:24:ARG:HD3	2.13	0.49
1:A:40:TRP:CE3	1:A:96:ALA:HB2	2.46	0.49
1:A:235:ARG:HB2	5:E:21:SER:HA	1.95	0.49
3:C:30:ALA:O	3:C:32:TRP:N	2.45	0.49
3:C:179:PHE:O	3:C:180:PHE:C	2.54	0.49
4:D:167:ASP:C	4:D:169:LEU:H	2.21	0.49
7:G:27:PRO:HD2	7:G:29:TYR:HD1	1.78	0.49
1:A:161:THR:HG21	1:A:235:ARG:N	2.28	0.49
1:A:334:MET:O	1:A:335:MET:C	2.54	0.49
3:C:127:THR:HG22	3:C:186:LEU:CB	2.42	0.49
4:D:164:ILE:CD1	4:D:182:VAL:HG13	2.35	0.49
5:E:71:MET:C	5:E:73:LYS:N	2.71	0.49
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.48	0.49
2:B:31:ASN:HB3	2:B:201:SER:OG	2.12	0.49
2:B:128:THR:HG21	2:B:223:LEU:HD12	1.94	0.49
2:B:370:MET:O	2:B:373:GLU:HG3	2.12	0.49
3:C:102:GLY:HA2	3:C:107:SER:HB2	1.94	0.49
3:C:139:MET:HE2	3:C:255:GLU:HB3	1.93	0.49
4:D:12:TRP:NE1	4:D:125:ASP:OD1	2.34	0.49
4:D:175:THR:O	4:D:177:ALA:N	2.46	0.49
6:F:13:LEU:N	6:F:13:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:O	1:A:58:PHE:C	2.56	0.49
1:A:103:SER:O	1:A:106:VAL:HG23	2.12	0.49
2:B:395:PRO:C	2:B:398:VAL:HG12	2.38	0.49
3:C:270:LYS:O	3:C:270:LYS:HG3	2.13	0.49
3:C:295:LEU:CG	12:C:383:SIG:H273	2.43	0.49
4:D:139:THR:C	4:D:141:VAL:H	2.20	0.49
5:E:62:MET:HG3	5:E:63:SER:N	2.26	0.49
5:E:62:MET:O	5:E:63:SER:C	2.56	0.49
8:H:35:GLU:O	8:H:39:LEU:HD13	2.12	0.49
2:B:430:LEU:O	2:B:433:THR:N	2.42	0.49
3:C:146:VAL:O	3:C:147:ILE:C	2.56	0.49
3:C:184:PHE:HA	11:C:381:HEM:CBC	2.43	0.49
4:D:128:PHE:O	4:D:129:SER:C	2.56	0.49
1:A:41:ILE:HD12	1:A:195:MET:SD	2.53	0.49
1:A:145:MET:O	1:A:149:VAL:HG12	2.12	0.49
1:A:210:GLU:O	1:A:214:LYS:CB	2.56	0.49
2:B:62:ASN:O	2:B:65:THR:HG22	2.13	0.49
2:B:83:PHE:CZ	2:B:87:ARG:HD2	2.48	0.49
2:B:90:GLU:C	2:B:92:VAL:H	2.20	0.49
4:D:130:LEU:HD11	4:D:158:ILE:CD1	2.43	0.49
1:A:16:VAL:HG22	1:A:26:ALA:HB2	1.95	0.48
1:A:64:PHE:O	1:A:66:GLY:N	2.45	0.48
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.48	0.48
2:B:305:ASN:CB	2:B:306:PRO:HD2	2.43	0.48
3:C:198:LEU:HD11	13:C:384:AMY:H9	1.93	0.48
3:C:369:THR:C	3:C:371:GLY:N	2.69	0.48
10:J:12:LEU:O	10:J:19:THR:HG21	2.13	0.48
1:A:94:HIS:NE2	1:A:381:ARG:HG2	2.29	0.48
1:A:147:GLU:O	1:A:148:VAL:C	2.56	0.48
1:A:327:ASP:O	1:A:328:ARG:C	2.56	0.48
2:B:72:ALA:CB	2:B:75:LEU:HD12	2.42	0.48
2:B:83:PHE:O	2:B:84:LYS:C	2.55	0.48
3:C:166:TRP:C	3:C:166:TRP:CD1	2.91	0.48
4:D:16:GLY:C	4:D:18:LEU:N	2.69	0.48
4:D:47:ALA:O	4:D:48:TYR:C	2.54	0.48
4:D:147:LEU:HD22	4:D:147:LEU:N	2.28	0.48
1:A:36:THR:HG22	1:A:100:LYS:HZ2	1.78	0.48
1:A:153:LEU:C	1:A:153:LEU:CD2	2.86	0.48
3:C:9:HIS:CD2	3:C:10:PRO:HG2	2.46	0.48
3:C:142:TRP:CE3	3:C:265:THR:HG22	2.48	0.48
3:C:242:THR:CA	4:D:208:MET:HE1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:271:PRO:HB3	12:C:383:SIG:C5	2.42	0.48
12:C:383:SIG:H353	12:C:383:SIG:C33	2.41	0.48
8:H:58:LEU:O	8:H:61:PHE:HB3	2.14	0.48
8:H:72:LYS:HA	8:H:75:ASN:HD21	1.77	0.48
1:A:240:GLN:HB3	1:A:422:VAL:HG12	1.95	0.48
3:C:63:ALA:HB2	3:C:176:LEU:HD21	1.95	0.48
3:C:110:TYR:O	3:C:111:LYS:C	2.56	0.48
3:C:137:GLY:N	3:C:140:SER:HB2	2.28	0.48
3:C:184:PHE:HD1	3:C:184:PHE:C	2.21	0.48
3:C:345:GLU:HB3	3:C:347:PRO:HD2	1.96	0.48
5:E:166:ASP:HB3	5:E:172:ARG:HH11	1.76	0.48
1:A:4:TYR:O	1:A:7:ALA:HB3	2.14	0.48
1:A:40:TRP:HZ3	1:A:89:TYR:OH	1.96	0.48
1:A:438:ARG:O	1:A:441:MET:HG2	2.13	0.48
2:B:102:ARG:NH1	2:B:174:ASP:O	2.47	0.48
2:B:248:ASN:C	2:B:248:ASN:ND2	2.64	0.48
3:C:64:PHE:CE2	3:C:259:PRO:HG3	2.48	0.48
3:C:139:MET:O	3:C:140:SER:C	2.56	0.48
5:E:40:THR:O	5:E:41:ALA:C	2.56	0.48
1:A:53:ASN:ND2	1:A:54:GLY:N	2.58	0.48
2:B:24:LEU:H	2:B:24:LEU:CD2	2.23	0.48
2:B:137:VAL:CG2	2:B:138:ALA:N	2.77	0.48
3:C:31:TRP:CD1	3:C:31:TRP:N	2.80	0.48
4:D:63:ALA:HA	4:D:66:GLU:HG3	1.95	0.48
4:D:144:ARG:NH1	4:D:147:LEU:HD21	2.28	0.48
4:D:204:MET:O	4:D:205:GLY:C	2.57	0.48
5:E:166:ASP:OD2	5:E:172:ARG:HD3	2.13	0.48
5:E:184:SER:O	5:E:196:GLY:N	2.36	0.48
6:F:58:ARG:HA	6:F:61:ARG:CZ	2.43	0.48
8:H:62:LEU:O	8:H:63:HIS:C	2.56	0.48
1:A:89:TYR:O	1:A:95:THR:HG23	2.13	0.48
3:C:285:ILE:O	3:C:285:ILE:HG13	2.13	0.48
1:A:428:ILE:O	1:A:429:GLU:C	2.57	0.48
2:B:70:ARG:HD3	2:B:100:SER:HB3	1.95	0.48
2:B:111:CYS:SG	2:B:112:LEU:N	2.87	0.48
2:B:171:ALA:O	2:B:172:LEU:HB3	2.14	0.48
2:B:281:ALA:O	2:B:285:VAL:HB	2.14	0.48
3:C:40:VAL:HG21	3:C:233:LEU:HD23	1.95	0.48
3:C:148:THR:C	3:C:150:LEU:H	2.21	0.48
5:E:32:ARG:HG3	5:E:32:ARG:HH11	1.78	0.48
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:VAL:C	2:B:191:LEU:N	2.71	0.48
3:C:104:TYR:O	3:C:105:TYR:CD1	2.67	0.48
3:C:127:THR:HG22	3:C:186:LEU:CD1	2.40	0.48
3:C:377:MET:HE2	6:F:20:TYR:CB	2.31	0.48
4:D:33:TYR:HA	4:D:37:CYS:SG	2.53	0.48
11:D:242:HEM:HMC1	11:D:242:HEM:CBC	2.44	0.48
1:A:40:TRP:N	1:A:40:TRP:CD1	2.81	0.48
3:C:267:PRO:O	3:C:268:HIS:CB	2.62	0.48
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.28	0.48
4:D:48:TYR:O	4:D:49:ARG:C	2.56	0.48
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.54	0.48
5:E:170:ARG:HA	5:E:179:ASN:CG	2.39	0.48
10:J:55:ILE:C	10:J:57:HIS:H	2.21	0.48
2:B:130:PRO:HB2	2:B:132:PHE:CE1	2.49	0.47
3:C:158:GLY:O	3:C:159:HIS:C	2.57	0.47
4:D:32:VAL:CG1	4:D:186:VAL:HG22	2.42	0.47
4:D:233:ARG:O	6:F:71:ARG:NH2	2.46	0.47
6:F:32:MET:HE3	6:F:87:VAL:CG2	2.43	0.47
10:J:41:ALA:O	10:J:42:ILE:C	2.55	0.47
1:A:36:THR:HG21	1:A:373:THR:OG1	2.13	0.47
2:B:137:VAL:C	2:B:139:ASP:H	2.22	0.47
2:B:160:ILE:O	2:B:161:GLU:C	2.56	0.47
2:B:195:VAL:HG13	2:B:199:PHE:HB2	1.95	0.47
3:C:100:GLY:O	3:C:101:ARG:C	2.56	0.47
4:D:56:TYR:CD2	4:D:60:GLU:HG2	2.49	0.47
4:D:216:VAL:CG2	4:D:217:PRO:CD	2.92	0.47
5:E:11:SER:CA	5:E:15:ARG:HD2	2.39	0.47
5:E:47:VAL:O	5:E:48:ALA:C	2.57	0.47
6:F:101:ARG:O	6:F:104:ARG:N	2.47	0.47
7:G:3:GLN:O	7:G:7:LEU:HD21	2.13	0.47
1:A:60:GLU:OE1	1:A:89:TYR:HA	2.13	0.47
3:C:40:VAL:HG21	3:C:233:LEU:CD2	2.44	0.47
3:C:64:PHE:CD2	3:C:259:PRO:HG3	2.49	0.47
3:C:161:LEU:HD23	3:C:161:LEU:O	2.13	0.47
3:C:184:PHE:HA	11:C:381:HEM:HBC2	1.95	0.47
3:C:186:LEU:O	3:C:187:PRO:C	2.57	0.47
3:C:191:ALA:CA	13:C:384:AMY:H251	2.44	0.47
5:E:170:ARG:HA	5:E:179:ASN:CB	2.43	0.47
7:G:26:PHE:CD1	7:G:26:PHE:N	2.71	0.47
2:B:277:HIS:C	2:B:279:LEU:N	2.69	0.47
2:B:370:MET:C	2:B:372:VAL:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:LEU:HD23	3:C:273:TRP:NE1	2.29	0.47
4:D:97:ASN:O	4:D:100:ALA:HB3	2.13	0.47
4:D:224:ARG:NH2	7:G:27:PRO:HG3	2.29	0.47
5:E:33:LYS:O	5:E:34:GLY:C	2.57	0.47
5:E:153:PHE:HD2	5:E:172:ARG:NH1	2.11	0.47
8:H:72:LYS:O	8:H:75:ASN:ND2	2.47	0.47
1:A:62:LEU:CD2	1:A:126:GLN:HG3	2.44	0.47
1:A:178:SER:C	1:A:180:ALA:N	2.67	0.47
3:C:5:ILE:C	3:C:7:LYS:H	2.21	0.47
3:C:191:ALA:HA	13:C:384:AMY:H251	1.96	0.47
5:E:17:PRO:HA	5:E:20:TYR:CE1	2.50	0.47
5:E:35:PHE:O	5:E:38:LEU:HB3	2.14	0.47
8:H:55:THR:O	8:H:58:LEU:HB3	2.14	0.47
1:A:26:ALA:O	1:A:27:SER:HB3	2.14	0.47
1:A:111:GLU:HB2	1:A:215:HIS:CD2	2.50	0.47
2:B:161:GLU:HA	2:B:161:GLU:OE1	2.14	0.47
2:B:345:LYS:C	2:B:347:ILE:N	2.72	0.47
3:C:87:GLY:O	3:C:88:ALA:C	2.57	0.47
3:C:241:LEU:HD23	3:C:241:LEU:HA	1.58	0.47
3:C:318:PHE:CG	6:F:26:PHE:HB3	2.50	0.47
4:D:21:LEU:HB3	4:D:26:ILE:HD11	1.95	0.47
5:E:70:ALA:C	5:E:72:SER:N	2.73	0.47
5:E:127:VAL:HG11	5:E:133:VAL:HA	1.96	0.47
1:A:99:ILE:HG22	1:A:100:LYS:N	2.30	0.47
1:A:138:LEU:HA	1:A:141:ASN:HD22	1.79	0.47
1:A:252:HIS:HB3	1:A:323:TYR:CE1	2.40	0.47
2:B:47:ILE:HD13	2:B:120:MET:SD	2.54	0.47
2:B:171:ALA:O	2:B:172:LEU:CB	2.63	0.47
2:B:180:ASP:O	2:B:182:ARG:N	2.48	0.47
2:B:213:HIS:O	2:B:213:HIS:HD2	1.97	0.47
3:C:5:ILE:C	3:C:7:LYS:N	2.72	0.47
3:C:153:ALA:HB1	3:C:289:LEU:HD12	1.97	0.47
4:D:83:ARG:O	4:D:83:ARG:HD2	2.13	0.47
5:E:44:THR:HG22	10:J:24:ILE:HG21	1.96	0.47
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.14	0.47
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.49	0.47
6:F:16:ILE:O	6:F:17:ARG:C	2.57	0.47
1:A:291:SER:O	1:A:293:PRO:CD	2.62	0.47
2:B:31:ASN:HD21	2:B:224:LEU:HD13	1.80	0.47
3:C:129:PHE:C	3:C:129:PHE:CD1	2.89	0.47
3:C:350:ILE:HD13	3:C:350:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:178:THR:O	4:D:182:VAL:HG12	2.15	0.47
4:D:235:LEU:O	4:D:236:ALA:HB2	2.13	0.47
5:E:53:ASN:O	5:E:57:GLN:HG3	2.15	0.47
5:E:153:PHE:CD2	5:E:172:ARG:HG3	2.50	0.47
7:G:7:LEU:HD22	7:G:7:LEU:N	2.30	0.47
10:J:20:PHE:CE1	10:J:24:ILE:HD11	2.50	0.47
1:A:61:HIS:CD2	1:A:134:ILE:HG12	2.45	0.47
2:B:307:PHE:CD2	2:B:308:ASP:N	2.82	0.47
2:B:410:VAL:O	2:B:411:ILE:C	2.57	0.47
2:B:424:MET:HG2	2:B:425:ALA:N	2.29	0.47
3:C:89:SER:O	3:C:90:PHE:C	2.58	0.47
3:C:135:PRO:HG2	3:C:140:SER:OG	2.15	0.47
3:C:161:LEU:HD23	3:C:161:LEU:C	2.40	0.47
3:C:277:PHE:CD2	3:C:278:ALA:N	2.83	0.47
3:C:318:PHE:CD2	6:F:26:PHE:HB3	2.49	0.47
3:C:352:GLY:O	3:C:353:GLN:C	2.56	0.47
4:D:195:GLU:OE2	4:D:201:ARG:NH2	2.47	0.47
1:A:8:LEU:O	1:A:11:VAL:HG23	2.15	0.47
1:A:72:GLN:HG2	1:A:76:GLU:OE1	2.15	0.47
1:A:320:PHE:CE2	1:A:415:ILE:HD11	2.46	0.47
2:B:318:ASP:O	2:B:319:SER:HB2	2.14	0.47
3:C:43:MET:CE	13:C:384:AMY:H242	2.45	0.47
3:C:138:GLN:HE21	3:C:261:ASN:N	2.09	0.47
3:C:148:THR:C	3:C:150:LEU:N	2.72	0.47
3:C:149:ASN:O	3:C:152:SER:CB	2.63	0.47
4:D:169:LEU:N	4:D:169:LEU:CD2	2.78	0.47
5:E:119:ASP:O	5:E:179:ASN:ND2	2.47	0.47
3:C:359:TYR:CD2	3:C:360:PHE:HD1	2.34	0.46
4:D:86:LYS:N	4:D:89:ASP:OD1	2.47	0.46
4:D:235:LEU:HB3	6:F:60:PHE:HE1	1.80	0.46
10:J:38:GLY:O	10:J:42:ILE:HG13	2.15	0.46
1:A:382:GLU:CG	1:A:390:ILE:H	2.26	0.46
3:C:107:SER:C	3:C:109:LEU:N	2.72	0.46
3:C:117:GLY:O	3:C:118:VAL:C	2.58	0.46
4:D:46:VAL:CG1	4:D:47:ALA:H	2.23	0.46
4:D:83:ARG:HD2	4:D:83:ARG:C	2.40	0.46
4:D:191:ARG:O	4:D:194:ALA:N	2.48	0.46
4:D:238:ARG:HG3	7:G:14:ILE:HD12	1.98	0.46
5:E:12:ASP:O	5:E:13:TYR:C	2.58	0.46
5:E:35:PHE:O	5:E:36:SER:C	2.58	0.46
5:E:170:ARG:HG2	5:E:179:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:HIS:C	10:J:60:GLU:H	2.17	0.46
10:J:57:HIS:HA	10:J:60:GLU:CA	2.46	0.46
1:A:59:LEU:C	1:A:61:HIS:N	2.72	0.46
1:A:64:PHE:CZ	1:A:86:LEU:HG	2.50	0.46
1:A:236:PHE:HB2	1:A:258:GLU:OE1	2.15	0.46
2:B:67:HIS:O	2:B:70:ARG:HB3	2.15	0.46
2:B:248:ASN:HD22	2:B:249:GLY:N	2.12	0.46
2:B:258:VAL:CG1	2:B:259:ALA:N	2.77	0.46
3:C:223:PRO:O	3:C:227:PHE:HD2	1.97	0.46
3:C:285:ILE:N	3:C:286:PRO:HD3	2.30	0.46
3:C:338:TRP:CE2	7:G:59:TYR:HD1	2.34	0.46
3:C:354:MET:O	3:C:357:LEU:CB	2.63	0.46
4:D:7:PRO:HA	4:D:8:PRO:HD2	1.76	0.46
4:D:227:TRP:O	4:D:228:SER:C	2.56	0.46
5:E:72:SER:CA	5:E:92:ARG:HD3	2.46	0.46
8:H:37:LEU:O	8:H:38:GLU:C	2.57	0.46
2:B:58:GLU:HB3	2:B:62:ASN:ND2	2.30	0.46
3:C:15:ILE:C	3:C:17:ASN:N	2.70	0.46
3:C:45:GLN:CB	11:C:381:HEM:HAB	2.46	0.46
3:C:89:SER:HB3	3:C:273:TRP:HZ2	1.80	0.46
3:C:335:ILE:O	3:C:337:THR:N	2.48	0.46
4:D:16:GLY:O	4:D:18:LEU:N	2.48	0.46
6:F:89:TYR:C	6:F:89:TYR:CD1	2.93	0.46
7:G:56:TYR:O	7:G:59:TYR:HB3	2.15	0.46
8:H:73:LEU:O	8:H:73:LEU:HD23	2.16	0.46
1:A:178:SER:O	1:A:182:LEU:HD23	2.16	0.46
1:A:280:TYR:CD2	1:A:281:ASP:N	2.84	0.46
5:E:38:LEU:HA	10:J:14:PHE:HE2	1.79	0.46
1:A:30:SER:N	1:A:201:GLY:O	2.45	0.46
1:A:85:HIS:CD2	9:I:314:UNK:CB	2.98	0.46
1:A:266:ASP:O	1:A:268:VAL:N	2.48	0.46
2:B:162:ASN:HB3	2:B:244:ILE:HD11	1.97	0.46
2:B:169:ARG:O	2:B:170:ASN:CG	2.58	0.46
2:B:284:HIS:C	2:B:286:LYS:N	2.73	0.46
3:C:65:SER:O	3:C:66:SER:C	2.59	0.46
5:E:189:SER:OG	5:E:192:MET:HB2	2.15	0.46
7:G:38:TRP:C	7:G:40:ARG:N	2.70	0.46
10:J:58:LYS:C	10:J:59:TYR:CG	2.94	0.46
1:A:142:ASP:OD1	5:E:2:HIS:HB3	2.16	0.46
2:B:140:LEU:HD12	2:B:140:LEU:O	2.16	0.46
2:B:307:PHE:CG	2:B:308:ASP:N	2.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.98	0.46
3:C:235:LEU:C	3:C:237:LEU:H	2.24	0.46
3:C:275:PHE:CD2	12:C:383:SIG:C33	2.98	0.46
3:C:275:PHE:CB	12:C:383:SIG:H332	2.45	0.46
3:C:350:ILE:HA	3:C:353:GLN:HE21	1.80	0.46
4:D:43:MET:HG2	4:D:43:MET:O	2.15	0.46
4:D:55:CYS:HG	4:D:56:TYR:HD1	1.54	0.46
1:A:261:GLY:O	1:A:262:TRP:C	2.59	0.46
2:B:146:ILE:C	2:B:148:LYS:N	2.73	0.46
2:B:207:VAL:CG1	2:B:208:GLY:N	2.75	0.46
2:B:213:HIS:N	2:B:214:PRO:CD	2.79	0.46
2:B:258:VAL:HG11	2:B:321:LEU:CB	2.38	0.46
3:C:138:GLN:O	3:C:142:TRP:HD1	1.98	0.46
3:C:239:PRO:O	3:C:240:PHE:C	2.59	0.46
4:D:44:ASP:O	4:D:90:TYR:HD2	1.98	0.46
4:D:135:CYS:O	4:D:149:PHE:HD2	1.98	0.46
4:D:220:TYR:O	4:D:221:TYR:C	2.57	0.46
1:A:405:ARG:HA	1:A:408:ARG:HE	1.81	0.46
2:B:101:THR:HG22	2:B:102:ARG:N	2.31	0.46
2:B:261:SER:O	2:B:262:ALA:O	2.33	0.46
3:C:34:PHE:O	3:C:98:HIS:ND1	2.49	0.46
3:C:249:ASN:O	3:C:250:LEU:C	2.59	0.46
3:C:354:MET:HA	3:C:354:MET:CE	2.42	0.46
4:D:130:LEU:HD11	4:D:158:ILE:HD11	1.98	0.46
5:E:28:SER:O	5:E:31:SER:HB3	2.15	0.46
5:E:87:MET:HG2	5:E:89:PHE:CZ	2.51	0.46
7:G:36:ASN:O	7:G:40:ARG:HG3	2.16	0.46
10:J:57:HIS:CB	10:J:61:ASN:O	2.59	0.46
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.51	0.46
2:B:24:LEU:HD11	2:B:392:TYR:CG	2.51	0.46
2:B:330:ALA:O	2:B:333:ALA:N	2.48	0.46
3:C:97:LEU:O	3:C:100:GLY:N	2.49	0.46
3:C:204:SER:O	3:C:205:GLY:C	2.57	0.46
4:D:144:ARG:HG3	4:D:147:LEU:HD23	1.98	0.46
5:E:57:GLN:C	5:E:59:VAL:H	2.23	0.46
5:E:153:PHE:CE2	5:E:172:ARG:HB3	2.51	0.46
1:A:259:GLY:HA3	1:A:318:GLY:HA3	1.98	0.45
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.98	0.45
2:B:430:LEU:C	2:B:432:HIS:N	2.74	0.45
3:C:207:ASN:O	3:C:208:ASN:CB	2.54	0.45
3:C:254:PRO:HG2	3:C:255:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:LEU:O	3:C:328:LEU:HB3	2.16	0.45
5:E:29:ASP:N	5:E:30:PRO:HD2	2.30	0.45
1:A:266:ASP:C	1:A:268:VAL:H	2.23	0.45
1:A:293:PRO:C	1:A:295:ALA:N	2.70	0.45
1:A:373:THR:HB	1:A:374:PRO:CD	2.45	0.45
