



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:51 AM UTC

PDB ID : 2E75 / pdb\_00002e75  
Title : Crystal Structure of the Cytochrome b6f Complex with 2-nonyl-4-hydroxyquinoline N-oxide (NQNO) from *M.laminosus*  
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.  
Deposited on : 2007-01-05  
Resolution : 3.55 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](mailto: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>.

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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)  
Xtrriage (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

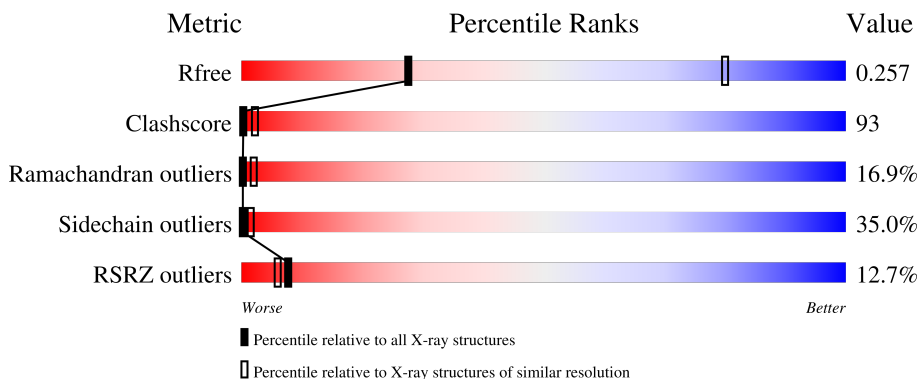
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 Å.

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



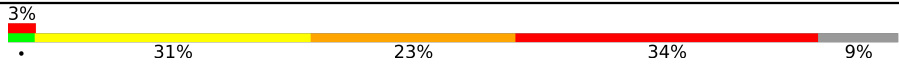
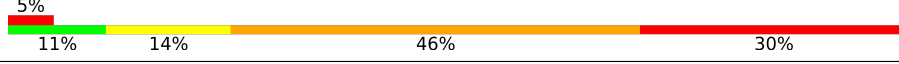
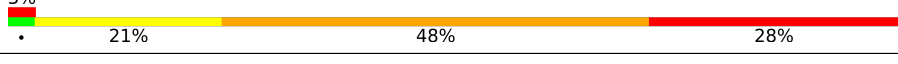
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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  $\geq 3$ , 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	215	
2	B	160	
3	C	289	
4	D	179	
5	E	32	

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Mol	Chain	Length	Quality of chain
6	F	35	
7	G	37	
8	H	29	

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
10	HEM	A	301	-	-	X	-
10	HEM	A	302	-	-	X	-
10	HEM	C	301	-	-	X	-
12	OPC	A	1002	-	-	X	-
13	UMQ	A	1102	X	-	-	-
13	UMQ	A	1103	X	-	-	-
13	UMQ	A	1104	X	-	-	-
13	UMQ	C	1101	X	-	-	-
14	QNO	A	501	X	-	-	-
15	CLA	B	201	X	-	-	-
16	FES	D	200	-	-	X	-
17	SQD	D	201	X	X	-	-
18	BCR	G	101	-	X	-	-

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 8046 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 Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1711	1140	272	288	11	0	0	0

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	1249	841	193	209	6	0	0	0

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	288	2216	1415	369	424	8	0	0	0

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	166	1260	805	218	230	7	0	0	0

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	32	248	179	34	34	1	0	0	0

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	32	242	165	35	40	2	0	0	0

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	37	Total 283	C 188	N 44	O 50	S 1	0	0	0

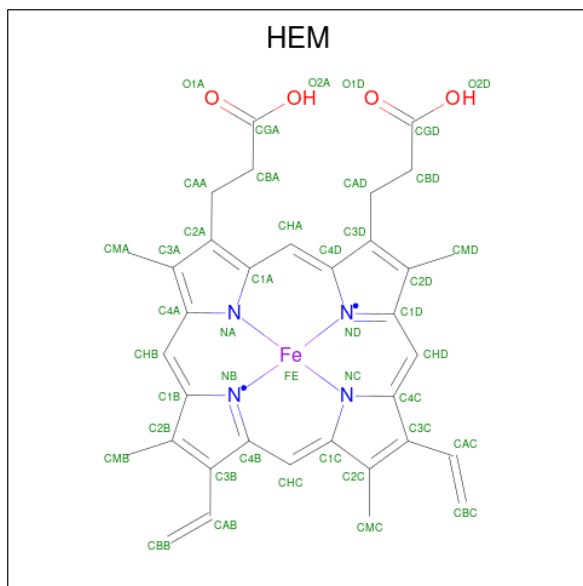
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	29	Total 230	C 156	N 36	O 36	S 2	0	0	0

- Molecule 9 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
9	A	1	Total 1	Cd 1	0	0
9	B	1	Total 1	Cd 1	0	0

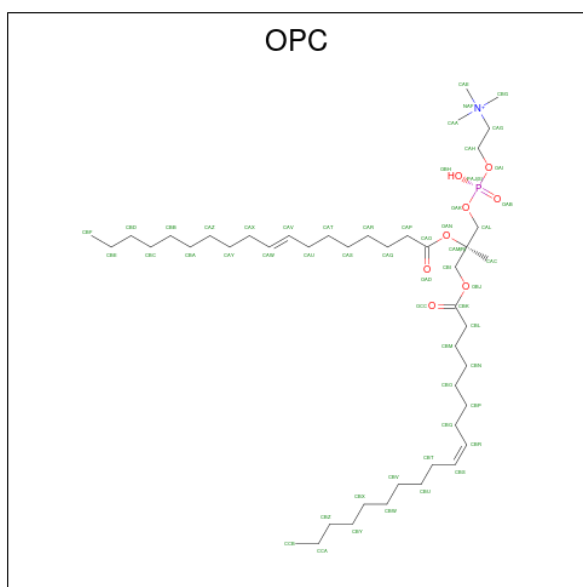
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

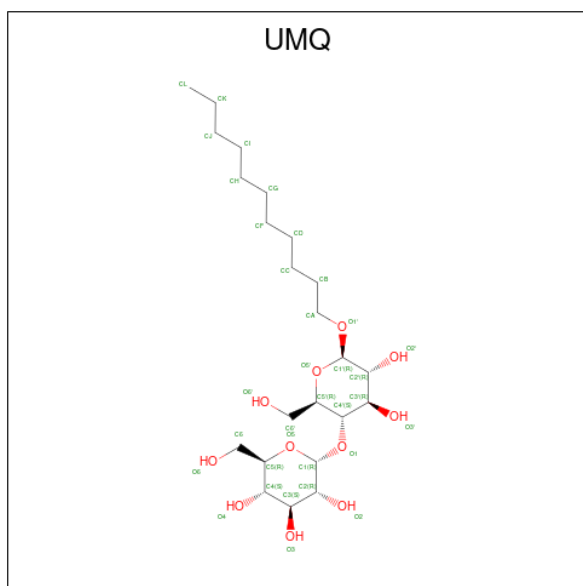
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
12	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 13 is UNDECYL-MALTOSE (CCD ID: UMQ) (formula:  $C_{23}H_{44}O_{11}$ ).