1:A:438:ARG:C	1:A:438:ARG:HD3	2.40	0.45
1:A:445:ARG:NH1	10:J:16:ARG:HG2	2.31	0.45
2:B:84:LYS:HG2	2:B:122:PHE:HE1	1.82	0.45
2:B:101:THR:O	2:B:102:ARG:C	2.59	0.45
3:C:27:ASN:HB3	6:F:70:MET:HB2	1.98	0.45
3:C:191:ALA:CB	13:C:384:AMY:H251	2.46	0.45
3:C:221:PHE:CD1	3:C:221:PHE:C	2.93	0.45
4:D:79:GLU:O	4:D:80:MET:C	2.60	0.45
5:E:148:ALA:HB2	5:E:156:TYR:HE1	1.80	0.45
1:A:67:THR:HG21	1:A:115:ASP:CG	2.41	0.45
1:A:209:LEU:O	1:A:213:GLN:N	2.37	0.45
1:A:278:GLY:O	1:A:307:PHE:HE1	1.99	0.45
3:C:16:ASN:HA	3:C:20:ILE:HB	1.98	0.45
3:C:73:ASN:O	5:E:66:ALA:HB3	2.16	0.45
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.87	0.45
4:D:138:PRO:HD3	8:H:58:LEU:HD23	1.99	0.45
5:E:10:PHE:O	5:E:11:SER:C	2.59	0.45
6:F:29:TYR:HB2	6:F:31:LEU:HD21	1.98	0.45
8:H:24:CYS:C	8:H:26:GLN:H	2.24	0.45
2:B:260:GLU:OE1	2:B:319:SER:OG	2.31	0.45
2:B:341:TYR:OH	2:B:439:LEU:HD22	2.16	0.45
2:B:341:TYR:O	2:B:342:ASN:C	2.59	0.45
3:C:105:TYR:O	3:C:106:GLY:C	2.56	0.45
3:C:109:LEU:C	3:C:111:LYS:N	2.71	0.45
3:C:138:GLN:NE2	3:C:138:GLN:HA	2.32	0.45
3:C:261:ASN:ND2	3:C:264:VAL:N	2.65	0.45
4:D:29:GLY:O	4:D:32:VAL:HG12	2.16	0.45
4:D:57:THR:O	4:D:60:GLU:HB3	2.16	0.45
4:D:66:GLU:C	4:D:68:VAL:H	2.23	0.45
4:D:148:TYR:N	4:D:148:TYR:CD1	2.84	0.45
8:H:37:LEU:C	8:H:37:LEU:HD13	2.42	0.45
10:J:48:GLU:HA	10:J:54:HIS:CE1	2.51	0.45
2:B:135:TRP:CD1	2:B:135:TRP:N	2.83	0.45
2:B:146:ILE:HA	2:B:149:ALA:HB3	1.99	0.45
2:B:207:VAL:CG1	2:B:208:GLY:H	2.29	0.45
3:C:52:LEU:HB3	11:C:381:HEM:HMD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:SER:C	4:D:3:LEU:H	2.24	0.45
4:D:116:ILE:HG23	4:D:117:VAL:H	1.80	0.45
1:A:146:ARG:NH2	9:I:206:UNK:HA	2.31	0.45
1:A:328:ARG:CG	1:A:427:PRO:HB2	2.44	0.45
2:B:43:PRO:HG2	2:B:44:GLY:H	1.81	0.45
2:B:59:ASN:C	2:B:61:SER:N	2.73	0.45
3:C:212:ILE:O	3:C:213:SER:C	2.59	0.45
3:C:258:THR:HG22	3:C:258:THR:O	2.16	0.45
3:C:339:ILE:O	3:C:339:ILE:CG2	2.64	0.45
4:D:37:CYS:C	4:D:39:SER:H	2.25	0.45
4:D:50:HIS:O	4:D:51:LEU:C	2.60	0.45
4:D:189:PHE:C	4:D:191:ARG:N	2.74	0.45
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.51	0.45
7:G:24:ARG:HA	7:G:25:PRO:HD2	1.67	0.45
1:A:152:TYR:OH	5:E:5:ILE:HD12	2.16	0.45
1:A:255:ILE:HG12	1:A:420:PRO:HB2	1.98	0.45
3:C:39:ALA:O	3:C:42:LEU:N	2.49	0.45
3:C:139:MET:HE3	3:C:253:ASP:OD2	2.16	0.45
3:C:338:TRP:CZ3	3:C:339:ILE:HD11	2.50	0.45
1:A:77:LYS:O	1:A:81:SER:CB	2.65	0.45
3:C:110:TYR:OH	3:C:207:ASN:HA	2.16	0.45
3:C:340:GLY:C	3:C:342:GLN:H	2.25	0.45
5:E:91:TRP:NE1	5:E:92:ARG:HG3	2.32	0.45
8:H:40:CYS:O	8:H:44:VAL:HG23	2.17	0.45
1:A:150:PHE:O	1:A:153:LEU:HB3	2.17	0.45
1:A:154:HIS:NE2	1:A:314:TYR:OH	2.34	0.45
1:A:428:ILE:C	1:A:430:GLN:N	2.73	0.45
3:C:142:TRP:HA	3:C:145:THR:OG1	2.17	0.45
3:C:361:THR:O	3:C:362:ILE:C	2.58	0.45
4:D:48:TYR:CD2	4:D:65:ALA:HB2	2.52	0.45
8:H:55:THR:O	8:H:58:LEU:N	2.49	0.45
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.98	0.45
2:B:66:SER:OG	2:B:67:HIS:N	2.44	0.45
2:B:101:THR:O	2:B:103:GLU:N	2.50	0.45
2:B:277:HIS:CD2	2:B:363:LYS:HB2	2.52	0.45
3:C:110:TYR:CD2	11:C:382:HEM:HBD2	2.52	0.45
5:E:45:LEU:CD2	10:J:24:ILE:O	2.65	0.45
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.98	0.45
1:A:104:LYS:HG2	1:A:104:LYS:O	2.17	0.44
2:B:112:LEU:N	2:B:112:LEU:CD2	2.81	0.44
2:B:395:PRO:O	2:B:398:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:TRP:O	11:C:382:HEM:O1A	2.35	0.44
3:C:276:LEU:O	3:C:277:PHE:C	2.59	0.44
3:C:295:LEU:HD21	12:C:383:SIG:H273	1.98	0.44
3:C:355:ALA:C	3:C:357:LEU:N	2.72	0.44
3:C:358:SER:O	3:C:362:ILE:HG13	2.17	0.44
4:D:147:LEU:C	4:D:148:TYR:CD1	2.95	0.44
4:D:161:ALA:O	4:D:163:PRO:HD3	2.17	0.44
1:A:59:LEU:O	1:A:61:HIS:N	2.49	0.44
1:A:72:GLN:O	1:A:73:ASN:C	2.60	0.44
2:B:141:GLN:C	2:B:143:GLN:N	2.75	0.44
3:C:124:LEU:HD13	3:C:124:LEU:C	2.42	0.44
3:C:132:TYR:HA	11:C:381:HEM:HAA2	1.99	0.44
3:C:214:SER:OG	3:C:218:LYS:HE3	2.16	0.44
4:D:120:ARG:O	4:D:121:HIS:C	2.60	0.44
5:E:15:ARG:HH12	5:E:19:ASP:HB3	1.74	0.44
5:E:35:PHE:O	5:E:38:LEU:N	2.50	0.44
5:E:86:ASN:HB2	5:E:99:ARG:HG3	1.98	0.44
1:A:61:HIS:NE2	1:A:137:GLU:OE2	2.50	0.44
1:A:85:HIS:CD2	9:I:314:UNK:HB2	2.52	0.44
1:A:102:LEU:C	1:A:104:LYS:N	2.75	0.44
1:A:182:LEU:O	1:A:185:TYR:HB3	2.17	0.44
1:A:297:ILE:HG21	1:A:337:VAL:CG1	2.35	0.44
1:A:372:THR:O	1:A:373:THR:C	2.60	0.44
1:A:391:PRO:CG	1:A:394:GLU:HB2	2.42	0.44
2:B:35:ILE:HD11	2:B:220:ALA:CB	2.48	0.44
2:B:141:GLN:O	2:B:143:GLN:N	2.50	0.44
3:C:42:LEU:HD23	13:C:384:AMY:H23	1.98	0.44
3:C:92:PHE:C	3:C:95:ILE:HG22	2.40	0.44
4:D:51:LEU:C	4:D:54:VAL:HG12	2.42	0.44
10:J:58:LYS:C	10:J:59:TYR:CD1	2.96	0.44
1:A:395:TRP:O	1:A:399:LEU:HG	2.17	0.44
2:B:56:ARG:O	2:B:171:ALA:HB1	2.17	0.44
2:B:71:LEU:O	2:B:73:SER:N	2.51	0.44
2:B:111:CYS:CB	2:B:119:LEU:HD22	2.46	0.44
2:B:259:ALA:O	2:B:260:GLU:C	2.59	0.44
2:B:272:PHE:HB3	2:B:322:PHE:CD2	2.53	0.44
2:B:399:LEU:O	2:B:402:ILE:HG22	2.18	0.44
3:C:81:ARG:HH11	3:C:81:ARG:HG3	1.82	0.44
3:C:121:LEU:O	3:C:122:LEU:C	2.59	0.44
4:D:5:LEU:HB2	8:H:59:PHE:CE1	2.53	0.44
7:G:64:GLN:O	7:G:65:GLU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:THR:O	1:A:238:GLY:C	2.61	0.44
1:A:279:HIS:HB2	1:A:307:PHE:O	2.18	0.44
1:A:305:GLN:HB3	9:I:203:UNK:HA	1.99	0.44
2:B:31:ASN:CB	2:B:201:SER:HB2	2.47	0.44
2:B:69:LEU:CD1	2:B:105:MET:HE1	2.41	0.44
2:B:169:ARG:O	2:B:170:ASN:HB3	2.17	0.44
2:B:273:SER:CB	2:B:364:LEU:HD11	2.45	0.44
3:C:67:VAL:O	3:C:68:ALA:C	2.60	0.44
3:C:92:PHE:HA	3:C:95:ILE:HG22	2.00	0.44
3:C:319:ARG:HH22	3:C:371:GLY:C	2.23	0.44
4:D:235:LEU:CD1	6:F:64:ARG:HA	2.48	0.44
5:E:193:VAL:HG13	5:E:193:VAL:O	2.18	0.44
7:G:42:ARG:HH11	7:G:42:ARG:HG2	1.82	0.44
1:A:74:ALA:O	1:A:78:GLU:N	2.46	0.44
1:A:370:ASP:O	1:A:374:PRO:HG3	2.17	0.44
2:B:70:ARG:HE	9:I:107:UNK:CB	2.31	0.44
2:B:409:ASP:O	2:B:411:ILE:N	2.51	0.44
3:C:9:HIS:HD2	3:C:10:PRO:CG	2.29	0.44
3:C:88:ALA:O	3:C:91:PHE:HB3	2.17	0.44
3:C:108:TYR:HB2	3:C:306:PRO:HG3	1.99	0.44
3:C:202:HIS:HD1	3:C:202:HIS:H	1.63	0.44
3:C:354:MET:O	3:C:357:LEU:HB3	2.18	0.44
4:D:57:THR:HG22	4:D:58:GLU:N	2.33	0.44
4:D:230:LEU:CB	6:F:70:MET:HE3	2.42	0.44
10:J:57:HIS:O	10:J:60:GLU:N	2.33	0.44
1:A:49:SER:HB2	1:A:52:ASN:CB	2.46	0.44
1:A:159:GLN:HE21	5:E:7:VAL:CG1	2.09	0.44
1:A:332:ASP:C	1:A:334:MET:N	2.75	0.44
2:B:120:MET:O	2:B:121:GLU:C	2.59	0.44
2:B:207:VAL:HG11	2:B:382:VAL:HG23	1.99	0.44
3:C:27:ASN:CB	6:F:69:ASN:ND2	2.72	0.44
3:C:43:MET:O	3:C:44:THR:C	2.60	0.44
3:C:70:THR:HA	3:C:74:VAL:HG23	2.00	0.44
3:C:78:TRP:CD2	3:C:79:LEU:N	2.86	0.44
3:C:113:THR:CG2	3:C:201:LEU:HA	2.47	0.44
3:C:352:GLY:C	3:C:354:MET:N	2.74	0.44
3:C:376:LYS:C	3:C:378:LEU:N	2.76	0.44
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.32	0.44
2:B:269:ALA:O	2:B:270:ASN:C	2.60	0.44
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.48	0.44
3:C:46:ILE:O	3:C:50:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:ILE:O	3:C:81:ARG:C	2.60	0.44
4:D:16:GLY:C	4:D:18:LEU:H	2.26	0.44
4:D:95:TYR:HE2	4:D:104:ALA:CB	2.30	0.44
4:D:129:SER:O	4:D:130:LEU:C	2.59	0.44
4:D:228:SER:O	4:D:232:SER:HB3	2.18	0.44
4:D:238:ARG:HD2	5:E:5:ILE:HD11	2.00	0.44
5:E:15:ARG:HH11	5:E:19:ASP:HB3	1.80	0.44
7:G:42:ARG:O	7:G:43:ALA:HB2	2.18	0.44
8:H:61:PHE:O	8:H:64:ALA:N	2.49	0.44
10:J:13:LEU:HA	10:J:19:THR:CG2	2.48	0.44
1:A:268:VAL:O	1:A:269:ALA:C	2.60	0.44
1:A:343:MET:C	1:A:347:THR:HG22	2.43	0.44
2:B:405:VAL:CG1	2:B:406:ALA:H	2.28	0.44
3:C:136:TRP:CD1	3:C:176:LEU:HD13	2.53	0.44
3:C:199:THR:O	3:C:200:PHE:C	2.60	0.44
4:D:29:GLY:HA3	4:D:185:ASP:O	2.18	0.44
1:A:114:ALA:HB2	1:A:216:PHE:CE1	2.52	0.43
1:A:123:GLU:HB3	1:A:126:GLN:CB	2.48	0.43
1:A:250:LEU:CD2	1:A:325:VAL:CG1	2.93	0.43
2:B:147:ASP:O	2:B:150:VAL:HG22	2.18	0.43
3:C:92:PHE:O	3:C:96:PHE:CD2	2.71	0.43
3:C:113:THR:HG22	3:C:201:LEU:N	2.32	0.43
3:C:173:ASN:O	3:C:174:PRO:C	2.60	0.43
3:C:282:LEU:HD23	3:C:295:LEU:HD22	2.00	0.43
3:C:326:PHE:O	3:C:329:LEU:N	2.51	0.43
4:D:167:ASP:O	4:D:168:VAL:C	2.60	0.43
11:D:242:HEM:HBB2	11:D:242:HEM:CMB	2.48	0.43
10:J:57:HIS:HA	10:J:60:GLU:HB2	1.99	0.43
1:A:15:GLN:HB3	1:A:205:HIS:CE1	2.53	0.43
1:A:134:ILE:O	1:A:138:LEU:N	2.50	0.43
1:A:335:MET:HG3	1:A:339:GLN:HE21	1.82	0.43
1:A:382:GLU:OE2	1:A:390:ILE:HB	2.19	0.43
2:B:240:ARG:NH1	2:B:242:GLY:HA3	2.33	0.43
2:B:430:LEU:C	2:B:432:HIS:H	2.25	0.43
3:C:56:TYR:OH	3:C:134:LEU:O	2.31	0.43
3:C:134:LEU:C	3:C:136:TRP:H	2.26	0.43
4:D:98:PRO:C	4:D:100:ALA:N	2.76	0.43
8:H:24:CYS:C	8:H:26:GLN:N	2.77	0.43
1:A:120:CYS:O	1:A:121:SER:C	2.61	0.43
1:A:382:GLU:HG2	1:A:390:ILE:N	2.32	0.43
1:A:411:CYS:O	1:A:415:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD21	2:B:223:LEU:HD23	2.00	0.43
3:C:95:ILE:HD13	3:C:121:LEU:CD1	2.47	0.43
3:C:106:GLY:C	3:C:108:TYR:N	2.74	0.43
3:C:186:LEU:O	3:C:189:ALA:N	2.45	0.43
3:C:345:GLU:C	3:C:347:PRO:HD2	2.43	0.43
5:E:166:ASP:OD2	5:E:170:ARG:NE	2.51	0.43
5:E:171:ILE:N	5:E:179:ASN:OD1	2.44	0.43
6:F:32:MET:SD	6:F:87:VAL:HG22	2.59	0.43
1:A:85:HIS:O	1:A:99:ILE:HA	2.18	0.43
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.44	0.43
1:A:206:GLN:HA	1:A:209:LEU:HD12	2.00	0.43
1:A:365:LEU:HD21	1:A:395:TRP:CB	2.48	0.43
2:B:65:THR:O	2:B:69:LEU:HB2	2.18	0.43
2:B:163:LEU:O	2:B:166:ALA:N	2.52	0.43
2:B:217:LYS:C	2:B:219:VAL:N	2.76	0.43
2:B:366:ALA:O	2:B:367:LYS:C	2.60	0.43
3:C:33:ASN:O	3:C:34:PHE:C	2.62	0.43
3:C:44:THR:O	3:C:48:THR:HG23	2.19	0.43
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.30	0.43
4:D:169:LEU:HD11	4:D:171:PHE:CE1	2.53	0.43
5:E:26:ARG:O	5:E:27:GLU:HG3	2.19	0.43
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.54	0.43
1:A:106:VAL:HG21	1:A:203:VAL:HG13	2.01	0.43
1:A:358:LYS:O	1:A:361:LEU:N	2.51	0.43
1:A:404:ALA:O	1:A:407:VAL:N	2.52	0.43
2:B:276:GLN:OE1	2:B:313:ASN:HB3	2.18	0.43
2:B:277:HIS:O	2:B:278:VAL:C	2.62	0.43
2:B:419:SER:O	2:B:420:ARG:O	2.36	0.43
3:C:7:LYS:O	3:C:13:LYS:HD2	2.18	0.43
3:C:204:SER:C	3:C:205:GLY:O	2.60	0.43
3:C:332:ASN:HD21	3:C:359:TYR:N	2.15	0.43
3:C:361:THR:CA	3:C:365:ILE:HG22	2.47	0.43
11:C:382:HEM:HMA1	11:C:382:HEM:HAA2	1.87	0.43
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.80	0.43
4:D:160:MET:HB2	11:D:242:HEM:C2D	2.54	0.43
4:D:161:ALA:O	4:D:162:PRO:C	2.61	0.43
4:D:218:LEU:CD1	5:E:42:VAL:HG12	2.48	0.43
4:D:234:LYS:O	7:G:15:THR:HA	2.19	0.43
5:E:42:VAL:O	5:E:45:LEU:HB3	2.18	0.43
7:G:50:PRO:CG	7:G:51:PRO:HD2	2.46	0.43
10:J:57:HIS:ND1	10:J:58:LYS:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SER:CB	1:A:199:ALA:O	2.67	0.43
1:A:296:SER:O	1:A:299:VAL:N	2.46	0.43
1:A:351:GLU:OE1	1:A:404:ALA:HB2	2.19	0.43
2:B:202:ALA:CB	2:B:229:GLY:HA2	2.48	0.43
3:C:117:GLY:O	3:C:120:LEU:HB2	2.19	0.43
3:C:157:ILE:O	3:C:157:ILE:HG13	2.18	0.43
3:C:276:LEU:HA	3:C:279:TYR:HB3	2.01	0.43
4:D:51:LEU:O	4:D:54:VAL:HG12	2.19	0.43
4:D:179:MET:O	4:D:180:SER:C	2.61	0.43
5:E:9:ASN:ND2	5:E:11:SER:HB3	2.33	0.43
5:E:48:ALA:O	5:E:49:TYR:C	2.61	0.43
6:F:58:ARG:O	6:F:59:MET:C	2.61	0.43
8:H:17:LEU:HD13	8:H:73:LEU:CD1	2.45	0.43
1:A:35:CYS:C	1:A:36:THR:HG23	2.44	0.43
3:C:22:LEU:HB3	3:C:221:PHE:HB2	1.99	0.43
3:C:112:GLU:O	3:C:113:THR:C	2.61	0.43
4:D:143:VAL:CG2	4:D:147:LEU:HB2	2.49	0.43
5:E:32:ARG:HH22	7:G:25:PRO:CD	2.27	0.43
5:E:63:SER:O	5:E:64:ALA:C	2.60	0.43
5:E:74:ILE:CG2	5:E:195:VAL:HB	2.48	0.43
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.87	0.43
10:J:57:HIS:CA	10:J:60:GLU:C	2.91	0.43
1:A:178:SER:O	1:A:180:ALA:N	2.52	0.43
1:A:438:ARG:C	1:A:440:GLY:N	2.70	0.43
2:B:53:ALA:O	2:B:104:ASN:N	2.52	0.43
3:C:89:SER:C	3:C:91:PHE:N	2.75	0.43
3:C:146:VAL:HG23	3:C:147:ILE:HG13	2.00	0.43
4:D:216:VAL:O	4:D:217:PRO:C	2.55	0.43
5:E:17:PRO:HA	5:E:20:TYR:HE1	1.83	0.43
5:E:52:LYS:C	5:E:52:LYS:CD	2.92	0.43
10:J:57:HIS:HA	10:J:60:GLU:CB	2.49	0.43
1:A:21:ASN:HD21	1:A:218:GLY:HA3	1.84	0.43
1:A:35:CYS:HA	1:A:372:THR:HG21	2.00	0.43
1:A:49:SER:CB	1:A:52:ASN:HB3	2.48	0.43
1:A:73:ASN:O	1:A:77:LYS:HB2	2.18	0.43
2:B:58:GLU:OE2	2:B:64:GLY:N	2.51	0.43
3:C:52:LEU:CD2	11:C:381:HEM:HBD1	2.49	0.43
3:C:141:PHE:O	3:C:144:ALA:HB3	2.18	0.43
3:C:148:THR:O	3:C:150:LEU:N	2.51	0.43
3:C:154:ILE:O	3:C:158:GLY:HA3	2.19	0.43
3:C:170:SER:O	3:C:171:VAL:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:331:ALA:C	3:C:333:LEU:N	2.74	0.43
4:D:168:VAL:O	4:D:168:VAL:HG12	2.18	0.43
5:E:9:ASN:HD21	5:E:11:SER:HB3	1.83	0.43
8:H:47:ARG:CD	8:H:48:SER:H	2.30	0.43
10:J:36:ASP:O	10:J:37:GLN:C	2.62	0.43
1:A:24:ARG:HG3	1:A:24:ARG:NH1	2.33	0.43
1:A:86:LEU:CB	1:A:99:ILE:HG12	2.49	0.43
1:A:140:GLU:C	1:A:142:ASP:N	2.76	0.43
2:B:187:THR:HG1	2:B:190:GLU:HG3	1.82	0.43
3:C:243:LEU:N	3:C:243:LEU:HD22	2.34	0.43
3:C:266:PRO:O	3:C:269:ILE:HG13	2.19	0.43
3:C:304:LEU:O	3:C:305:ILE:C	2.59	0.43
4:D:224:ARG:O	4:D:225:HIS:C	2.62	0.43
5:E:117:LEU:O	5:E:120:PRO:HD3	2.19	0.43
1:A:39:VAL:HG22	1:A:41:ILE:HD13	2.01	0.42
1:A:274:ASN:O	1:A:309:THR:HG21	2.19	0.42
1:A:431:LEU:HD23	1:A:432:PRO:N	2.33	0.42
2:B:37:SER:O	2:B:38:LEU:HB2	2.19	0.42
2:B:135:TRP:O	2:B:136:GLU:C	2.61	0.42
2:B:209:LEU:O	2:B:211:VAL:N	2.52	0.42
4:D:83:ARG:HH12	4:D:86:LYS:HG3	1.80	0.42
4:D:175:THR:O	4:D:176:PRO:C	2.60	0.42
5:E:85:LYS:HG2	5:E:86:ASN:N	2.32	0.42
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.54	0.42
6:F:101:ARG:O	6:F:102:LYS:C	2.62	0.42
7:G:38:TRP:C	7:G:40:ARG:H	2.26	0.42
9:I:105:UNK:O	9:I:106:UNK:CB	2.67	0.42
2:B:61:SER:C	2:B:63:LEU:H	2.27	0.42
3:C:198:LEU:O	3:C:199:THR:C	2.61	0.42
3:C:284:SER:C	3:C:286:PRO:HD3	2.44	0.42
3:C:359:TYR:CD2	3:C:360:PHE:CD1	3.07	0.42
4:D:211:MET:O	4:D:212:MET:C	2.62	0.42
5:E:19:ASP:O	5:E:20:TYR:CD1	2.72	0.42
6:F:32:MET:O	6:F:33:ARG:C	2.62	0.42
1:A:64:PHE:C	1:A:66:GLY:N	2.76	0.42
2:B:378:PHE:C	2:B:380:GLU:H	2.26	0.42
3:C:48:THR:O	3:C:51:LEU:HB3	2.19	0.42
3:C:129:PHE:C	3:C:130:VAL:O	2.60	0.42
3:C:184:PHE:O	3:C:184:PHE:CD1	2.71	0.42
3:C:191:ALA:O	3:C:195:ILE:HG12	2.19	0.42
3:C:201:LEU:O	3:C:202:HIS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:SER:N	3:C:248:PRO:HD3	2.35	0.42
4:D:233:ARG:C	6:F:71:ARG:NH2	2.76	0.42
10:J:16:ARG:C	10:J:18:SER:N	2.77	0.42
10:J:45:HIS:ND1	10:J:45:HIS:C	2.77	0.42
10:J:57:HIS:C	10:J:57:HIS:ND1	2.77	0.42
1:A:146:ARG:HG2	1:A:146:ARG:NH1	2.35	0.42
1:A:262:TRP:O	1:A:263:ALA:C	2.61	0.42
2:B:69:LEU:C	2:B:69:LEU:HD13	2.44	0.42
3:C:175:THR:O	3:C:179:PHE:CD1	2.72	0.42
5:E:29:ASP:OD2	7:G:22:GLU:OE1	2.38	0.42
6:F:34:ASP:C	6:F:36:THR:N	2.78	0.42
1:A:91:SER:OG	1:A:92:ARG:N	2.52	0.42
1:A:92:ARG:NE	1:A:154:HIS:CD2	2.87	0.42
1:A:269:ALA:CB	1:A:410:VAL:HG21	2.49	0.42
1:A:294:LEU:HD11	1:A:334:MET:CE	2.50	0.42
1:A:310:PHE:HE1	1:A:322:PHE:N	2.17	0.42
2:B:50:PHE:C	2:B:51:ILE:HG13	2.45	0.42
2:B:117:GLU:O	2:B:120:MET:HB2	2.19	0.42
2:B:372:VAL:O	2:B:372:VAL:HG12	2.18	0.42
2:B:395:PRO:HA	2:B:398:VAL:HG12	2.00	0.42
3:C:42:LEU:HD21	3:C:191:ALA:HA	2.02	0.42
3:C:130:VAL:CG1	3:C:179:PHE:HB3	2.46	0.42
1:A:146:ARG:NH2	9:I:206:UNK:CB	2.82	0.42
1:A:165:GLN:HE21	1:A:165:GLN:HB2	1.66	0.42
1:A:236:PHE:CD2	1:A:258:GLU:HB2	2.54	0.42
1:A:262:TRP:HH2	1:A:381:ARG:HH21	1.66	0.42
1:A:322:PHE:C	1:A:322:PHE:CD1	2.97	0.42
1:A:350:SER:O	1:A:353:GLU:HB2	2.19	0.42
3:C:233:LEU:CD1	3:C:237:LEU:HD22	2.48	0.42
5:E:53:ASN:O	5:E:54:VAL:C	2.62	0.42
5:E:101:ARG:HH12	5:E:123:ASP:CG	2.27	0.42
1:A:102:LEU:H	1:A:102:LEU:CD1	2.26	0.42
1:A:167:VAL:HB	1:A:168:GLU:OE2	2.20	0.42
2:B:37:SER:O	2:B:38:LEU:CB	2.67	0.42
2:B:270:ASN:O	2:B:273:SER:HB2	2.20	0.42
3:C:37:LEU:O	3:C:38:LEU:C	2.62	0.42
3:C:42:LEU:O	3:C:46:ILE:HG13	2.20	0.42
3:C:63:ALA:O	3:C:66:SER:OG	2.35	0.42
3:C:238:THR:N	3:C:239:PRO:CD	2.83	0.42
3:C:344:VAL:C	3:C:349:ILE:HD11	2.44	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TYR:O	1:A:435:ASN:C	2.62	0.42
2:B:276:GLN:O	2:B:279:LEU:O	2.38	0.42
2:B:277:HIS:CB	2:B:360:ALA:HB1	2.48	0.42
2:B:374:SER:O	2:B:377:GLY:N	2.50	0.42
2:B:410:VAL:C	2:B:412:LYS:N	2.77	0.42
3:C:69:HIS:O	3:C:71:CYS:N	2.53	0.42
3:C:239:PRO:O	3:C:243:LEU:HD23	2.19	0.42
3:C:327:TRP:HE3	3:C:330:VAL:HG11	1.84	0.42
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.55	0.42
4:D:57:THR:O	4:D:58:GLU:C	2.63	0.42
4:D:144:ARG:NH1	4:D:147:LEU:CD2	2.83	0.42
4:D:160:MET:HB2	11:D:242:HEM:C1D	2.55	0.42
5:E:26:ARG:C	5:E:28:SER:N	2.68	0.42
5:E:121:GLN:OE1	5:E:126:ARG:HD2	2.20	0.42
10:J:54:HIS:O	10:J:57:HIS:NE2	2.53	0.42
1:A:114:ALA:HA	1:A:216:PHE:CE1	2.53	0.42
1:A:250:LEU:HD23	1:A:251:ALA:O	2.19	0.42
3:C:27:ASN:HD22	6:F:69:ASN:HD21	1.61	0.42
3:C:93:ILE:O	3:C:94:CYS:C	2.63	0.42
3:C:130:VAL:HG13	3:C:179:PHE:CD2	2.55	0.42
3:C:308:LEU:HD13	3:C:364:LEU:HA	2.01	0.42
12:C:383:SIG:H343	12:C:383:SIG:H23	1.97	0.42
4:D:98:PRO:HG2	4:D:99:GLU:OE2	2.20	0.42
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.55	0.42
1:A:65:LYS:HZ1	9:I:310:UNK:C	2.33	0.42
2:B:353:SER:C	2:B:355:GLU:N	2.77	0.42
3:C:63:ALA:CB	3:C:176:LEU:HD21	2.50	0.42
3:C:86:ASN:O	3:C:87:GLY:C	2.63	0.42
3:C:295:LEU:CD1	12:C:383:SIG:H273	2.50	0.42
11:D:242:HEM:CBB	11:D:242:HEM:CMB	2.97	0.42
5:E:136:ILE:O	5:E:180:LEU:HD22	2.20	0.42
1:A:8:LEU:O	1:A:11:VAL:HB	2.20	0.41
1:A:245:GLU:C	1:A:247:GLY:H	2.28	0.41
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.79	0.41
1:A:396:GLU:O	1:A:400:ALA:N	2.53	0.41
1:A:419:CYS:SG	1:A:438:ARG:NH2	2.78	0.41
2:B:269:ALA:O	2:B:271:ALA:N	2.53	0.41
3:C:108:TYR:CE1	3:C:109:LEU:CD2	3.03	0.41
3:C:147:ILE:O	3:C:150:LEU:CB	2.56	0.41
3:C:162:VAL:HA	3:C:165:ALA:HB2	2.01	0.41
3:C:316:MET:HB3	3:C:319:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:THR:CA	4:D:179:MET:HE2	2.45	0.41
5:E:49:TYR:O	5:E:50:ALA:C	2.61	0.41
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.32	0.41
1:A:14:THR:HG23	1:A:27:SER:O	2.21	0.41
1:A:103:SER:C	1:A:105:ASP:N	2.78	0.41
1:A:405:ARG:HG2	1:A:405:ARG:NH1	2.35	0.41
2:B:228:GLY:O	2:B:229:GLY:C	2.63	0.41
2:B:264:ILE:HD11	2:B:317:SER:HA	2.02	0.41
3:C:194:THR:O	3:C:197:HIS:HB3	2.19	0.41
4:D:214:LEU:O	4:D:217:PRO:HG2	2.20	0.41
5:E:78:LEU:HD11	5:E:193:VAL:HB	2.02	0.41
5:E:171:ILE:HD12	5:E:172:ARG:H	1.85	0.41
6:F:12:TRP:CB	6:F:15:GLY:H	2.32	0.41
9:I:117:UNK:O	9:I:118:UNK:CB	2.67	0.41
1:A:23:VAL:CG2	1:A:192:ALA:HB1	2.46	0.41
1:A:192:ALA:N	1:A:193:PRO:HD2	2.34	0.41
2:B:56:ARG:HG3	2:B:56:ARG:HH11	1.85	0.41
2:B:268:GLU:O	2:B:268:GLU:HG2	2.20	0.41
3:C:139:MET:HB2	3:C:256:ASN:OD1	2.21	0.41
3:C:166:TRP:HB2	3:C:175:THR:HG21	1.96	0.41
4:D:23:HIS:HB2	10:J:50:LYS:O	2.20	0.41
5:E:14:ARG:O	5:E:15:ARG:O	2.38	0.41
5:E:171:ILE:O	5:E:171:ILE:HG23	2.19	0.41
6:F:40:ASN:O	6:F:41:ASP:C	2.62	0.41
6:F:58:ARG:HA	6:F:61:ARG:NH2	2.35	0.41
6:F:62:ILE:O	6:F:66:LEU:HG	2.20	0.41
6:F:67:ASP:O	6:F:71:ARG:HG3	2.20	0.41
7:G:73:ASN:O	7:G:74:PRO:C	2.62	0.41
1:A:39:VAL:O	1:A:39:VAL:CG1	2.68	0.41
1:A:40:TRP:CE3	1:A:96:ALA:CB	3.03	0.41
1:A:161:THR:HG21	1:A:234:CYS:CA	2.47	0.41
1:A:205:HIS:O	1:A:206:GLN:C	2.64	0.41
1:A:343:MET:CA	1:A:343:MET:CE	2.97	0.41
3:C:120:LEU:H	3:C:120:LEU:HD22	1.86	0.41
3:C:324:THR:O	3:C:325:LEU:C	2.62	0.41
5:E:126:ARG:HG2	5:E:126:ARG:HH11	1.85	0.41
7:G:53:LEU:O	7:G:57:LEU:HD23	2.20	0.41
8:H:59:PHE:O	8:H:61:PHE:N	2.54	0.41
1:A:64:PHE:CE1	1:A:86:LEU:CG	3.03	0.41
1:A:155:ALA:O	5:E:7:VAL:HG21	2.20	0.41
2:B:200:THR:HG22	2:B:226:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:LYS:O	3:C:112:GLU:C	2.62	0.41
3:C:271:PRO:HG3	3:C:279:TYR:CG	2.56	0.41
4:D:192:TRP:O	4:D:193:ALA:C	2.64	0.41
5:E:91:TRP:CZ2	5:E:92:ARG:NE	2.89	0.41
5:E:97:PHE:O	5:E:134:ILE:HA	2.21	0.41
5:E:127:VAL:CG1	5:E:133:VAL:HA	2.49	0.41
6:F:32:MET:N	6:F:35:ASP:OD2	2.52	0.41
8:H:68:CYS:O	8:H:69:VAL:C	2.62	0.41
1:A:144:SER:C	1:A:146:ARG:N	2.78	0.41
1:A:251:ALA:HB1	1:A:428:ILE:HG22	2.02	0.41
2:B:39:GLU:HG3	2:B:41:TYR:CD1	2.55	0.41
2:B:137:VAL:C	2:B:139:ASP:N	2.78	0.41
2:B:168:TYR:CD1	2:B:168:TYR:N	2.87	0.41
3:C:9:HIS:HA	3:C:10:PRO:HD2	1.72	0.41
3:C:76:TYR:CE2	5:E:57:GLN:HG2	2.56	0.41
3:C:210:LEU:HD23	3:C:210:LEU:HA	1.87	0.41
3:C:325:LEU:HD21	3:C:362:ILE:HG23	2.00	0.41
3:C:335:ILE:O	3:C:338:TRP:N	2.53	0.41
3:C:335:ILE:C	3:C:337:THR:N	2.76	0.41
4:D:150:ASN:HA	4:D:151:PRO:HD2	1.81	0.41
4:D:155:GLY:C	4:D:157:ALA:N	2.79	0.41
8:H:15:ASP:HA	8:H:16:PRO:HD2	1.82	0.41
10:J:33:ARG:O	10:J:37:GLN:HG3	2.21	0.41
1:A:102:LEU:O	1:A:103:SER:OG	2.37	0.41
1:A:114:ALA:CB	1:A:216:PHE:CE1	3.04	0.41
2:B:282:ASN:HB2	2:B:283:PRO:CD	2.51	0.41
2:B:397:THR:C	2:B:399:LEU:N	2.78	0.41
2:B:410:VAL:O	2:B:413:ALA:N	2.54	0.41
3:C:52:LEU:HD21	11:C:381:HEM:O2D	2.21	0.41
3:C:75:GLN:C	3:C:77:GLY:H	2.27	0.41
3:C:229:ASP:OD2	13:C:384:AMY:O1	2.39	0.41
4:D:26:ILE:HG23	4:D:189:PHE:HA	2.02	0.41
4:D:118:ARG:NH1	4:D:195:GLU:OE1	2.54	0.41
7:G:11:ARG:O	7:G:12:HIS:HB2	2.20	0.41
1:A:106:VAL:HB	1:A:107:PRO:HD3	2.02	0.41
2:B:189:VAL:O	2:B:190:GLU:C	2.63	0.41
2:B:221:GLU:HG3	2:B:222:GLN:H	1.86	0.41
3:C:146:VAL:O	3:C:150:LEU:N	2.52	0.41
3:C:346:HIS:O	3:C:347:PRO:C	2.62	0.41
4:D:22:ASP:HA	10:J:50:LYS:HB3	2.02	0.41
4:D:200:HIS:O	4:D:204:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD13	5:E:132:TRP:CE2	2.55	0.41
6:F:34:ASP:C	6:F:36:THR:H	2.28	0.41
6:F:87:VAL:O	6:F:89:TYR:N	2.47	0.41
6:F:87:VAL:HA	6:F:88:PRO:HD2	1.91	0.41
7:G:53:LEU:O	7:G:56:TYR:HB3	2.21	0.41
1:A:36:THR:CG2	1:A:100:LYS:NZ	2.83	0.41
1:A:72:GLN:O	1:A:74:ALA:N	2.54	0.41
1:A:145:MET:CB	1:A:252:HIS:CD2	3.04	0.41
1:A:239:SER:CB	7:G:18:LEU:HA	2.51	0.41
1:A:245:GLU:C	1:A:247:GLY:N	2.79	0.41
1:A:250:LEU:HB2	1:A:326:CYS:O	2.21	0.41
1:A:266:ASP:O	1:A:267:LEU:C	2.64	0.41
1:A:365:LEU:HD21	1:A:395:TRP:HB3	2.02	0.41
1:A:388:ARG:HG2	1:A:389:ARG:N	2.34	0.41
1:A:428:ILE:O	1:A:430:GLN:N	2.54	0.41
1:A:431:LEU:HA	1:A:432:PRO:HD2	1.83	0.41
2:B:24:LEU:HD11	2:B:392:TYR:CD2	2.55	0.41
2:B:31:ASN:ND2	2:B:224:LEU:HD13	2.35	0.41
2:B:166:ALA:HB1	2:B:242:GLY:C	2.45	0.41
3:C:4:ASN:OD1	3:C:7:LYS:CB	2.69	0.41
3:C:45:GLN:CG	11:C:381:HEM:HAB	2.46	0.41
3:C:76:TYR:CE1	4:D:200:HIS:HE1	2.25	0.41
3:C:104:TYR:CZ	3:C:316:MET:CB	3.02	0.41
3:C:143:GLY:O	3:C:144:ALA:C	2.63	0.41
3:C:183:HIS:O	3:C:184:PHE:C	2.63	0.41
3:C:212:ILE:HD12	6:F:62:ILE:HG23	2.03	0.41
3:C:319:ARG:NH2	3:C:374:GLU:OE2	2.53	0.41
3:C:319:ARG:HH21	3:C:371:GLY:HA2	1.84	0.41
3:C:331:ALA:C	3:C:333:LEU:H	2.29	0.41
3:C:374:GLU:HB3	6:F:20:TYR:CZ	2.56	0.41
4:D:26:ILE:O	4:D:27:ARG:C	2.63	0.41
4:D:46:VAL:HB	4:D:91:PHE:CE2	2.56	0.41
4:D:97:ASN:HB2	4:D:98:PRO:HD2	2.03	0.41
4:D:127:VAL:O	4:D:128:PHE:C	2.63	0.41
5:E:78:LEU:HG	5:E:193:VAL:CG1	2.51	0.41
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.50	0.41
5:E:153:PHE:CD2	5:E:172:ARG:NH1	2.88	0.41
1:A:32:GLN:HA	1:A:33:PRO:HD2	1.71	0.41
1:A:36:THR:HG23	1:A:372:THR:HG1	1.83	0.41
1:A:48:GLU:OE1	1:A:53:ASN:ND2	2.54	0.41
1:A:111:GLU:O	1:A:112:LEU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLU:C	1:A:149:VAL:N	2.78	0.41
2:B:176:LEU:HD12	2:B:176:LEU:O	2.20	0.41
2:B:277:HIS:HD2	2:B:363:LYS:HB2	1.86	0.41
3:C:131:GLY:HA2	3:C:134:LEU:CD2	2.46	0.41
3:C:134:LEU:CD1	3:C:134:LEU:H	2.33	0.41
3:C:158:GLY:C	3:C:160:THR:N	2.77	0.41
3:C:172:ASP:CG	3:C:173:ASN:N	2.79	0.41
3:C:214:SER:C	3:C:216:SER:N	2.77	0.41
3:C:233:LEU:C	3:C:233:LEU:HD13	2.45	0.41
11:C:382:HEM:HMA2	13:C:384:AMY:O7	2.21	0.41
5:E:102:THR:H	5:E:105:GLU:HB2	1.86	0.41
6:F:43:VAL:O	6:F:46:ALA:HB3	2.20	0.41
6:F:80:TRP:N	6:F:80:TRP:CD1	2.89	0.41
7:G:48:VAL:O	7:G:51:PRO:HG2	2.21	0.41
1:A:37:VAL:HG23	1:A:113:LEU:HD11	2.03	0.40
1:A:55:ALA:O	1:A:56:GLY:C	2.63	0.40
1:A:158:PHE:O	1:A:159:GLN:C	2.64	0.40
1:A:343:MET:HE2	1:A:343:MET:N	2.35	0.40
1:A:433:ASP:OD2	1:A:435:ASN:ND2	2.54	0.40
2:B:206:LEU:O	2:B:206:LEU:HG	2.20	0.40
2:B:385:GLN:OE1	2:B:393:ASN:N	2.48	0.40
3:C:26:SER:HA	3:C:219:ILE:HD13	2.03	0.40
3:C:86:ASN:HD22	3:C:86:ASN:HA	1.70	0.40
4:D:16:GLY:HA2	4:D:17:PRO:HD2	1.90	0.40
6:F:19:TRP:O	6:F:20:TYR:C	2.64	0.40
8:H:15:ASP:OD1	8:H:15:ASP:C	2.63	0.40
8:H:55:THR:O	8:H:56:GLU:C	2.64	0.40
1:A:48:GLU:HB3	1:A:53:ASN:HA	2.03	0.40
1:A:378:ASP:O	1:A:382:GLU:HB2	2.22	0.40
1:A:405:ARG:HG2	1:A:405:ARG:HH11	1.87	0.40
2:B:135:TRP:CD1	2:B:135:TRP:H	2.37	0.40
2:B:137:VAL:HA	2:B:140:LEU:HB3	2.03	0.40
3:C:63:ALA:O	3:C:64:PHE:C	2.62	0.40
3:C:117:GLY:HA2	3:C:120:LEU:HD23	2.04	0.40
3:C:290:GLY:O	3:C:291:GLY:C	2.64	0.40
4:D:6:HIS:HA	4:D:7:PRO:HD2	1.69	0.40
4:D:10:TYR:CD1	4:D:10:TYR:N	2.89	0.40
5:E:121:GLN:HA	5:E:125:GLU:OE2	2.21	0.40
6:F:76:PRO:O	6:F:78:GLU:N	2.54	0.40
7:G:66:PHE:CZ	7:G:70:LYS:HE3	2.56	0.40
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLU:O	1:A:398:ARG:C	2.64	0.40
2:B:157:THR:HG23	2:B:158:HIS:N	2.36	0.40
2:B:162:ASN:O	2:B:163:LEU:C	2.65	0.40
2:B:223:LEU:HG	2:B:223:LEU:O	2.22	0.40
3:C:9:HIS:HB3	3:C:12:LEU:CB	2.47	0.40
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.78	0.40
3:C:238:THR:HG21	4:D:212:MET:HG3	2.03	0.40
4:D:66:GLU:C	4:D:68:VAL:N	2.79	0.40
4:D:98:PRO:O	4:D:100:ALA:N	2.55	0.40
4:D:148:TYR:CZ	4:D:161:ALA:HB2	2.56	0.40
4:D:233:ARG:CB	6:F:71:ARG:NH2	2.80	0.40
5:E:43:THR:O	5:E:44:THR:C	2.65	0.40
5:E:142:LEU:HD23	5:E:142:LEU:HA	1.88	0.40
6:F:93:TYR:O	6:F:94:LEU:C	2.65	0.40
10:J:13:LEU:N	10:J:13:LEU:CD1	2.84	0.40
1:A:54:GLY:O	1:A:55:ALA:C	2.64	0.40
1:A:318:GLY:O	1:A:319:LEU:HD23	2.22	0.40
1:A:335:MET:O	1:A:338:LEU:N	2.54	0.40
2:B:227:ARG:O	2:B:228:GLY:C	2.64	0.40
2:B:375:SER:HA	2:B:378:PHE:HB3	2.04	0.40
3:C:6:ARG:HA	3:C:12:LEU:CD2	2.44	0.40
3:C:100:GLY:O	3:C:103:LEU:N	2.55	0.40
3:C:173:ASN:O	3:C:176:LEU:HB3	2.21	0.40
4:D:218:LEU:HD22	5:E:39:VAL:HG13	2.03	0.40
5:E:27:GLU:C	5:E:30:PRO:HG2	2.46	0.40
5:E:78:LEU:HD13	5:E:132:TRP:NE1	2.36	0.40
5:E:108:GLN:O	5:E:112:VAL:HG23	2.21	0.40
5:E:110:ALA:C	5:E:112:VAL:H	2.28	0.40
1:A:244:ARG:NE	7:G:10:VAL:HB	2.37	0.40
1:A:252:HIS:HB2	1:A:425:PRO:HD2	2.03	0.40
1:A:310:PHE:N	1:A:310:PHE:CD1	2.89	0.40
2:B:145:LYS:HG3	2:B:183:ILE:HG21	2.03	0.40
2:B:162:ASN:O	2:B:165:ALA:HB3	2.22	0.40
2:B:383:GLY:O	2:B:384:SER:C	2.65	0.40
3:C:49:GLY:HA3	11:C:381:HEM:C4C	2.55	0.40
3:C:220:PRO:O	3:C:221:PHE:C	2.64	0.40
3:C:263:LEU:CD1	3:C:263:LEU:N	2.84	0.40
3:C:297:ALA:O	3:C:298:SER:C	2.62	0.40
4:D:51:LEU:HA	4:D:54:VAL:CG1	2.51	0.40
6:F:95:LYS:O	6:F:96:GLU:C	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:165:TYR:OH	6:F:14:GLU:OE2[3_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	440/446 (99%)	310 (70%)	103 (23%)	27 (6%)	1	14
2	B	404/422 (96%)	281 (70%)	83 (20%)	40 (10%)	0	6
3	C	377/380 (99%)	235 (62%)	106 (28%)	36 (10%)	0	7
4	D	239/241 (99%)	175 (73%)	47 (20%)	17 (7%)	1	12
5	E	194/196 (99%)	141 (73%)	39 (20%)	14 (7%)	1	12
6	F	98/109 (90%)	74 (76%)	17 (17%)	7 (7%)	1	12
7	G	76/81 (94%)	52 (68%)	17 (22%)	7 (9%)	0	8
8	H	64/78 (82%)	42 (66%)	19 (30%)	3 (5%)	2	18
10	J	57/62 (92%)	37 (65%)	13 (23%)	7 (12%)	0	4
All	All	1949/2015 (97%)	1347 (69%)	444 (23%)	158 (8%)	1	9