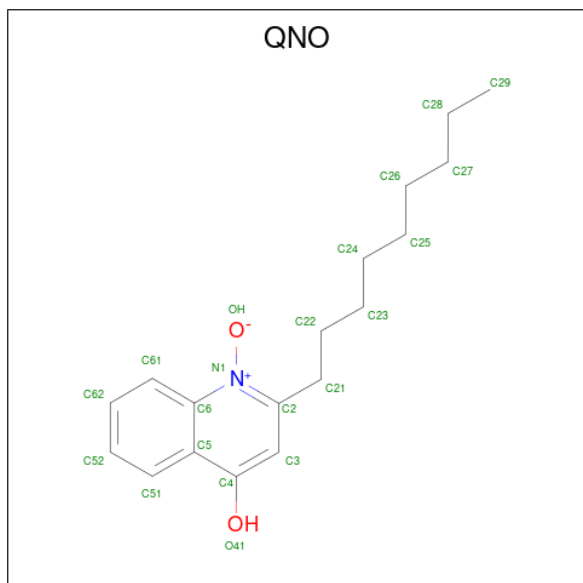
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		
13	A	1	Total	C	O	0	0
			34	23	11		

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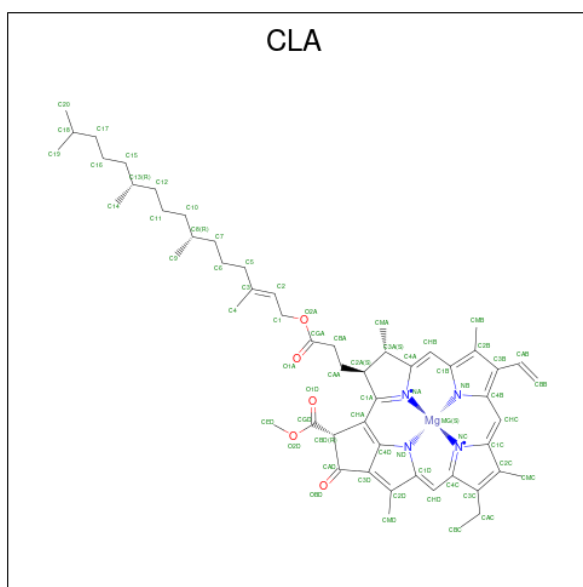
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		
13	C	1	Total	C	O	0	0
			34	23	11		

- Molecule 14 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (CCD ID: QNO) (formula:  $C_{18}H_{25}NO_2$ ).



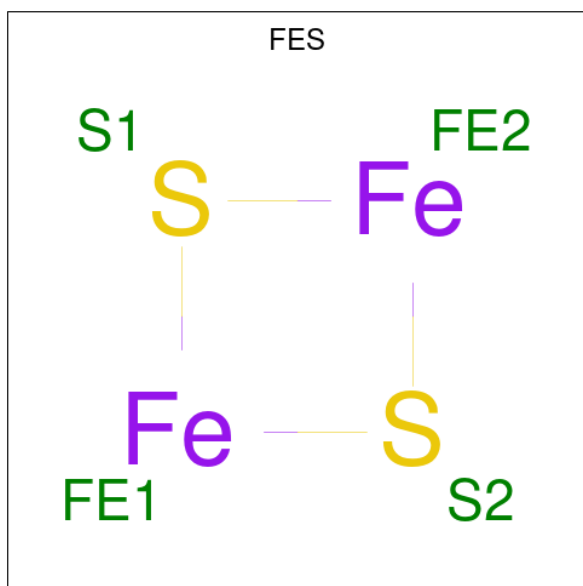
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



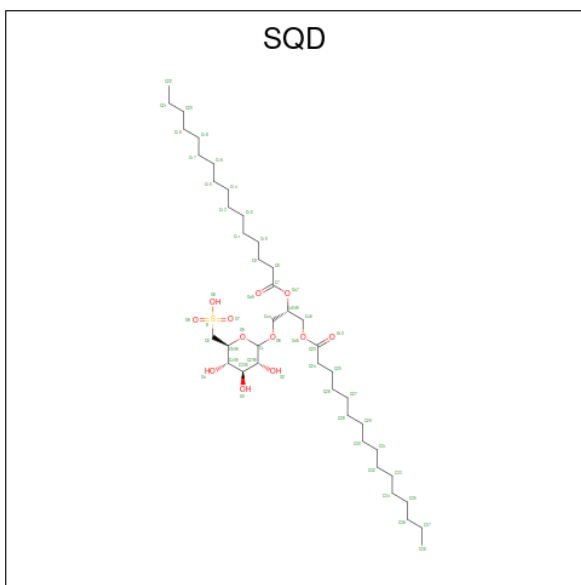
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
15	B	1	65	55	1	4	5	0	0

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



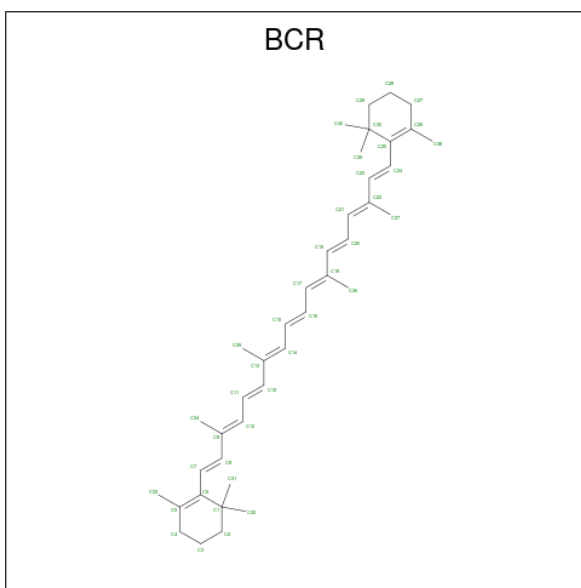
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	Fe			S
16	D	1	4	2	2	0	0