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	282	ARG
1	A	284	TYR
1	A	289	HIS
2	B	19	PRO
2	B	20	HIS
2	B	38	LEU
2	B	113	ARG
2	B	170	ASN

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Mol	Chain	Res	Type
2	B	171	ALA
2	B	228	GLY
2	B	233	SER
2	B	262	ALA
2	B	305	ASN
2	B	330	ALA
2	B	375	SER
2	B	406	ALA
2	B	410	VAL
2	B	420	ARG
3	C	60	THR
3	C	111	LYS
3	C	167	GLY
3	C	202	HIS
3	C	207	ASN
3	C	208	ASN
3	C	218	LYS
3	C	284	SER
3	C	349	ILE
4	D	67	GLU
4	D	73	GLY
4	D	106	ASN
4	D	168	VAL
4	D	198	HIS
4	D	233	ARG
5	E	11	SER
5	E	15	ARG
5	E	72	SER
7	G	27	PRO
7	G	43	ALA
10	J	5	LEU
10	J	60	GLU
10	J	61	ASN
1	A	58	PHE
1	A	65	LYS
1	A	72	GLN
1	A	81	SER
1	A	205	HIS
1	A	222	THR
1	A	281	ASP
1	A	291	SER
1	A	292	SER

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Mol	Chain	Res	Type
1	A	333	ASP
1	A	382	GLU
1	A	433	ASP
1	A	444	LEU
2	B	132	PHE
2	B	181	TYR
2	B	229	GLY
2	B	261	SER
2	B	346	THR
3	C	164	TRP
3	C	205	GLY
3	C	224	TYR
3	C	268	HIS
3	C	352	GLY
4	D	75	ASN
4	D	78	GLY
4	D	190	LEU
4	D	236	ALA
5	E	21	SER
5	E	27	GLU
5	E	65	SER
5	E	70	ALA
5	E	180	LEU
6	F	53	ASN
6	F	97	VAL
7	G	33	GLY
7	G	69	SER
10	J	32	GLU
1	A	73	ASN
1	A	245	GLU
2	B	76	THR
2	B	102	ARG
2	B	111	CYS
2	B	190	GLU
2	B	201	SER
2	B	210	GLY
2	B	218	ASN
2	B	249	GLY
2	B	260	GLU
2	B	270	ASN
2	B	431	GLY
3	C	31	TRP

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Mol	Chain	Res	Type
3	C	58	ALA
3	C	149	ASN
3	C	201	LEU
3	C	222	HIS
3	C	274	TYR
3	C	287	ASN
3	C	353	GLN
4	D	133	GLY
4	D	172	ASP
5	E	30	PRO
5	E	141	HIS
6	F	19	TRP
6	F	77	LYS
8	H	61	PHE
10	J	25	VAL
10	J	58	LYS
1	A	159	GLN
1	A	181	ASP
1	A	209	LEU
1	A	268	VAL
1	A	332	ASP
1	A	405	ARG
2	B	23	ASP
2	B	269	ALA
2	B	319	SER
2	B	331	ALA
2	B	371	SER
2	B	430	LEU
3	C	16	ASN
3	C	64	PHE
3	C	105	TYR
3	C	163	GLU
3	C	235	LEU
4	D	55	CYS
5	E	17	PRO
5	E	177	PRO
6	F	37	ILE
8	H	65	ARG
10	J	20	PHE
2	B	72	ALA
2	B	366	ALA
3	C	12	LEU

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Mol	Chain	Res	Type
3	C	173	ASN
3	C	286	PRO
3	C	300	LEU
4	D	51	LEU
4	D	176	PRO
5	E	62	MET
6	F	69	ASN
1	A	60	GLU
3	C	239	PRO
7	G	74	PRO
8	H	60	ASP
3	C	147	ILE
3	C	171	VAL
4	D	162	PRO
5	E	137	GLY
2	B	21	PRO
7	G	26	PHE
1	A	312	ILE
7	G	50	PRO
3	C	119	ILE
3	C	130	VAL
6	F	98	ILE
4	D	98	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	359/376 (96%)	339 (94%)	20 (6%)	19	46
2	B	307/336 (91%)	289 (94%)	18 (6%)	18	44
3	C	326/329 (99%)	307 (94%)	19 (6%)	18	45
4	D	201/207 (97%)	190 (94%)	11 (6%)	19	46
5	E	165/169 (98%)	150 (91%)	15 (9%)	9	33
6	F	90/98 (92%)	82 (91%)	8 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	60/72 (83%)	53 (88%)	7 (12%)	5	24
8	H	51/74 (69%)	50 (98%)	1 (2%)	48	64
10	J	41/52 (79%)	39 (95%)	2 (5%)	22	48
All	All	1600/1713 (93%)	1499 (94%)	101 (6%)	16	43

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	100	LYS
1	A	102	LEU
1	A	108	LYS
1	A	148	VAL
1	A	165	GLN
1	A	168	GLU
1	A	220	PRO
1	A	250	LEU
1	A	279	HIS
1	A	281	ASP
1	A	316	GLU
1	A	361	LEU
1	A	382	GLU
1	A	384	LEU
1	A	388	ARG
1	A	395	TRP
1	A	409	GLU
1	A	443	TRP
1	A	444	LEU
2	B	21	PRO
2	B	24	LEU
2	B	57	TYR
2	B	62	ASN
2	B	109	VAL
2	B	112	LEU
2	B	135	TRP
2	B	170	ASN
2	B	181	TYR
2	B	221	GLU
2	B	225	ASN
2	B	247	GLN
2	B	248	ASN

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Mol	Chain	Res	Type
2	B	325	TYR
2	B	343	GLN
2	B	402	ILE
2	B	435	PHE
2	B	437	ASP
3	C	28	ILE
3	C	43	MET
3	C	104	TYR
3	C	136	TRP
3	C	164	TRP
3	C	182	LEU
3	C	199	THR
3	C	208	ASN
3	C	216	SER
3	C	250	LEU
3	C	254	PRO
3	C	258	THR
3	C	259	PRO
3	C	265	THR
3	C	282	LEU
3	C	285	ILE
3	C	317	THR
3	C	350	ILE
3	C	354	MET
4	D	36	VAL
4	D	82	MET
4	D	99	GLU
4	D	136	GLU
4	D	156	GLN
4	D	163	PRO
4	D	169	LEU
4	D	181	GLN
4	D	192	TRP
4	D	197	GLU
4	D	224	ARG
5	E	9	ASN
5	E	32	ARG
5	E	36	SER
5	E	45	LEU
5	E	69	LEU
5	E	79	SER
5	E	81	ILE

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Mol	Chain	Res	Type
5	E	83	GLU
5	E	113	GLU
5	E	123	ASP
5	E	136	ILE
5	E	147	ILE
5	E	171	ILE
5	E	186	GLU
5	E	191	ASP
6	F	12	TRP
6	F	31	LEU
6	F	37	ILE
6	F	59	MET
6	F	70	MET
6	F	76	PRO
6	F	84	GLU
6	F	107	TRP
7	G	4	PHE
7	G	16	TYR
7	G	22	GLU
7	G	26	PHE
7	G	27	PRO
7	G	41	LEU
7	G	77	TYR
8	H	73	LEU
10	J	14	PHE
10	J	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	53	ASN
1	A	69	ASN
1	A	87	ASN
1	A	94	HIS
1	A	118	GLN
1	A	141	ASN
1	A	165	GLN
1	A	173	ASN
1	A	189	HIS
1	A	213	GLN
1	A	252	HIS

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Mol	Chain	Res	Type
1	A	274	ASN
1	A	279	HIS
1	A	308	GLN
1	A	339	GLN
1	A	341	GLN
2	B	22	GLN
2	B	62	ASN
2	B	125	ASN
2	B	141	GLN
2	B	225	ASN
2	B	248	ASN
2	B	277	HIS
2	B	313	ASN
2	B	342	ASN
2	B	343	GLN
2	B	351	ASN
2	B	356	ASN
2	B	393	ASN
2	B	421	GLN
2	B	429	ASN
3	C	9	HIS
3	C	16	ASN
3	C	17	ASN
3	C	73	ASN
3	C	82	ASN
3	C	86	ASN
3	C	222	HIS
3	C	249	ASN
3	C	261	ASN
3	C	313	GLN
3	C	342	GLN
3	C	353	GLN
4	D	6	HIS
4	D	35	GLN
4	D	156	GLN
4	D	181	GLN
4	D	200	HIS
5	E	9	ASN
5	E	86	ASN
5	E	164	HIS
6	F	69	ASN
7	G	64	GLN

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Mol	Chain	Res	Type
7	G	79	ASN
8	H	23	GLN
8	H	75	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
12	SIG	C	383	-	35,36,36	1.51	8 (22%)	42,50,50	1.60	7 (16%)
11	HEM	C	382	3	50,50,50	1.99	12 (24%)	67,82,82	2.61	26 (38%)
13	AMY	C	384	-	39,39,39	3.98	17 (43%)	33,53,53	4.00	10 (30%)
14	FES	E	197	5	0,4,4	-	-	-	-	-
11	HEM	D	242	4	50,50,50	1.69	9 (18%)	67,82,82	2.21	21 (31%)
11	HEM	C	381	3	50,50,50	2.30	13 (26%)	67,82,82	3.07	33 (49%)

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
12	SIG	C	383	-	-	17/30/30/30	0/2/2/2
11	HEM	C	382	3	-	8/14/54/54	-
13	AMY	C	384	-	-	15/37/52/52	0/1/2/2
14	FES	E	197	5	-	-	0/1/1/1
11	HEM	D	242	4	-	10/14/54/54	-
11	HEM	C	381	3	-	8/14/54/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	AMY	O6-C14	12.06	1.51	1.21
13	C	384	AMY	O7-C20	10.30	1.47	1.21
11	C	381	HEM	FE-NA	-8.85	1.65	1.95
13	C	384	AMY	O5-C14	8.80	1.54	1.34
13	C	384	AMY	C27-C11	-7.69	1.33	1.51
13	C	384	AMY	O4-C20	6.22	1.48	1.34
11	C	381	HEM	FE-NB	-6.14	1.76	1.94
13	C	384	AMY	O9-C21	5.37	1.38	1.22
11	C	382	HEM	FE-NA	-5.20	1.78	1.95
11	D	242	HEM	CBB-CAB	4.67	1.52	1.30
11	D	242	HEM	CBC-CAC	4.64	1.52	1.30
13	C	384	AMY	C4-C5	4.50	1.46	1.38
13	C	384	AMY	C8-N1	-4.39	1.28	1.34
11	C	381	HEM	FE-NC	-4.33	1.80	1.95
13	C	384	AMY	C26-C10	-4.32	1.41	1.51
11	C	381	HEM	C3B-C2B	-4.28	1.28	1.37
11	C	382	HEM	CAB-C3B	-4.19	1.36	1.47
13	C	384	AMY	C15-C13	4.17	1.61	1.54
11	C	382	HEM	C2A-C3A	-4.09	1.28	1.38
11	C	381	HEM	CAB-C3B	-3.98	1.36	1.47
11	C	382	HEM	FE-ND	-3.88	1.83	1.94
12	C	383	SIG	O14-C5	3.80	1.43	1.37
11	C	382	HEM	C3B-C2B	-3.77	1.29	1.37
11	D	242	HEM	C3B-C2B	-3.61	1.29	1.37
13	C	384	AMY	C13-C12	3.56	1.59	1.53
13	C	384	AMY	C6-C1	3.44	1.47	1.41
11	C	382	HEM	CHA-C4D	-3.43	1.31	1.38
11	C	382	HEM	C4A-NA	-3.33	1.33	1.39
11	D	242	HEM	C2A-C3A	-3.25	1.30	1.38
11	C	382	HEM	CAC-C3C	-3.21	1.38	1.47
13	C	384	AMY	C12-C11	3.02	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	383	SIG	C1-C2	2.99	1.44	1.40
11	C	381	HEM	CAC-C3C	-2.96	1.39	1.47
11	C	381	HEM	C2A-C3A	-2.88	1.31	1.38
11	D	242	HEM	C3C-C2C	-2.82	1.31	1.37
12	C	383	SIG	C4-C5	2.80	1.45	1.40
11	C	381	HEM	CHA-C4D	-2.77	1.33	1.38
11	C	381	HEM	C3D-C2D	-2.76	1.30	1.36
12	C	383	SIG	C37-C36	2.74	1.35	1.33
13	C	384	AMY	O5-C10	2.72	1.50	1.46
11	C	381	HEM	CHB-C1B	-2.70	1.33	1.38
13	C	384	AMY	O3-C7	2.69	1.29	1.23
11	C	382	HEM	CHA-C1A	-2.62	1.33	1.39
13	C	384	AMY	C4-C3	2.54	1.43	1.38
11	C	382	HEM	FE-NB	-2.52	1.87	1.94
11	C	381	HEM	CHB-C4A	-2.47	1.33	1.39
12	C	383	SIG	C9-C10	2.40	1.53	1.47
11	D	242	HEM	C1A-NA	-2.40	1.35	1.39
11	C	381	HEM	C4C-NC	2.34	1.44	1.39
11	D	242	HEM	CHA-C1A	-2.23	1.34	1.39
11	C	382	HEM	C3C-C2C	-2.21	1.32	1.37
12	C	383	SIG	C21-C22	2.17	1.59	1.54
11	D	242	HEM	FE-NC	-2.15	1.88	1.95
11	D	242	HEM	CAD-C3D	2.12	1.56	1.51
13	C	384	AMY	C25-C23	-2.12	1.40	1.51
11	C	382	HEM	CHC-C4B	-2.11	1.34	1.39
11	C	381	HEM	CHD-C1D	-2.04	1.34	1.39
12	C	383	SIG	C6-C1	2.02	1.42	1.38
12	C	383	SIG	C20-C8	2.01	1.54	1.49