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			S
17	D	1	54	41	12	1	0	0

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
18	G	1	40	40	0	0

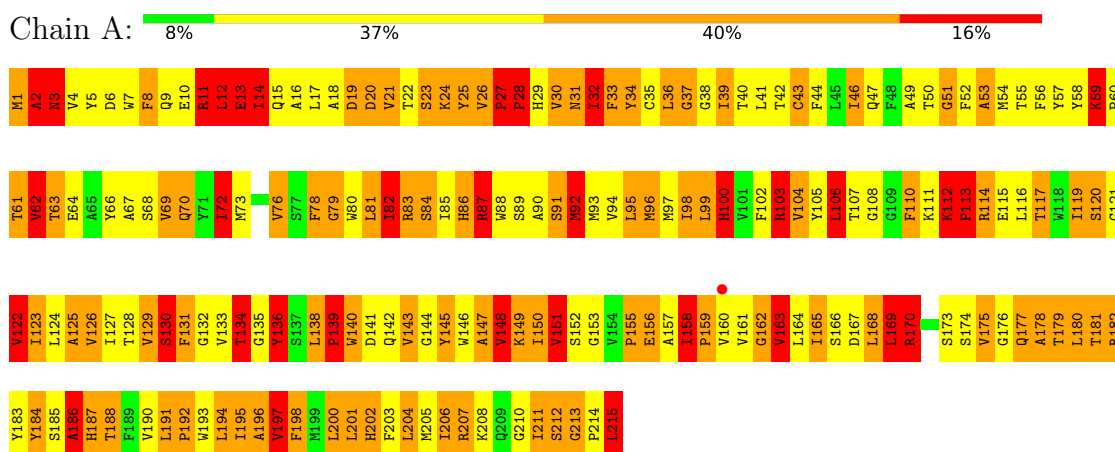
- Molecule 19 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
19	A	3	Total 3	O 3	0	0
19	B	2	Total 2	O 2	0	0

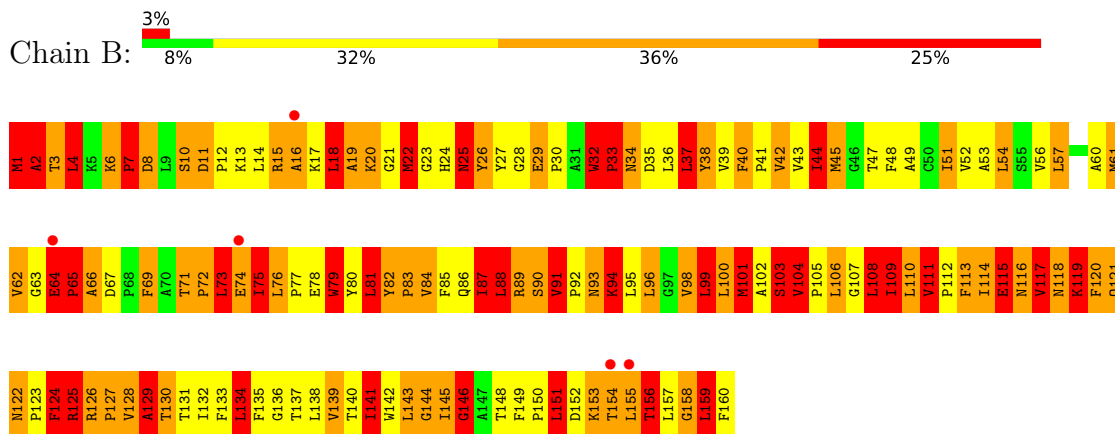
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