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	384	AMY	O5-C14-O6	-13.34	107.56	124.10
13	C	384	AMY	O4-C20-O7	-13.09	107.87	124.10
11	C	381	HEM	C3B-C4B-NB	8.67	115.70	109.47
11	C	381	HEM	C1B-NB-C4B	-7.88	95.87	105.21
11	C	381	HEM	C4D-ND-C1D	-7.27	96.60	105.21
13	C	384	AMY	O8-C21-O9	-7.18	106.92	123.70
11	C	382	HEM	C3B-C4B-NB	6.85	114.39	109.47
11	C	381	HEM	C3D-C4D-ND	6.45	117.24	110.17
11	D	242	HEM	CBA-CAA-C2A	6.34	130.05	112.53
11	D	242	HEM	CAD-C3D-C4D	6.26	135.60	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	382	HEM	C3D-C4D-ND	6.01	116.76	110.17
13	C	384	AMY	O9-C21-C22	-5.76	111.26	124.65
11	C	382	HEM	CMB-C2B-C1B	5.69	133.92	125.03
11	C	381	HEM	C2B-C1B-NB	5.56	116.23	109.84
13	C	384	AMY	O2-C8-N1	-5.49	118.19	125.72
11	C	381	HEM	CAD-C3D-C4D	5.47	134.22	124.70
11	C	381	HEM	C2A-C1A-NA	5.25	115.97	110.15
11	C	382	HEM	C2A-C1A-NA	5.15	115.87	110.15
11	C	381	HEM	C4A-NA-C1A	-5.14	97.44	105.82
11	C	381	HEM	C4C-NC-C1C	-5.03	97.62	105.82
11	C	382	HEM	C1B-NB-C4B	-5.01	99.27	105.21
12	C	383	SIG	C24-C23-C22	4.99	118.17	113.89
11	C	382	HEM	CAA-C2A-C1A	4.95	134.60	124.94
11	D	242	HEM	C3D-C4D-ND	4.60	115.21	110.17
11	C	381	HEM	CMB-C2B-C1B	4.39	131.89	125.03
11	C	382	HEM	C4A-NA-C1A	-4.35	98.72	105.82
11	C	382	HEM	CBD-CAD-C3D	4.25	124.30	112.53
11	D	242	HEM	CBC-CAC-C3C	-4.19	106.61	127.53
11	C	382	HEM	C2B-C1B-NB	4.18	114.64	109.84
11	C	382	HEM	C4D-ND-C1D	-4.12	100.33	105.21
11	D	242	HEM	CBD-CAD-C3D	4.09	123.84	112.53
12	C	383	SIG	C39-C36-C32	-4.03	111.94	118.09
11	C	381	HEM	C2D-C1D-ND	3.99	114.51	109.90
11	D	242	HEM	CMC-C2C-C1C	3.98	131.74	124.73
13	C	384	AMY	C16-C15-C13	3.92	121.20	114.28
11	D	242	HEM	CBB-CAB-C3B	-3.67	109.19	127.53
11	D	242	HEM	C2A-C1A-NA	3.66	114.22	110.15
11	D	242	HEM	C4D-C3D-C2D	-3.61	101.64	106.89
11	C	381	HEM	CHC-C4B-NB	-3.57	120.58	124.42
11	C	381	HEM	C3A-C4A-NA	3.52	115.79	110.14
11	C	382	HEM	C4C-NC-C1C	-3.46	100.18	105.82
11	C	382	HEM	CHB-C1B-NB	-3.45	120.10	124.37
11	C	381	HEM	C2C-C1C-NC	3.37	115.87	109.64
11	C	382	HEM	CAD-C3D-C4D	3.34	130.52	124.70
11	C	381	HEM	C3B-C2B-C1B	-3.33	103.91	106.41
11	C	382	HEM	C1A-C2A-C3A	-3.21	101.90	106.87
11	D	242	HEM	CHC-C4B-NB	-3.17	121.01	124.42
11	C	381	HEM	C4C-CHD-C1D	-3.17	119.29	126.02
11	D	242	HEM	CMC-C2C-C3C	-3.14	120.82	128.43
13	C	384	AMY	O8-C12-C11	3.12	115.16	107.97
11	C	381	HEM	CHA-C4D-ND	-3.12	120.51	124.37
11	C	381	HEM	C4A-CHB-C1B	-3.09	118.97	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	382	HEM	CHD-C4C-NC	-3.08	121.10	124.45
11	C	381	HEM	CMD-C2D-C1D	3.06	129.82	125.03
13	C	384	AMY	O8-C21-C22	-3.02	106.02	111.43
11	C	381	HEM	CHB-C4A-C3A	-2.99	118.73	127.43
11	C	382	HEM	CAC-C3C-C4C	2.99	131.96	124.82
11	C	381	HEM	CAD-C3D-C2D	-2.98	122.29	127.87
11	D	242	HEM	C4A-NA-C1A	-2.96	100.99	105.82
11	C	382	HEM	C4D-C3D-C2D	-2.92	102.64	106.89
11	C	381	HEM	CHA-C1A-C2A	-2.90	118.96	125.30
11	C	382	HEM	C4C-C3C-C2C	-2.88	104.31	106.81
13	C	384	AMY	O3-C7-C6	-2.83	115.84	121.03
11	C	382	HEM	C3B-C2B-C1B	-2.79	104.31	106.41
11	C	382	HEM	CMB-C2B-C3B	-2.75	121.76	128.43
11	D	242	HEM	CAD-C3D-C2D	-2.74	122.73	127.87
11	C	381	HEM	CBD-CAD-C3D	2.73	120.07	112.53
11	D	242	HEM	C4D-ND-C1D	-2.68	102.04	105.21
11	C	381	HEM	CHB-C1B-NB	-2.67	121.06	124.37
12	C	383	SIG	O14-C5-C4	2.64	119.58	115.84
12	C	383	SIG	C5-C4-C3	2.60	121.50	116.87
11	D	242	HEM	C3B-C4B-NB	2.57	111.31	109.47
11	C	382	HEM	C2C-C1C-NC	2.51	114.29	109.64
11	D	242	HEM	CMD-C2D-C1D	2.48	128.92	125.03
11	D	242	HEM	CMB-C2B-C1B	2.47	128.90	125.03
12	C	383	SIG	C6-C5-C4	-2.45	117.52	121.79
11	C	382	HEM	CMA-C3A-C4A	2.45	129.15	125.42
11	C	382	HEM	CHA-C4D-C3D	-2.40	120.80	125.23
11	C	381	HEM	C4B-C3B-C2B	-2.39	105.09	107.28
11	C	381	HEM	C4C-C3C-C2C	-2.37	104.76	106.81
11	C	381	HEM	C4D-C3D-C2D	-2.35	103.47	106.89
11	C	381	HEM	CAA-C2A-C1A	2.35	129.53	124.94
12	C	383	SIG	O7-C8-C9	-2.33	119.76	121.81
11	C	381	HEM	CHD-C4C-C3C	-2.33	121.29	125.21
11	D	242	HEM	C1B-NB-C4B	-2.27	102.52	105.21
11	D	242	HEM	C1D-C2D-C3D	2.27	109.36	106.98
11	C	381	HEM	CMC-C2C-C1C	2.17	128.56	124.73
11	C	382	HEM	CBA-CAA-C2A	2.16	118.51	112.53
11	D	242	HEM	CHA-C4D-ND	-2.13	121.73	124.37
13	C	384	AMY	C26-C10-C9	-2.11	109.04	114.22
11	D	242	HEM	CMB-C2B-C3B	-2.09	123.37	128.43
12	C	383	SIG	C3-C4-C10	-2.06	116.46	119.99
11	C	381	HEM	O2D-CGD-CBD	2.05	120.46	114.00
11	C	381	HEM	CHC-C1C-C2C	-2.04	121.25	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	382	HEM	CMA-C3A-C2A	-2.04	121.30	125.62
11	C	381	HEM	O1D-CGD-CBD	-2.03	116.65	123.09
11	C	382	HEM	CHC-C4B-NB	-2.02	122.25	124.42

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	HEM	C2B-C3B-CAB-CBB
11	C	381	HEM	C4B-C3B-CAB-CBB
11	C	382	HEM	C1A-C2A-CAA-CBA
11	C	382	HEM	C2B-C3B-CAB-CBB
11	D	242	HEM	C3A-C2A-CAA-CBA
11	D	242	HEM	C2C-C3C-CAC-CBC
12	C	383	SIG	C21-C20-C8-O7
12	C	383	SIG	C21-C20-C8-C9
12	C	383	SIG	C21-C22-C23-C24
12	C	383	SIG	C21-C22-C23-C28
12	C	383	SIG	C27-C22-C23-C24
12	C	383	SIG	C27-C22-C23-C28
12	C	383	SIG	C22-C23-C24-C25
12	C	383	SIG	C28-C23-C24-C25
12	C	383	SIG	C28-C23-C24-C35
12	C	383	SIG	C31-C32-C36-C37
12	C	383	SIG	C31-C32-C36-C39
13	C	384	AMY	C13-C14-O5-C10
13	C	384	AMY	C9-C10-O5-C14
13	C	384	AMY	C26-C10-O5-C14
13	C	384	AMY	O2-C8-N1-C2
13	C	384	AMY	C27-C11-O4-C20
13	C	384	AMY	C11-C12-O8-C21
13	C	384	AMY	C13-C12-O8-C21
13	C	384	AMY	C9-C20-O4-C11
13	C	384	AMY	O7-C20-O4-C11
11	D	242	HEM	C4D-C3D-CAD-CBD
12	C	383	SIG	C20-C21-C22-C23
13	C	384	AMY	O9-C21-O8-C12
11	D	242	HEM	C1A-C2A-CAA-CBA
12	C	383	SIG	C20-C21-C22-C27
11	D	242	HEM	C2D-C3D-CAD-CBD
12	C	383	SIG	C29-C30-C31-C32
12	C	383	SIG	C30-C31-C32-C36

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Mol	Chain	Res	Type	Atoms
13	C	384	AMY	C15-C16-C17-C18
11	C	382	HEM	C2C-C3C-CAC-CBC
11	C	382	HEM	C4B-C3B-CAB-CBB
11	C	382	HEM	C4C-C3C-CAC-CBC
12	C	383	SIG	C22-C23-C24-C35
13	C	384	AMY	C1-C6-C7-O3
13	C	384	AMY	C1-C6-C7-N2
11	C	381	HEM	C2C-C3C-CAC-CBC
13	C	384	AMY	C1-C2-N1-C8
11	C	381	HEM	CAA-CBA-CGA-O2A
11	C	382	HEM	CAA-CBA-CGA-O2A
11	C	381	HEM	CAA-CBA-CGA-O1A
11	C	381	HEM	CAD-CBD-CGD-O2D
11	D	242	HEM	CAD-CBD-CGD-O2D
11	C	382	HEM	CAA-CBA-CGA-O1A
11	D	242	HEM	CAA-CBA-CGA-O2A
11	D	242	HEM	CAD-CBD-CGD-O1D
11	C	381	HEM	C4C-C3C-CAC-CBC
11	D	242	HEM	C4C-C3C-CAC-CBC
11	C	381	HEM	CAD-CBD-CGD-O1D
11	C	382	HEM	C2A-CAA-CBA-CGA
11	D	242	HEM	CAA-CBA-CGA-O1A
12	C	383	SIG	C8-C20-C21-C22
13	C	384	AMY	O9-C21-C22-C23

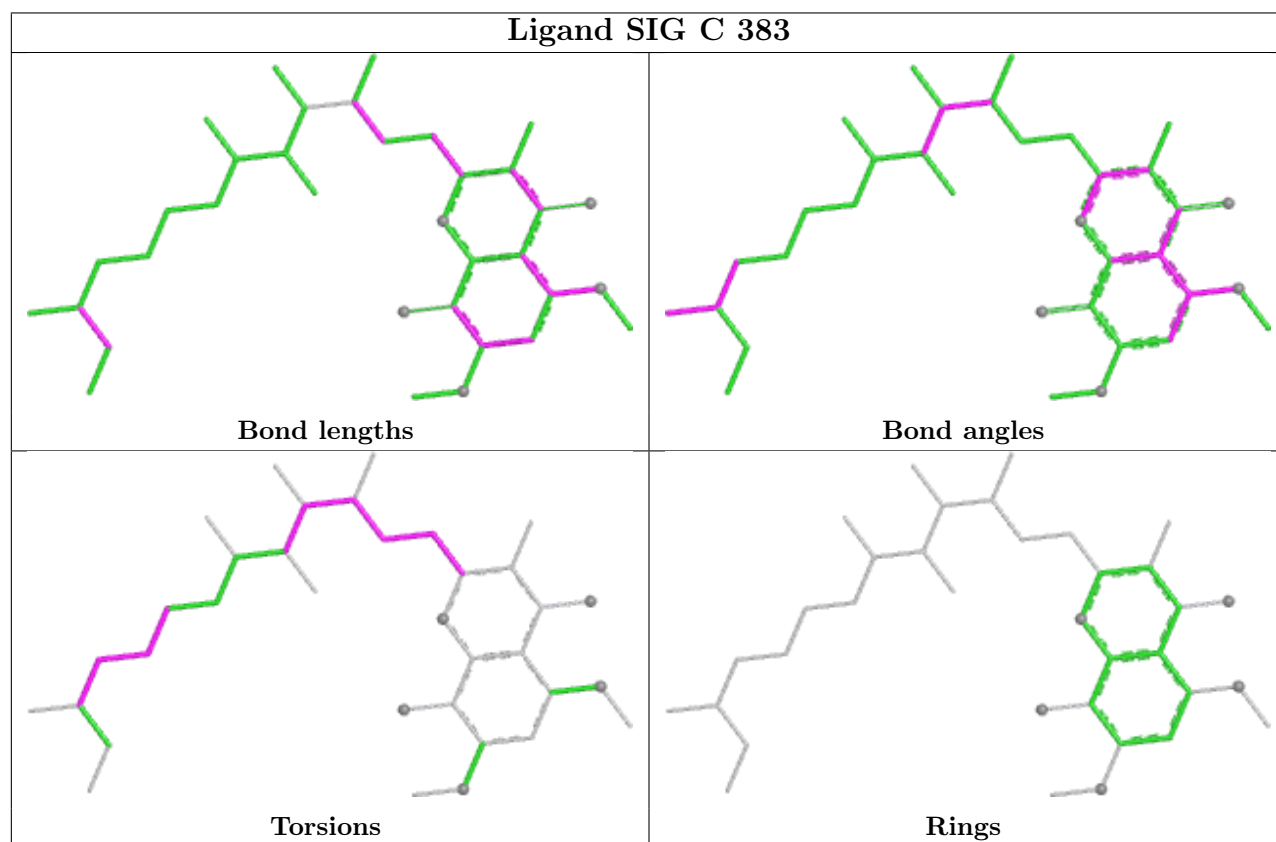
There are no ring outliers.

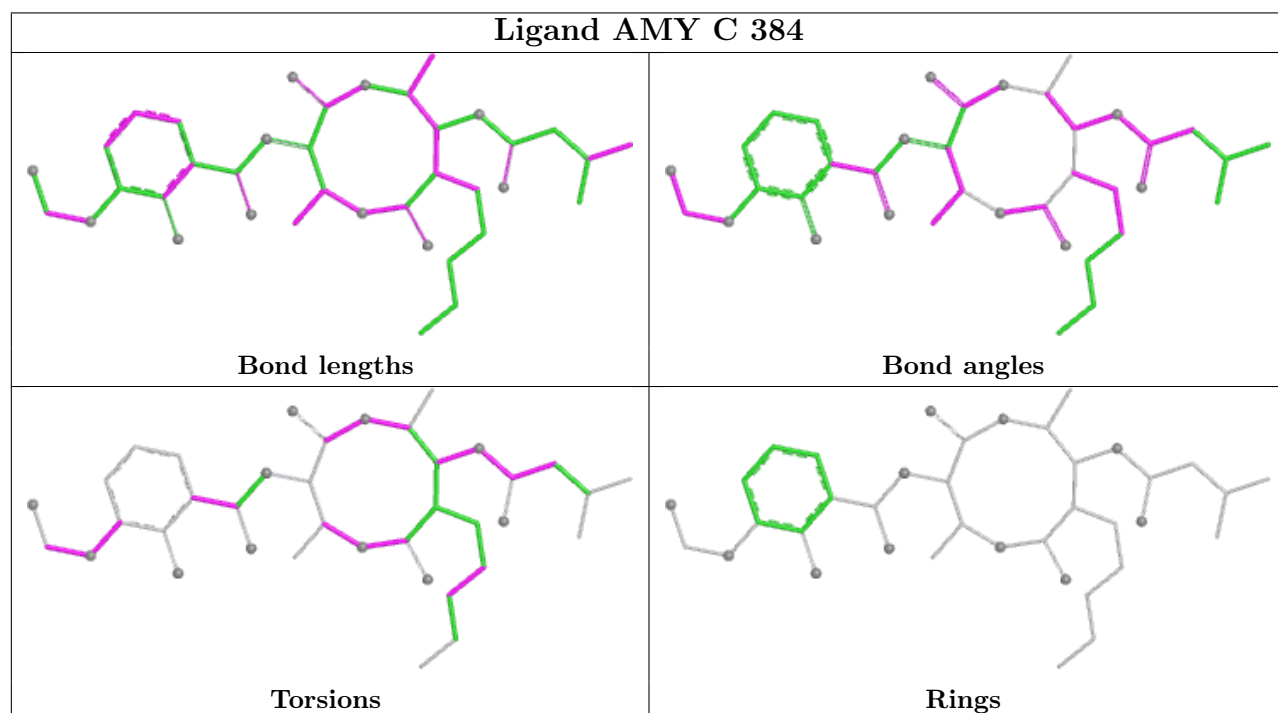
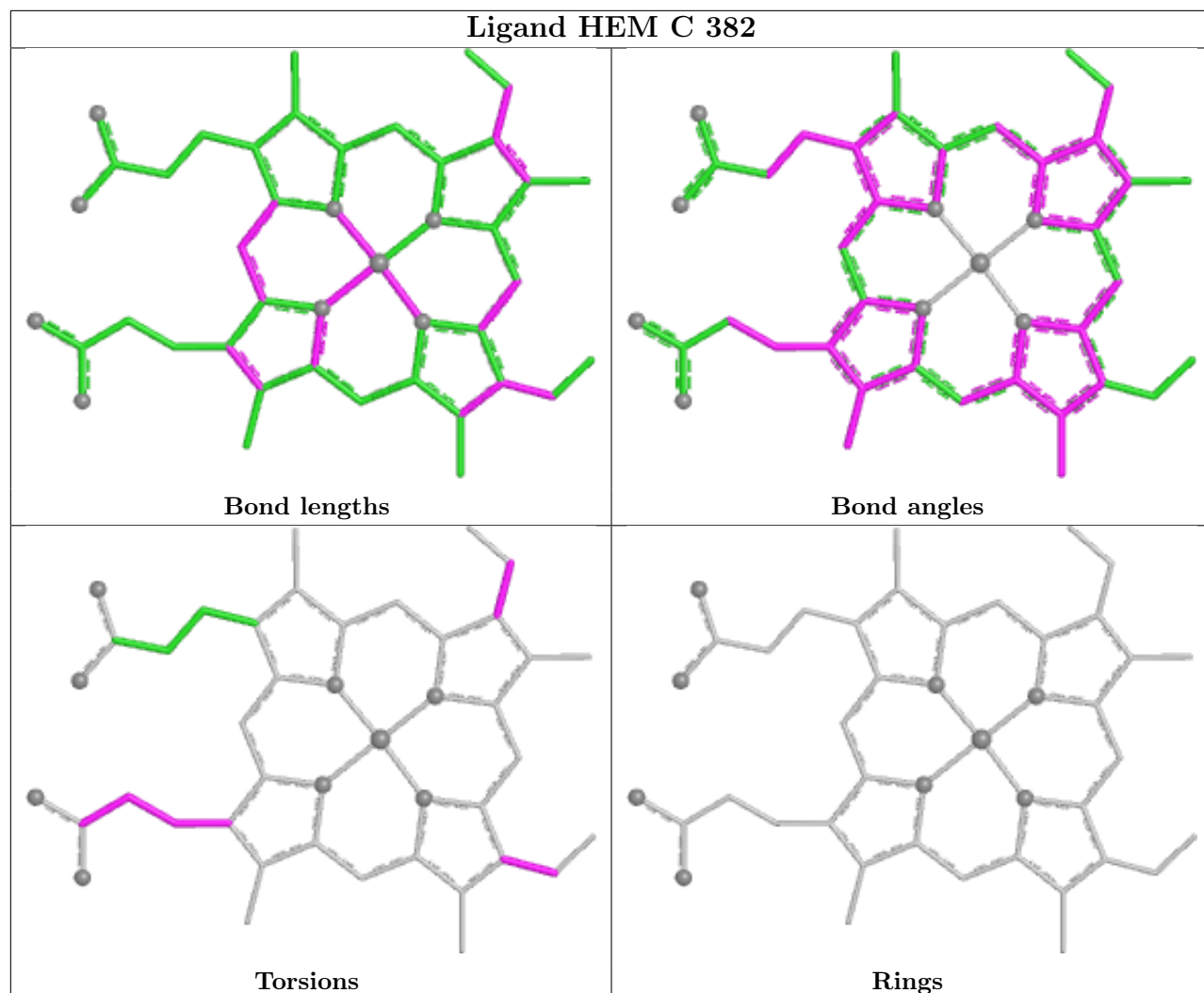
6 monomers are involved in 60 short contacts:

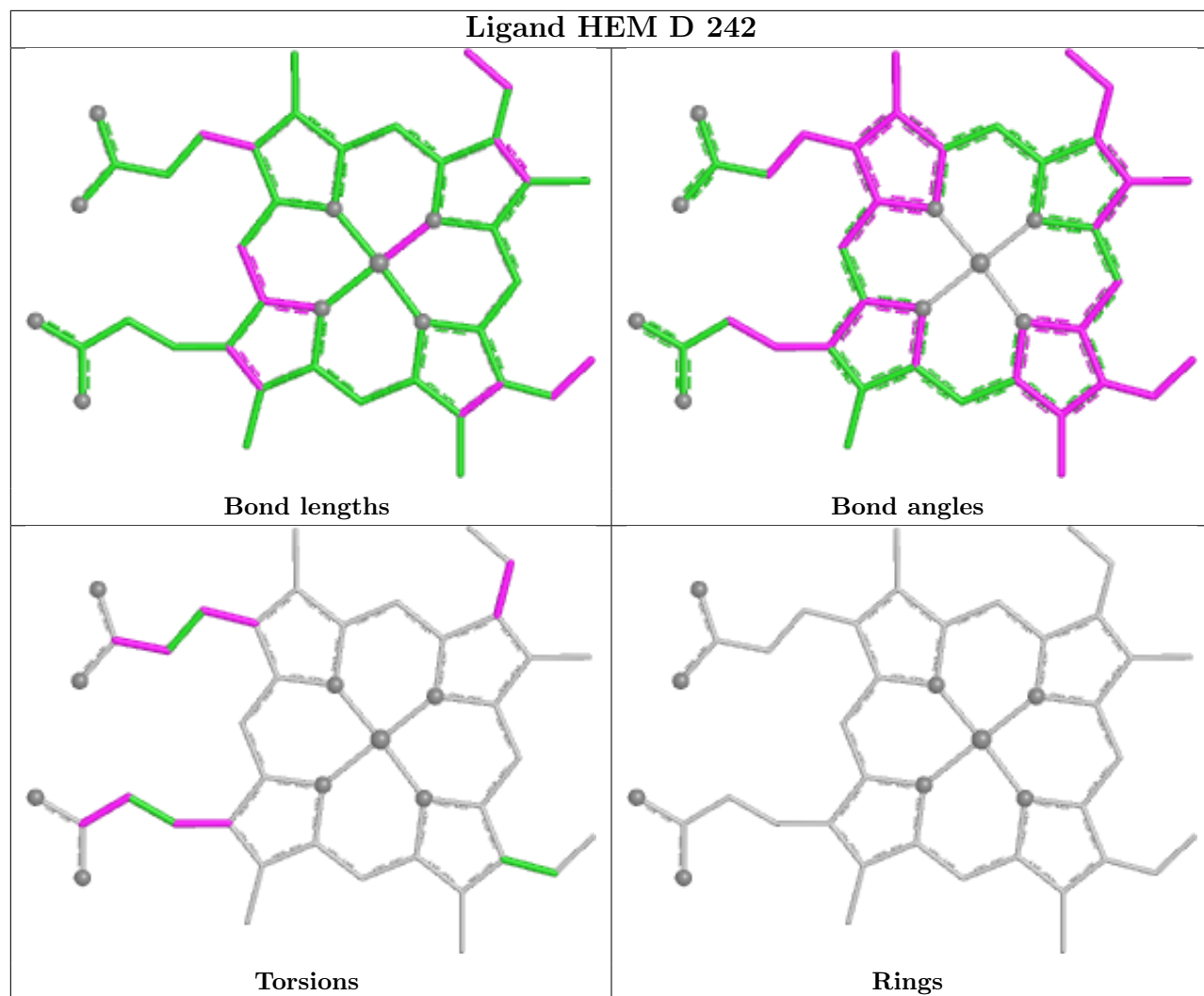
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	383	SIG	15	0
11	C	382	HEM	11	0
13	C	384	AMY	15	0
14	E	197	FES	2	0
11	D	242	HEM	6	0
11	C	381	HEM	12	0

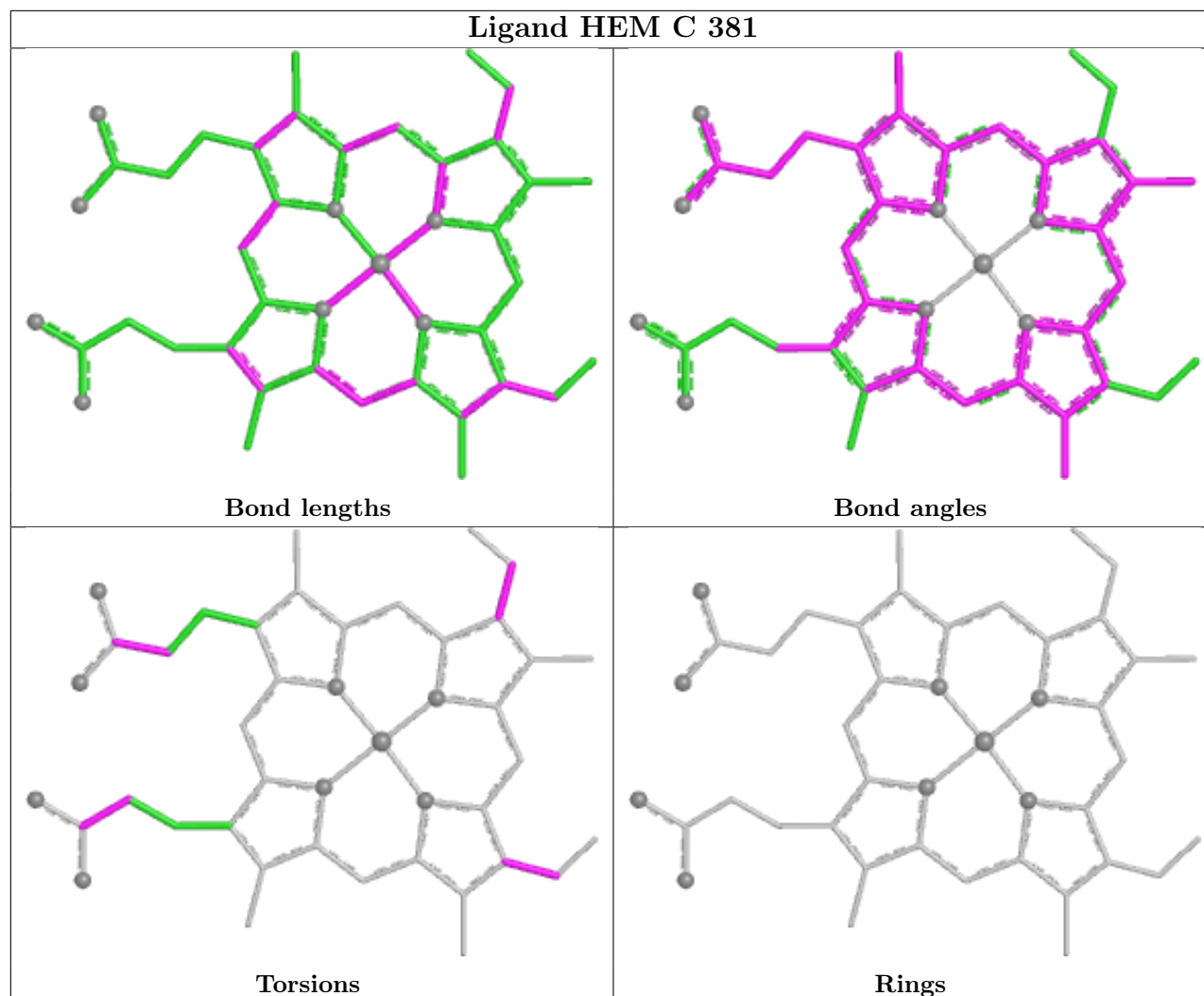
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:UNK	C	309:UNK	N	33.28
1	I	121:UNK	C	202:UNK	N	28.55