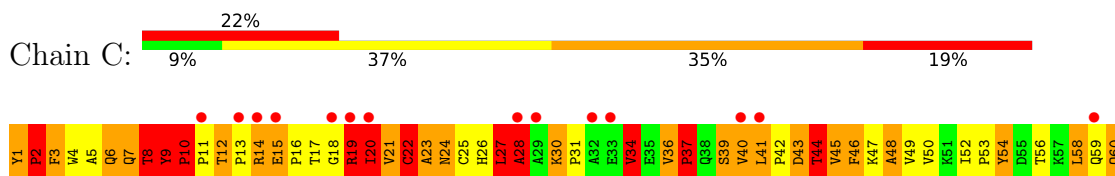
#### • Molecule 1: Cytochrome b6

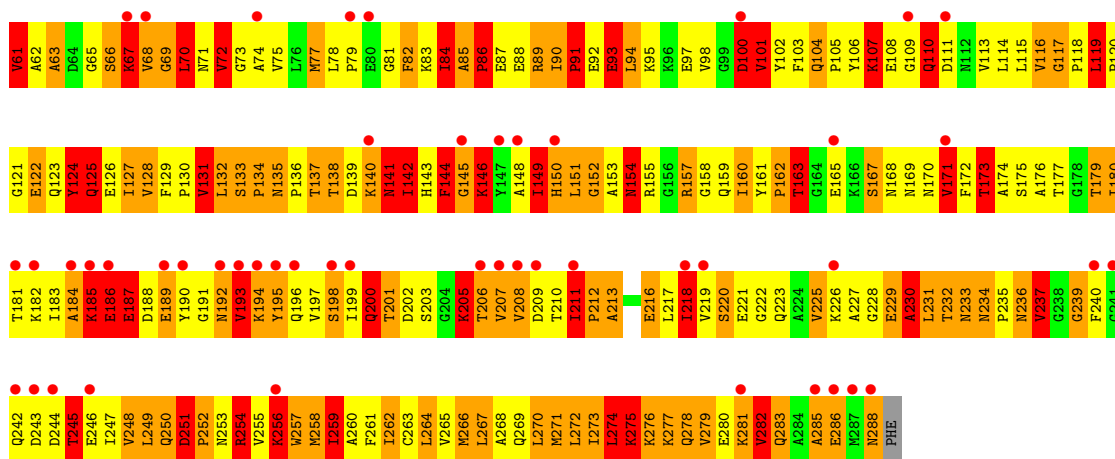


#### • Molecule 2: Cytochrome b6-f complex subunit 4

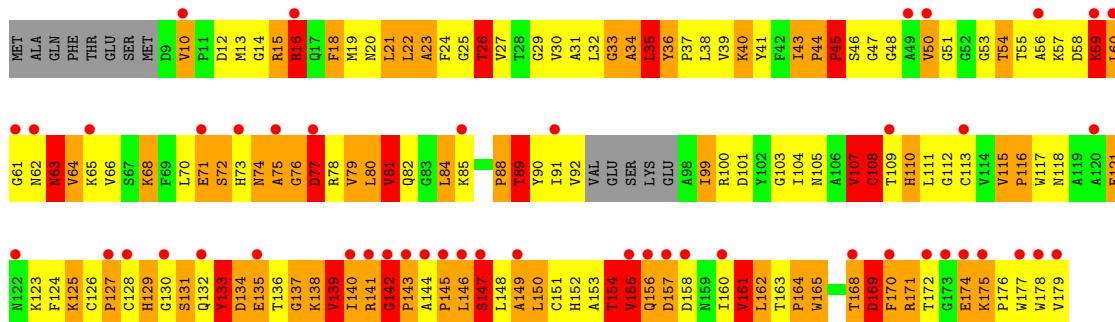


#### • Molecule 3: Apocytochrome f

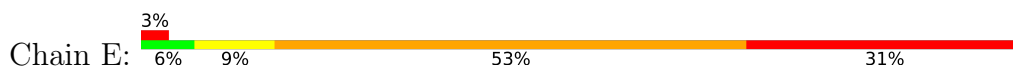




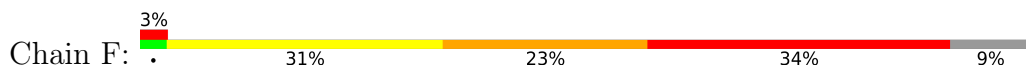
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



• Molecule 5: Cytochrome b6-f complex subunit 6



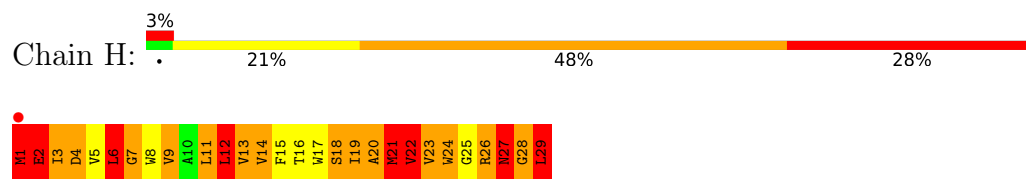
• Molecule 6: Cytochrome b6-f complex subunit 7



• Molecule 7: Cytochrome b6-f complex subunit 5



- Molecule 8: Cytochrome b6-f complex subunit 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.16Å 159.16Å 362.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.94 – 3.55 49.94 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.94-3.55) 99.7 (49.94-3.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.89 (at 3.57Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.267 0.198 , 0.257	Depositor DCC
$R_{free}$ test set	1703 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.2	Xtrriage
Anisotropy	0.189	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 70.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8046	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CD, UMQ, CLA, QNO, FES, HEM, SQD, HEC, OPC, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	2.41	81/1763 (4.6%)	2.56	145/2405 (6.0%)
2	B	2.17	45/1288 (3.5%)	2.47	90/1765 (5.1%)
3	C	1.93	62/2264 (2.7%)	2.22	124/3082 (4.0%)
4	D	1.67	17/1292 (1.3%)	1.86	43/1760 (2.4%)
5	E	2.26	11/253 (4.3%)	2.22	15/340 (4.4%)
6	F	2.58	17/246 (6.9%)	2.29	14/331 (4.2%)
7	G	2.03	6/289 (2.1%)	2.26	18/391 (4.6%)
8	H	2.35	15/236 (6.4%)	2.38	16/323 (5.0%)
All	All	2.10	254/7631 (3.3%)	2.30	465/10397 (4.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	7
3	C	0	8
5	E	0	4
6	F	0	1
7	G	0	4
8	H	0	2
All	All	0	32

All (254) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	VAL	CA-CB	-19.91	1.33	1.54
2	B	84	VAL	CA-CB	-12.42	1.39	1.54
1	A	49	ALA	CA-CB	-10.74	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	ARG	CZ-NH1	10.58	1.47	1.32
1	A	67	ALA	CA-CB	-10.53	1.36	1.53
4	D	34	ALA	CA-CB	-10.47	1.37	1.53
4	D	50	VAL	CA-CB	10.27	1.68	1.54
3	C	148	ALA	CA-CB	-10.11	1.36	1.53
1	A	59	LYS	C-O	-9.97	1.15	1.25
3	C	142	ILE	CA-CB	-9.75	1.42	1.54
1	A	134	THR	C-O	9.32	1.35	1.24
1	A	62	VAL	CA-CB	-9.27	1.42	1.54
1	A	85	ILE	CA-CB	-9.21	1.44	1.54
3	C	84	ILE	CA-CB	-9.17	1.42	1.53
2	B	141	ILE	CA-CB	-8.81	1.42	1.54
1	A	26	VAL	CA-CB	8.72	1.63	1.53
6	F	16	ILE	CA-CB	-8.63	1.44	1.54
6	F	9	ALA	CA-CB	-8.55	1.39	1.53
2	B	71	THR	CA-CB	-8.52	1.36	1.53
3	C	87	GLU	N-CA	8.46	1.56	1.46
3	C	40	VAL	CA-CB	-8.46	1.44	1.54
1	A	125	ALA	CA-CB	-8.44	1.40	1.53
1	A	131	PHE	C-O	8.36	1.34	1.24
3	C	144	PHE	N-CA	8.34	1.56	1.46
5	E	11	PHE	C-O	8.34	1.33	1.24
6	F	2	THR	CA-CB	8.32	1.66	1.54
1	A	145	TYR	CA-CB	-8.30	1.39	1.53
3	C	256	LYS	CG-CD	8.27	1.77	1.52
3	C	142	ILE	C-O	8.24	1.34	1.24
1	A	39	ILE	CA-CB	-8.24	1.44	1.54
3	C	16	PRO	C-O	8.21	1.34	1.24
1	A	61	THR	CB-CG2	8.12	1.79	1.52
8	H	23	VAL	CA-CB	-8.11	1.45	1.54
6	F	20	TRP	C-O	8.11	1.33	1.24
5	E	20	VAL	CA-CB	-8.03	1.43	1.54
6	F	29	ILE	CA-CB	7.82	1.65	1.54
3	C	50	VAL	CA-CB	-7.77	1.45	1.54
4	D	54	THR	CA-CB	7.74	1.66	1.53
8	H	29	LEU	CG-CD2	7.74	1.78	1.52
6	F	8	ALA	CA-CB	-7.65	1.40	1.53
3	C	218	ILE	CA-CB	7.63	1.64	1.54
2	B	104	VAL	CA-CB	-7.62	1.44	1.54
1	A	127	ILE	CA-CB	-7.60	1.46	1.54
1	A	180	LEU	C-O	7.59	1.32	1.24
3	C	40	VAL	CA-C	-7.54	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	LYS	CD-CE	7.51	1.75	1.52
7	G	21	LEU	C-O	7.49	1.32	1.24
2	B	108	LEU	CA-C	7.41	1.62	1.52
3	C	87	GLU	CA-CB	7.39	1.65	1.53
2	B	40	PHE	CA-C	7.37	1.61	1.52
3	C	45	VAL	CA-CB	-7.37	1.45	1.54
8	H	14	VAL	N-CA	7.35	1.55	1.46
1	A	188	THR	CA-C	-7.33	1.43	1.52
1	A	140	TRP	C-O	7.22	1.33	1.24
6	F	10	LEU	CA-C	-7.21	1.43	1.52
1	A	139	PRO	CA-CB	-7.20	1.43	1.53
1	A	181	THR	C-O	7.20	1.33	1.24
3	C	256	LYS	CD-CE	7.18	1.74	1.52
5	E	12	ILE	CG1-CD1	7.18	1.79	1.51
1	A	204	LEU	CA-C	-7.17	1.43	1.52
1	A	123	ILE	CA-C	7.16	1.61	1.52
3	C	208	VAL	CA-C	7.15	1.61	1.52
6	F	6	LEU	CG-CD2	7.05	1.75	1.52
2	B	88	LEU	CG-CD1	6.99	1.75	1.52
2	B	108	LEU	C-O	6.97	1.32	1.24
1	A	186	ALA	CA-C	-6.93	1.43	1.52
8	H	3	ILE	CA-CB	-6.90	1.46	1.54
1	A	206	ILE	CA-CB	-6.87	1.46	1.54
2	B	56	VAL	CA-CB	-6.83	1.45	1.54
5	E	26	ILE	CA-CB	6.77	1.61	1.54
5	E	12	ILE	CA-CB	-6.76	1.46	1.54
4	D	31	ALA	CA-CB	-6.75	1.42	1.53
2	B	124	PHE	CA-C	6.75	1.61	1.52
1	A	53	ALA	CA-CB	-6.73	1.42	1.53
5	E	5	ALA	CA-CB	-6.72	1.42	1.53
3	C	90	ILE	N-CA	-6.69	1.39	1.47
1	A	207	ARG	C-O	6.69	1.32	1.24
5	E	10	VAL	C-O	6.69	1.32	1.24
1	A	24	LYS	CB-CG	6.69	1.72	1.52
1	A	100	HIS	CA-CB	6.68	1.63	1.53
3	C	237	VAL	CA-CB	-6.67	1.45	1.54
2	B	115	GLU	CG-CD	6.64	1.68	1.52
2	B	35	ASP	CA-C	-6.60	1.46	1.53
1	A	69	VAL	CA-CB	-6.57	1.47	1.54
8	H	26	ARG	CZ-NH1	6.57	1.42	1.32
2	B	26	TYR	CA-C	-6.56	1.44	1.52
6	F	12	SER	C-O	6.53	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	50	VAL	N-CA	6.51	1.54	1.46
1	A	190	VAL	CA-CB	-6.47	1.46	1.54
4	D	133	TYR	CA-C	6.47	1.61	1.52
4	D	155	VAL	CA-CB	6.47	1.63	1.54
1	A	157	ALA	N-CA	6.46	1.54	1.46
8	H	29	LEU	CB-CG	6.46	1.66	1.53
3	C	145	GLY	CA-C	6.46	1.62	1.52
7	G	16	ALA	CA-C	6.43	1.61	1.52
4	D	50	VAL	CA-C	6.42	1.60	1.52
2	B	98	VAL	CA-CB	-6.41	1.47	1.54
1	A	179	THR	CA-CB	-6.41	1.43	1.53
3	C	135	ASN	C-O	-6.38	1.18	1.24
8	H	6	LEU	CA-C	6.36	1.61	1.52
3	C	154	ASN	N-CA	6.35	1.53	1.45
1	A	90	ALA	N-CA	6.35	1.53	1.46
2	B	61	MET	C-O	6.32	1.32	1.23
2	B	115	GLU	C-O	6.32	1.32	1.24
3	C	21	VAL	CA-CB	-6.32	1.46	1.54
1	A	186	ALA	CA-CB	-6.28	1.42	1.53
1	A	26	VAL	CA-C	6.27	1.58	1.53
5	E	9	ILE	CA-C	6.26	1.60	1.52
3	C	90	ILE	CA-CB	-6.26	1.46	1.54
1	A	195	ILE	CA-CB	-6.26	1.47	1.54
8	H	28	GLY	N-CA	6.22	1.50	1.44
1	A	149	LYS	CA-C	-6.21	1.44	1.52
8	H	1	MET	CB-CG	6.21	1.71	1.52
3	C	110	GLN	N-CA	6.21	1.54	1.46
3	C	128	VAL	CA-CB	-6.20	1.44	1.54
1	A	24	LYS	CG-CD	6.19	1.71	1.52
1	A	207	ARG	CZ-NH2	6.19	1.41	1.33
4	D	36	TYR	N-CA	-6.19	1.42	1.46
6	F	17	PHE	C-O	6.19	1.31	1.24
1	A	156	GLU	CA-C	6.17	1.61	1.52
1	A	196	ALA	CA-CB	-6.17	1.43	1.53
2	B	8	ASP	CA-C	-6.17	1.46	1.53
2	B	88	LEU	CG-CD2	6.14	1.72	1.52
1	A	197	VAL	CA-CB	-6.14	1.46	1.54
3	C	36	VAL	C-O	-6.13	1.16	1.24
1	A	114	ARG	N-CA	6.12	1.51	1.46