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/446 (99%)	1.32	100 (22%) 2 3	36, 84, 100, 100	0
2	B	406/422 (96%)	1.63	132 (32%) 1 1	58, 95, 100, 100	0
3	C	379/380 (99%)	0.64	29 (7%) 19 15	13, 43, 72, 92	0
4	D	241/241 (100%)	0.96	33 (13%) 6 8	27, 65, 95, 100	0
5	E	196/196 (100%)	1.63	67 (34%) 1 1	32, 95, 100, 100	0
6	F	100/109 (91%)	0.90	10 (10%) 12 13	39, 64, 93, 99	0
7	G	78/81 (96%)	1.22	15 (19%) 3 4	35, 74, 97, 99	0
8	H	66/78 (84%)	1.30	13 (19%) 3 3	63, 91, 98, 100	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	1.38	14 (23%) 2 2	56, 71, 95, 100	0
All	All	1967/2048 (96%)	1.22	413 (20%) 2 3	13, 78, 100, 100	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	73	LYS	8.4
5	E	188	THR	7.5
2	B	260	GLU	6.5
2	B	114	ASP	6.2
2	B	138	ALA	6.2
1	A	215	HIS	5.7
2	B	239	TYR	5.3
2	B	235	ALA	5.1
1	A	22	GLY	5.0
10	J	61	ASN	4.9
5	E	189	SER	4.9
5	E	160	CYS	4.9
1	A	44	GLY	4.9
2	B	205	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
5	E	171	ILE	4.7
1	A	406	MET	4.7
2	B	212	SER	4.7
4	D	139	THR	4.7
2	B	124	LEU	4.6
2	B	193	ASP	4.6
2	B	427	SER	4.5
1	A	368	HIS	4.5
5	E	147	ILE	4.4
8	H	68	CYS	4.4
1	A	306	SER	4.3
1	A	191	THR	4.2
2	B	285	VAL	4.2
5	E	80	ASP	4.1
3	C	163	GLU	4.1
1	A	407	VAL	4.0
7	G	73	ASN	4.0
3	C	6	ARG	4.0
1	A	223	TYR	4.0
2	B	153	GLN	4.0
2	B	203	ARG	3.9
7	G	75	ALA	3.9
1	A	193	PRO	3.9
5	E	78	LEU	3.9
5	E	82	PRO	3.9
1	A	385	THR	3.9
2	B	214	PRO	3.8
1	A	19	LEU	3.8
1	A	140	GLU	3.8
5	E	71	MET	3.8
2	B	412	LYS	3.7
6	F	70	MET	3.7
1	A	4	TYR	3.6
2	B	340	ALA	3.6
2	B	402	ILE	3.6
10	J	14	PHE	3.6
2	B	49	VAL	3.6
8	H	41	ASP	3.6
6	F	12	TRP	3.6
5	E	96	LEU	3.6
2	B	261	SER	3.6
2	B	222	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	33	LEU	3.5
1	A	52	ASN	3.5
2	B	421	GLN	3.5
1	A	369	LEU	3.5
5	E	69	LEU	3.5
1	A	228	VAL	3.5
10	J	54	HIS	3.5
1	A	282	ARG	3.5
1	A	284	TYR	3.5
8	H	76	SER	3.5
1	A	69	ASN	3.5
2	B	31	ASN	3.5
1	A	363	ASN	3.5
1	A	260	PRO	3.5
10	J	47	ASN	3.4
7	G	25	PRO	3.4
5	E	159	PRO	3.4
6	F	11	ARG	3.4
5	E	106	ILE	3.4
1	A	389	ARG	3.4
1	A	206	GLN	3.4
3	C	66	SER	3.4
1	A	443	TRP	3.3
1	A	40	TRP	3.3
1	A	194	ARG	3.3
5	E	101	ARG	3.3
2	B	38	LEU	3.3
5	E	143	GLY	3.3
7	G	77	TYR	3.3
4	D	136	GLU	3.3
5	E	100	HIS	3.3
8	H	45	SER	3.3
4	D	69	GLU	3.2
2	B	106	ALA	3.2
1	A	15	GLN	3.2
2	B	338	LYS	3.2
1	A	246	ASP	3.2
4	D	15	ARG	3.2
5	E	150	ALA	3.2
7	G	76	ALA	3.2
7	G	28	HIS	3.2
1	A	53	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	346	CYS	3.1
2	B	172	LEU	3.1
2	B	423	SER	3.1
5	E	30	PRO	3.1
3	C	371	GLY	3.1
2	B	185	LYS	3.1
2	B	41	TYR	3.1
3	C	161	LEU	3.1
1	A	38	GLY	3.1
4	D	57	THR	3.1
1	A	88	ALA	3.1
1	A	251	ALA	3.1
10	J	55	ILE	3.1
5	E	185	TYR	3.1
8	H	50	THR	3.1
2	B	164	HIS	3.1
2	B	201	SER	3.0
2	B	391	SER	3.0
2	B	263	ALA	3.0
4	D	174	GLY	3.0
1	A	6	GLN	3.0
2	B	227	ARG	3.0
2	B	210	GLY	3.0
2	B	397	THR	3.0
8	H	49	GLN	3.0
1	A	216	PHE	3.0
2	B	81	SER	3.0
5	E	128	LYS	3.0
1	A	61	HIS	3.0
5	E	126	ARG	3.0
5	E	16	PRO	3.0
2	B	274	VAL	3.0
4	D	24	THR	3.0
5	E	72	SER	3.0
4	D	105	ASN	2.9
1	A	440	GLY	2.9
3	C	137	GLY	2.9
5	E	190	ASP	2.9
2	B	152	PHE	2.9
1	A	220	PRO	2.9
5	E	9	ASN	2.9
5	E	56	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	376	LYS	2.9
10	J	6	THR	2.9
2	B	118	ILE	2.9
1	A	394	GLU	2.9
2	B	283	PRO	2.8
2	B	416	LYS	2.8
1	A	189	HIS	2.8
1	A	444	LEU	2.8
3	C	328	LEU	2.8
1	A	231	LEU	2.8
2	B	60	SER	2.8
2	B	218	ASN	2.8
1	A	378	ASP	2.8
6	F	13	LEU	2.8
5	E	114	VAL	2.8
6	F	102	LYS	2.8
1	A	234	CYS	2.8
2	B	26	ILE	2.8
1	A	12	PRO	2.8
2	B	80	ALA	2.8
1	A	235	ARG	2.7
7	G	47	ARG	2.7
2	B	50	PHE	2.7
4	D	231	LYS	2.7
1	A	13	GLU	2.7
2	B	171	ALA	2.7
5	E	40	THR	2.7
2	B	23	ASP	2.7
1	A	30	SER	2.7
2	B	168	TYR	2.7
5	E	83	GLU	2.7
1	A	262	TRP	2.7
6	F	10	SER	2.7
2	B	221	GLU	2.7
3	C	372	THR	2.7
5	E	179	ASN	2.7
1	A	289	HIS	2.7
4	D	77	ASP	2.7
2	B	220	ALA	2.7
2	B	359	ALA	2.7
3	C	53	ALA	2.7
5	E	64	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLU	2.7
1	A	411	CYS	2.7
8	H	35	GLU	2.7
1	A	8	LEU	2.7
1	A	217	GLY	2.7
8	H	25	GLU	2.7
1	A	326	CYS	2.7
2	B	319	SER	2.7
1	A	71	PRO	2.6
1	A	32	GLN	2.6
2	B	115	ASP	2.6
3	C	156	TYR	2.6
2	B	200	THR	2.6
2	B	264	ILE	2.6
5	E	164	HIS	2.6
6	F	15	GLY	2.6
6	F	106	GLU	2.6
1	A	73	ASN	2.6
2	B	20	HIS	2.6
1	A	302	LYS	2.6
5	E	165	TYR	2.6
1	A	80	GLU	2.6
2	B	226	ILE	2.6
4	D	118	ARG	2.6
2	B	217	LYS	2.6
4	D	115	TYR	2.6
1	A	37	VAL	2.6
2	B	98	VAL	2.6
7	G	24	ARG	2.6
2	B	394	PRO	2.6
5	E	192	MET	2.6
5	E	156	TYR	2.6
1	A	210	GLU	2.6
7	G	69	SER	2.6
2	B	189	VAL	2.6
10	J	16	ARG	2.6
2	B	281	ALA	2.6
2	B	306	PRO	2.6
4	D	8	PRO	2.6
2	B	128	THR	2.5
2	B	215	VAL	2.5
2	B	140	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	331	ALA	2.5
2	B	335	GLN	2.5
8	H	70	ALA	2.5
2	B	101	THR	2.5
5	E	76	ILE	2.5
6	F	95	LYS	2.5
1	A	124	ASP	2.5
5	E	148	ALA	2.5
2	B	433	THR	2.5
1	A	135	VAL	2.5
1	A	172	GLU	2.5
3	C	338	TRP	2.5
10	J	26	VAL	2.5
1	A	29	GLN	2.5
2	B	165	ALA	2.5
3	C	271	PRO	2.5
3	C	168	GLY	2.5
10	J	56	LYS	2.5
4	D	102	ARG	2.5
7	G	31	SER	2.5
2	B	34	VAL	2.5
5	E	27	GLU	2.5
1	A	349	ILE	2.5
2	B	360	ALA	2.5
4	D	63	ALA	2.5
5	E	81	ILE	2.5
10	J	40	ASP	2.5
1	A	408	ARG	2.5
1	A	34	THR	2.5
2	B	252	LEU	2.5
5	E	113	GLU	2.5
3	C	90	PHE	2.5
1	A	213	GLN	2.5
4	D	238	ARG	2.5
5	E	123	ASP	2.5
5	E	68	VAL	2.5
2	B	373	GLU	2.4
5	E	104	LYS	2.4
1	A	62	LEU	2.4
5	E	19	ASP	2.4
5	E	119	ASP	2.4
5	E	63	SER	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	68	VAL	2.4
5	E	153	PHE	2.4
5	E	111	ALA	2.4
1	A	398	ARG	2.4
3	C	70	THR	2.4
1	A	313	CYS	2.4
2	B	243	GLU	2.4
4	D	133	GLY	2.4
2	B	422	LYS	2.4
2	B	116	VAL	2.4
2	B	111	CYS	2.4
2	B	400	GLN	2.4
4	D	31	GLN	2.4
2	B	21	PRO	2.4
2	B	145	LYS	2.4
2	B	159	VAL	2.4
4	D	185	ASP	2.4
5	E	13	TYR	2.4
2	B	39	GLU	2.4
5	E	99	ARG	2.4
2	B	267	ALA	2.4
3	C	313	GLN	2.4
7	G	44	CYS	2.4
10	J	37	GLN	2.4
1	A	202	GLY	2.4
4	D	74	PRO	2.4
2	B	55	SER	2.4
1	A	23	VAL	2.4
2	B	157	THR	2.4
1	A	376	CYS	2.3
4	D	81	PHE	2.3
5	E	31	SER	2.3
2	B	126	VAL	2.3
8	H	55	THR	2.3
2	B	181	TYR	2.3
3	C	294	ALA	2.3
1	A	33	PRO	2.3
2	B	213	HIS	2.3
2	B	231	GLY	2.3
3	C	149	ASN	2.3
4	D	146	GLY	2.3
2	B	258	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	127	VAL	2.3
1	A	164	ALA	2.3
1	A	42	ASP	2.3
1	A	118	GLN	2.3
5	E	191	ASP	2.3
2	B	230	LEU	2.3
2	B	45	SER	2.3
8	H	67	HIS	2.3
5	E	176	ALA	2.3
2	B	250	ASP	2.3
2	B	352	VAL	2.3
4	D	32	VAL	2.3
7	G	70	LYS	2.3
10	J	15	ARG	2.3
1	A	5	ALA	2.3
2	B	368	TYR	2.3
3	C	255	GLU	2.3
2	B	277	HIS	2.3
8	H	43	ARG	2.3
6	F	90	LEU	2.3
3	C	129	PHE	2.3
1	A	130	GLU	2.3
2	B	310	SER	2.3
2	B	376	GLU	2.3
2	B	428	GLY	2.3
5	E	195	VAL	2.3
3	C	285	ILE	2.2
2	B	57	TYR	2.2
1	A	330	SER	2.2
2	B	354	ASN	2.2
3	C	15	ILE	2.2
10	J	57	HIS	2.2
4	D	88	SER	2.2
2	B	102	ARG	2.2
4	D	145	GLU	2.2
1	A	230	THR	2.2
2	B	197	ASN	2.2
10	J	45	HIS	2.2
2	B	196	GLN	2.2
2	B	204	MET	2.2
1	A	175	ARG	2.2
1	A	83	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	142	PRO	2.2
2	B	377	GLY	2.2
5	E	109	GLU	2.2
4	D	117	VAL	2.2
2	B	268	GLU	2.2
2	B	322	PHE	2.2
8	H	74	PHE	2.2
1	A	51	LYS	2.2
1	A	352	SER	2.1
2	B	401	GLN	2.1
2	B	420	ARG	2.1
1	A	203	VAL	2.1
1	A	101	ALA	2.1
5	E	51	ALA	2.1
3	C	178	ARG	2.1
2	B	37	SER	2.1
1	A	176	LYS	2.1
2	B	64	GLY	2.1
4	D	212	MET	2.1
1	A	146	ARG	2.1
4	D	198	HIS	2.1
5	E	85	LYS	2.1
1	A	384	LEU	2.1
2	B	25	GLU	2.1
2	B	163	LEU	2.1
2	B	187	THR	2.1
2	B	173	ALA	2.1
2	B	407	ASP	2.1
3	C	316	MET	2.1
4	D	110	PRO	2.1
4	D	67	GLU	2.1
1	A	356	ARG	2.1
2	B	272	PHE	2.1
2	B	307	PHE	2.1
7	G	37	VAL	2.1
1	A	115	ASP	2.1
5	E	155	GLY	2.1
5	E	162	GLY	2.1
2	B	46	THR	2.1
1	A	35	CYS	2.1
1	A	197	LEU	2.1
2	B	219	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	117	LEU	2.1
2	B	249	GLY	2.0
4	D	84	PRO	2.0
7	G	38	TRP	2.0
4	D	178	THR	2.0
2	B	385	GLN	2.0
3	C	380	TYR	2.0
3	C	5	ILE	2.0
5	E	118	ARG	2.0
5	E	91	TRP	2.0
1	A	209	LEU	2.0
2	B	315	SER	2.0
3	C	2	ALA	2.0
7	G	30	PHE	2.0
5	E	196	GLY	2.0
5	E	130	PRO	2.0
3	C	84	HIS	2.0
1	A	236	PHE	2.0
2	B	339	ALA	2.0
2	B	371	SER	2.0
5	E	88	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	SIG	C	383	35/35	0.91	0.13	17,37,61,71	0
13	AMY	C	384	38/38	0.92	0.13	15,37,60,64	0

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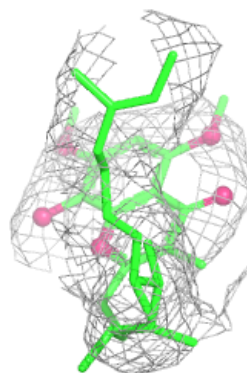
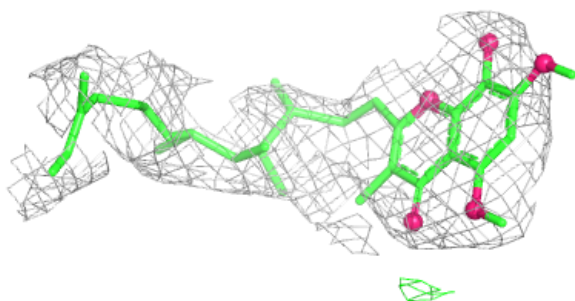
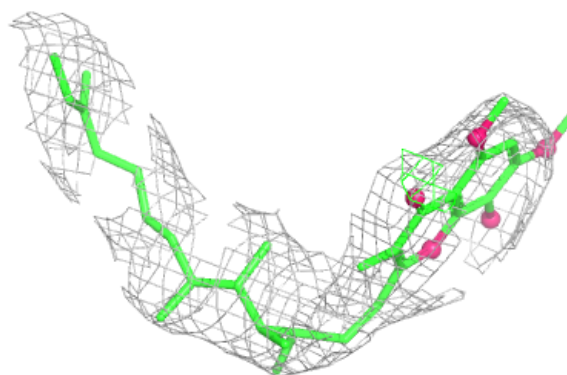
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	HEM	D	242	43/43	0.93	0.14	34,40,53,61	0
11	HEM	C	382	43/43	0.94	0.15	22,34,43,47	0
14	FES	E	197	4/4	0.95	0.10	71,84,87,88	0
11	HEM	C	381	43/43	0.97	0.12	22,34,42,44	0

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.

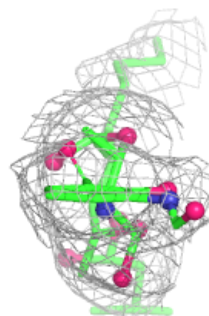
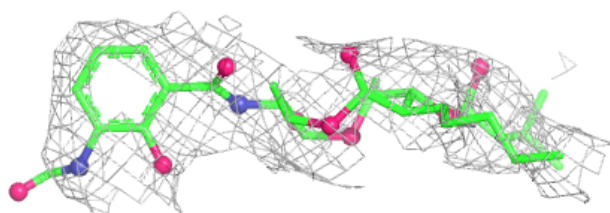
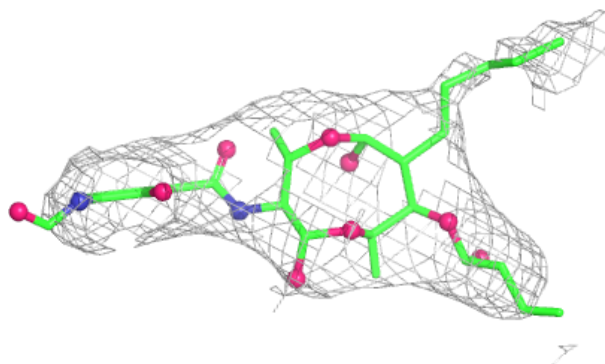
Electron density around SIG C 383:

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



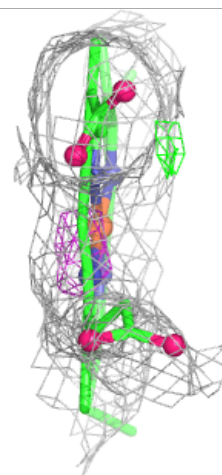
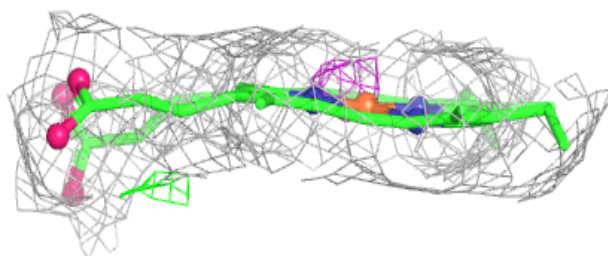
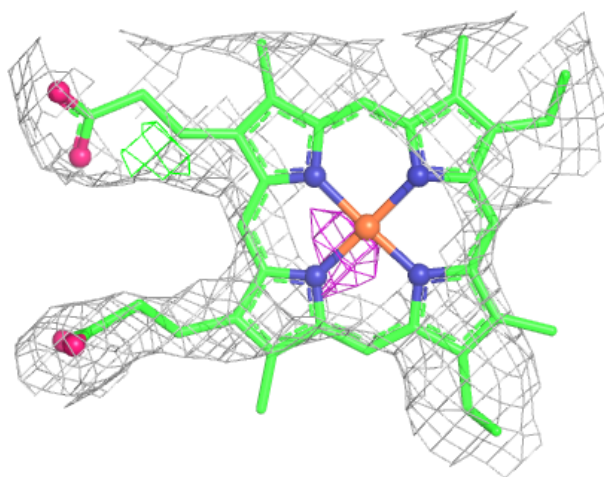
Electron density around AMY C 384:

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



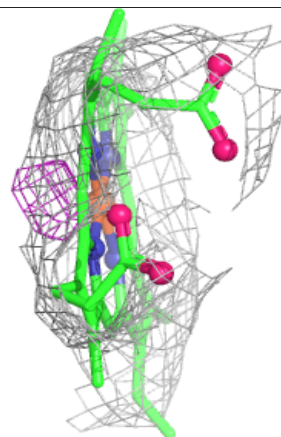
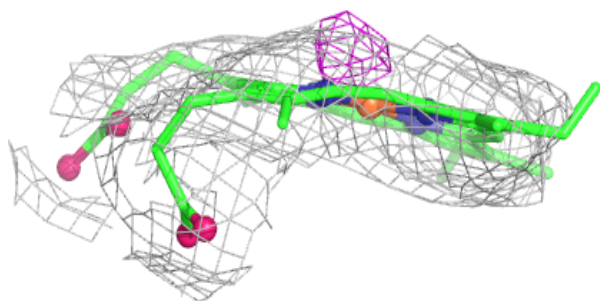
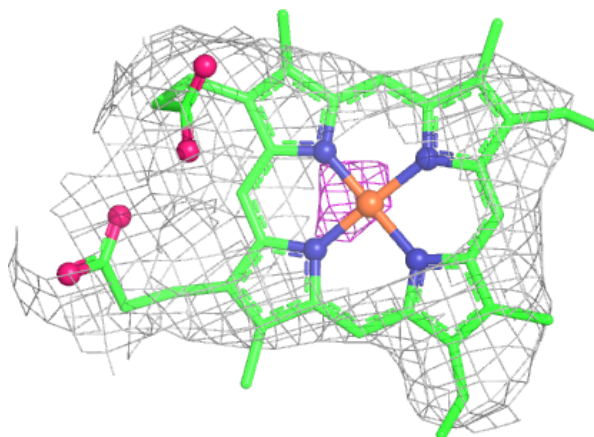
Electron density around HEM D 242:

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



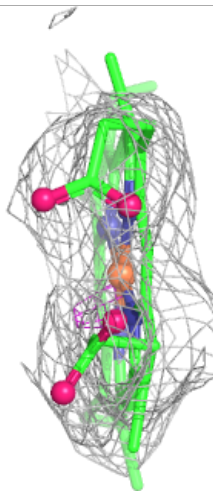
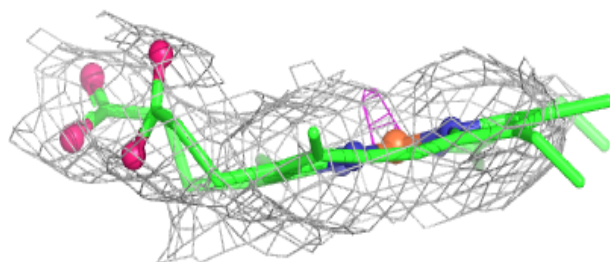
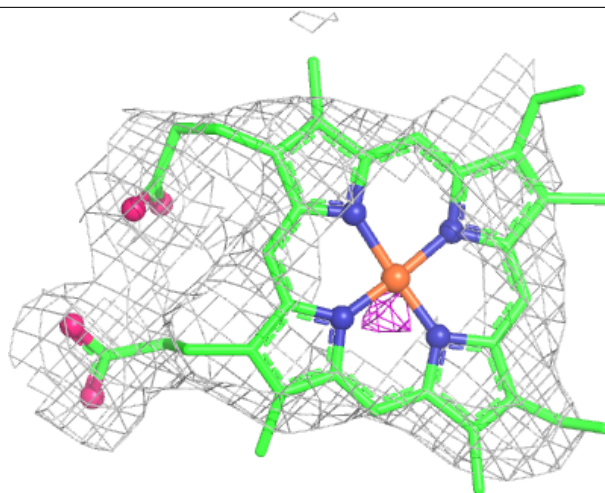
Electron density around HEM C 382:

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



Electron density around HEM C 381:

$2mF_o-DF_c$ (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.