3	C	213	ALA	CA-CB	-6.11	1.44	1.53
2	B	72	PRO	CA-C	-6.11	1.45	1.52
3	C	179	THR	CA-CB	6.06	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	ALA	N-CA	-6.06	1.38	1.46
2	B	119	LYS	CB-CG	6.04	1.70	1.52
1	A	39	ILE	CG1-CD1	-6.01	1.28	1.51
3	C	72	VAL	CB-CG1	-5.99	1.32	1.52
1	A	136	TYR	C-O	-5.98	1.16	1.24
3	C	20	ILE	CA-C	5.94	1.60	1.52
3	C	87	GLU	CG-CD	5.93	1.66	1.52
2	B	44	ILE	CA-C	5.93	1.60	1.52
2	B	62	VAL	CA-CB	5.91	1.61	1.54
3	C	49	VAL	CA-CB	-5.89	1.46	1.54
2	B	43	VAL	CA-CB	-5.89	1.48	1.54
7	G	11	LEU	N-CA	5.89	1.53	1.46
1	A	153	GLY	CA-C	5.88	1.58	1.51
2	B	116	ASN	CG-OD1	5.88	1.34	1.23
1	A	59	LYS	CE-NZ	5.87	1.67	1.49
4	D	107	VAL	N-CA	5.87	1.53	1.46
3	C	259	ILE	CA-CB	5.86	1.62	1.54
1	A	122	VAL	CA-C	-5.82	1.46	1.52
1	A	178	ALA	C-O	5.80	1.30	1.24
1	A	193	TRP	C-O	5.79	1.30	1.24
3	C	230	ALA	CA-C	5.77	1.60	1.52
8	H	1	MET	CG-SD	5.76	1.95	1.80
2	B	120	PHE	N-CA	5.75	1.53	1.46
3	C	46	PHE	CA-C	-5.75	1.45	1.52
1	A	76	VAL	N-CA	5.75	1.53	1.46
3	C	173	THR	CA-CB	5.72	1.63	1.52
5	E	3	LEU	CA-C	5.71	1.60	1.52
1	A	126	VAL	CA-CB	-5.71	1.48	1.54
1	A	198	PHE	CA-CB	-5.71	1.44	1.53
3	C	141	ASN	CA-C	5.71	1.61	1.52
1	A	215	LEU	CA-C	5.71	1.65	1.52
6	F	17	PHE	CD2-CE2	5.69	1.55	1.38
3	C	160	ILE	CA-CB	-5.68	1.46	1.54
1	A	110	PHE	CA-CB	-5.68	1.45	1.53
2	B	122	ASN	CG-OD1	5.67	1.34	1.23
1	A	62	VAL	CA-C	-5.67	1.44	1.52
3	C	167	SER	CA-C	-5.66	1.45	1.52
1	A	174	SER	N-CA	5.65	1.53	1.45
3	C	207	VAL	CA-C	5.64	1.59	1.52
1	A	63	THR	CA-CB	-5.64	1.44	1.53
2	B	42	VAL	CA-CB	-5.63	1.48	1.54
3	C	21	VAL	CA-C	-5.63	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	HIS	C-O	5.63	1.30	1.24
1	A	78	PHE	CA-C	5.58	1.61	1.52
1	A	120	SER	CA-C	5.58	1.60	1.52
5	E	3	LEU	C-O	5.58	1.30	1.24
1	A	157	ALA	CA-CB	5.54	1.62	1.53
3	C	20	ILE	N-CA	5.54	1.53	1.46
3	C	82	PHE	CA-C	5.54	1.59	1.52
2	B	109	ILE	CA-CB	-5.53	1.47	1.54
3	C	39	SER	CA-C	5.52	1.59	1.52
1	A	119	ILE	CA-C	5.49	1.59	1.52
6	F	11	LEU	C-O	5.48	1.30	1.24
1	A	190	VAL	CA-C	5.47	1.59	1.52
1	A	191	LEU	C-O	5.46	1.31	1.24
2	B	79	TRP	N-CA	-5.46	1.39	1.46
3	C	100	ASP	CA-C	5.45	1.60	1.52
3	C	145	GLY	N-CA	5.45	1.56	1.45
6	F	24	VAL	CA-CB	-5.42	1.47	1.54
3	C	256	LYS	CA-CB	5.42	1.62	1.53
2	B	128	VAL	CA-CB	-5.42	1.48	1.54
1	A	123	ILE	C-O	5.42	1.30	1.24
1	A	28	PRO	N-CA	-5.41	1.40	1.47
2	B	119	LYS	CG-CD	5.40	1.68	1.52
8	H	14	VAL	CA-CB	5.40	1.60	1.54
3	C	171	VAL	N-CA	5.40	1.52	1.46
4	D	81	VAL	CA-CB	-5.40	1.47	1.54
3	C	16	PRO	N-CA	5.39	1.54	1.47
3	C	143	HIS	N-CA	5.39	1.52	1.45
1	A	11	ARG	C-O	5.38	1.30	1.24
1	A	207	ARG	CA-CB	5.37	1.62	1.53
1	A	20	ASP	CB-CG	5.35	1.65	1.52
1	A	112	LYS	CG-CD	5.35	1.68	1.52
2	B	2	ALA	CA-CB	5.34	1.62	1.53
3	C	132	LEU	C-O	5.33	1.30	1.24
3	C	266	MET	CA-C	5.33	1.59	1.52
1	A	184	TYR	CZ-OH	5.30	1.49	1.38
1	A	145	TYR	CA-C	-5.28	1.45	1.52
8	H	28	GLY	C-O	-5.27	1.17	1.23
2	B	106	LEU	C-O	5.26	1.30	1.24
6	F	17	PHE	CD1-CE1	5.25	1.54	1.38
3	C	131	VAL	CA-C	-5.25	1.46	1.52
4	D	65	LYS	CA-C	5.24	1.59	1.52
1	A	215	LEU	N-CA	5.23	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	ALA	C-O	5.22	1.30	1.24
1	A	8	PHE	CA-CB	-5.21	1.45	1.53
2	B	67	ASP	N-CA	5.21	1.52	1.46
2	B	98	VAL	C-O	5.21	1.30	1.24
3	C	142	ILE	CA-C	5.21	1.59	1.52
4	D	26	THR	CA-CB	-5.21	1.45	1.53
4	D	116	PRO	CA-C	5.20	1.59	1.52
2	B	37	LEU	N-CA	-5.20	1.39	1.46
3	C	8	THR	N-CA	5.20	1.52	1.46
1	A	16	ALA	CA-CB	-5.19	1.45	1.53
2	B	4	LEU	N-CA	5.19	1.52	1.46
3	C	30	LYS	N-CA	5.18	1.52	1.46
3	C	44	THR	CA-CB	-5.18	1.45	1.54
3	C	259	ILE	CG1-CD1	5.17	1.72	1.51
5	E	12	ILE	C-O	5.17	1.29	1.24
3	C	146	LYS	CE-NZ	5.15	1.64	1.49
2	B	29	GLU	CB-CG	5.14	1.67	1.52
6	F	13	PHE	CA-C	5.14	1.59	1.52
1	A	187	HIS	C-O	-5.13	1.17	1.24
1	A	187	HIS	CA-C	-5.13	1.45	1.52
1	A	113	PRO	N-CA	5.11	1.53	1.47
4	D	125	LYS	CA-C	-5.10	1.46	1.52
7	G	31	ARG	CA-C	-5.09	1.46	1.52
8	H	9	VAL	CA-CB	-5.09	1.47	1.54
3	C	48	ALA	CA-CB	-5.08	1.45	1.53
2	B	29	GLU	CA-CB	5.07	1.61	1.53
6	F	17	PHE	CE1-CZ	5.07	1.53	1.38
4	D	89	THR	CA-CB	5.05	1.61	1.53
7	G	14	VAL	CA-CB	-5.05	1.47	1.54
7	G	26	TYR	CA-CB	-5.05	1.45	1.53
8	H	12	LEU	CA-C	5.05	1.59	1.52
2	B	79	TRP	CA-C	5.03	1.59	1.52
3	C	108	GLU	N-CA	5.03	1.52	1.46
1	A	145	TYR	N-CA	-5.02	1.39	1.46
1	A	52	PHE	CB-CG	-5.02	1.39	1.50
3	C	91	PRO	N-CA	-5.02	1.40	1.47
2	B	19	ALA	CA-C	-5.01	1.46	1.52
8	H	11	LEU	CA-C	-5.01	1.46	1.52
4	D	129	HIS	N-CA	5.01	1.52	1.46
6	F	14	GLY	C-O	5.00	1.30	1.23
2	B	92	PRO	N-CA	-5.00	1.44	1.47

All (465) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LYS	CA-C-N	-19.77	95.13	119.84
1	A	112	LYS	C-N-CA	-19.77	95.13	119.84
3	C	9	TYR	CA-C-N	16.48	137.36	120.38
3	C	9	TYR	C-N-CA	16.48	137.36	120.38
3	C	85	ALA	CA-C-N	15.21	138.85	119.84
3	C	85	ALA	C-N-CA	15.21	138.85	119.84
4	D	44	PRO	CA-C-N	14.41	135.35	119.93
4	D	44	PRO	C-N-CA	14.41	135.35	119.93
2	B	111	VAL	CA-C-N	-14.29	104.61	120.04
2	B	111	VAL	C-N-CA	-14.29	104.61	120.04
3	C	280	GLU	N-CA-C	-12.92	96.78	112.54
3	C	125	GLN	N-CA-C	-12.90	97.29	113.55
2	B	15	ARG	NE-CZ-NH2	-12.28	108.15	119.20
7	G	3	GLU	CA-C-N	11.91	134.73	119.84
7	G	3	GLU	C-N-CA	11.91	134.73	119.84
1	A	26	VAL	N-CA-C	10.90	118.34	107.55
1	A	24	LYS	N-CA-C	-10.65	92.82	109.76
1	A	153	GLY	N-CA-C	10.34	125.15	112.64
2	B	11	ASP	CA-C-N	10.31	129.92	119.82
2	B	11	ASP	C-N-CA	10.31	129.92	119.82
2	B	91	VAL	CA-C-N	-10.29	109.21	120.94
2	B	91	VAL	C-N-CA	-10.29	109.21	120.94
3	C	104	GLN	CA-C-N	10.18	130.83	119.83
3	C	104	GLN	C-N-CA	10.18	130.83	119.83
3	C	207	VAL	N-CA-C	9.98	123.33	109.55
1	A	52	PHE	N-CA-C	-9.81	99.62	111.69
4	D	43	ILE	CA-C-N	9.56	130.22	120.38
4	D	43	ILE	C-N-CA	9.56	130.22	120.38
4	D	107	VAL	N-CA-C	9.30	120.93	109.30
1	A	187	HIS	CA-C-N	-9.14	107.73	122.26
1	A	187	HIS	C-N-CA	-9.14	107.73	122.26
5	E	26	ILE	CB-CA-C	9.12	123.63	111.87
3	C	202	ASP	N-CA-C	9.06	121.16	111.28
2	B	64	GLU	N-CA-C	-9.02	97.85	110.29
3	C	70	LEU	N-CA-C	9.01	123.49	109.52
2	B	22	MET	N-CA-C	8.94	129.85	110.80
4	D	43	ILE	CB-CA-C	-8.92	100.42	110.68
4	D	107	VAL	CB-CA-C	-8.92	98.04	111.33
3	C	141	ASN	N-CA-C	8.92	123.72	113.02
3	C	133	SER	CA-C-N	8.90	130.96	119.84
3	C	133	SER	C-N-CA	8.90	130.96	119.84
7	G	23	TYR	CA-C-N	-8.87	106.92	122.26
7	G	23	TYR	C-N-CA	-8.87	106.92	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	PRO	CA-C-N	8.85	130.90	119.84
1	A	27	PRO	C-N-CA	8.85	130.90	119.84
2	B	156	THR	N-CA-C	-8.84	101.93	112.89
8	H	23	VAL	N-CA-CB	8.80	120.60	110.65
3	C	149	ILE	CA-C-N	-8.79	111.08	122.77
3	C	149	ILE	C-N-CA	-8.79	111.08	122.77
2	B	2	ALA	CA-C-N	-8.77	108.94	122.62
2	B	2	ALA	C-N-CA	-8.77	108.94	122.62
2	B	143	LEU	N-CA-C	-8.77	101.68	112.38
2	B	84	VAL	CB-CA-C	-8.73	100.36	112.14
2	B	64	GLU	CA-C-N	8.71	130.73	119.84
2	B	64	GLU	C-N-CA	8.71	130.73	119.84
7	G	28	GLN	N-CA-C	-8.71	104.69	114.62
8	H	23	VAL	CB-CA-C	-8.52	100.88	111.87
1	A	61	THR	CA-CB-CG2	8.51	124.97	110.50
2	B	154	THR	N-CA-C	8.50	121.39	111.02
3	C	41	LEU	CA-C-N	-8.37	111.40	119.85
3	C	41	LEU	C-N-CA	-8.37	111.40	119.85
3	C	39	SER	CA-C-N	-8.34	112.34	123.10
3	C	39	SER	C-N-CA	-8.34	112.34	123.10
2	B	32	TRP	CA-C-N	8.31	130.23	119.84
2	B	32	TRP	C-N-CA	8.31	130.23	119.84
1	A	100	HIS	CB-CA-C	8.30	124.01	110.90
4	D	64	VAL	CB-CA-C	-8.30	100.20	110.99
3	C	34	VAL	CB-CA-C	-8.27	98.39	110.63
1	A	184	TYR	N-CA-C	-8.26	102.24	111.82
3	C	218	ILE	CB-CA-C	8.21	119.49	110.62
1	A	207	ARG	N-CA-C	-8.16	102.32	111.71
2	B	73	LEU	N-CA-C	-8.14	95.63	108.90
8	H	1	MET	CB-CG-SD	8.10	137.01	112.70
3	C	172	PHE	N-CA-C	7.98	122.80	112.26
3	C	5	ALA	N-CA-C	-7.98	102.28	110.97
3	C	208	VAL	N-CA-C	7.94	121.40	109.17
1	A	122	VAL	CA-CB-CG2	-7.94	96.91	110.40
1	A	86	HIS	N-CA-C	-7.92	101.74	111.33
7	G	32	PRO	N-CA-C	7.92	123.15	110.40
1	A	61	THR	CA-CB-OG1	-7.90	97.75	109.60
1	A	129	VAL	N-CA-CB	7.87	119.24	110.51
1	A	136	TYR	CA-C-N	-7.86	108.66	122.26
1	A	136	TYR	C-N-CA	-7.86	108.66	122.26
4	D	43	ILE	N-CA-CB	7.81	118.84	110.17
1	A	3	ASN	N-CA-C	7.80	127.42	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	101	VAL	CA-C-N	-7.78	110.53	122.05
3	C	101	VAL	C-N-CA	-7.78	110.53	122.05
1	A	20	ASP	N-CA-CB	7.78	122.47	109.78
3	C	201	THR	N-CA-C	7.73	127.27	110.80
1	A	151	VAL	CB-CA-C	-7.72	101.99	111.88
3	C	251	ASP	CA-C-N	7.72	129.49	119.84
3	C	251	ASP	C-N-CA	7.72	129.49	119.84
1	A	59	LYS	CD-CE-NZ	7.69	136.51	111.90
1	A	83	ARG	NE-CZ-NH1	-7.67	113.83	121.50
4	D	80	LEU	N-CA-C	7.67	120.75	108.41
5	E	12	ILE	N-CA-CB	7.63	118.93	110.62
1	A	61	THR	N-CA-C	-7.60	96.24	108.55
3	C	68	VAL	CB-CA-C	-7.57	101.18	111.63
1	A	69	VAL	CB-CA-C	-7.55	102.37	111.81
4	D	64	VAL	N-CA-C	7.53	119.25	107.28
1	A	149	LYS	N-CA-C	-7.51	103.08	111.71
2	B	64	GLU	N-CA-CB	7.47	119.06	110.03
3	C	160	ILE	CB-CA-C	-7.45	99.06	111.29
8	H	3	ILE	N-CA-CB	-7.44	101.85	110.55
1	A	24	LYS	CB-CA-C	7.42	121.93	109.84
3	C	234	ASN	N-CA-C	7.39	124.30	109.01
1	A	186	ALA	CA-C-N	7.37	131.51	120.31
1	A	186	ALA	C-N-CA	7.37	131.51	120.31
2	B	62	VAL	N-CA-C	7.34	118.47	107.75
2	B	125	ARG	NE-CZ-NH1	-7.34	114.16	121.50
2	B	157	LEU	N-CA-C	-7.34	104.79	113.38
1	A	79	GLY	N-CA-C	-7.33	104.00	112.50
3	C	27	LEU	N-CA-C	7.31	126.36	110.80
1	A	64	GLU	N-CA-C	7.29	122.46	113.50
2	B	40	PHE	CA-C-N	7.29	127.14	119.05
2	B	40	PHE	C-N-CA	7.29	127.14	119.05
2	B	66	ALA	CA-C-N	7.29	131.75	122.64
2	B	66	ALA	C-N-CA	7.29	131.75	122.64
6	F	11	LEU	CA-CB-CG	-7.28	90.82	116.30
1	A	12	LEU	N-CA-C	7.26	119.27	111.36
1	A	106	LEU	CB-CG-CD1	-7.26	88.93	110.70
4	D	16	ARG	N-CA-C	-7.25	103.37	111.71
3	C	142	ILE	N-CA-CB	-7.23	102.83	110.72
6	F	10	LEU	N-CA-CB	7.22	120.80	109.82
4	D	77	ASP	N-CA-C	7.21	126.17	110.80
1	A	112	LYS	N-CA-C	7.20	125.73	109.81
1	A	129	VAL	CB-CA-C	-7.20	102.66	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	MET	CB-CG-SD	-7.18	91.17	112.70
1	A	113	PRO	CA-C-N	7.15	132.17	120.23
1	A	113	PRO	C-N-CA	7.15	132.17	120.23
6	F	10	LEU	CA-C-N	-7.15	110.14	120.29
6	F	10	LEU	C-N-CA	-7.15	110.14	120.29
1	A	122	VAL	CA-C-N	-7.13	109.14	121.97
1	A	122	VAL	C-N-CA	-7.13	109.14	121.97
8	H	28	GLY	N-CA-C	7.11	123.86	112.06
2	B	25	ASN	N-CA-C	-7.09	102.60	112.25
3	C	239	GLY	N-CA-C	7.09	123.31	112.81
2	B	61	MET	N-CA-C	7.08	119.67	110.53
1	A	145	TYR	N-CA-C	-7.08	104.67	113.38
1	A	203	PHE	N-CA-C	7.07	118.98	111.28
4	D	142	GLY	CA-C-N	7.04	128.64	119.84
4	D	142	GLY	C-N-CA	7.04	128.64	119.84
4	D	135	GLU	N-CA-C	-6.98	104.24	112.89
3	C	49	VAL	CA-C-N	-6.95	114.17	122.93
3	C	49	VAL	C-N-CA	-6.95	114.17	122.93
6	F	12	SER	N-CA-C	-6.94	103.40	110.97
3	C	30	LYS	CA-C-N	6.92	128.49	119.84
3	C	30	LYS	C-N-CA	6.92	128.49	119.84
5	E	16	PHE	N-CA-C	-6.92	102.81	111.11
4	D	149	ALA	N-CA-C	6.89	120.68	110.48
1	A	138	LEU	CA-C-N	6.84	126.53	119.56
1	A	138	LEU	C-N-CA	6.84	126.53	119.56
2	B	25	ASN	CA-C-N	-6.83	111.63	122.29
2	B	25	ASN	C-N-CA	-6.83	111.63	122.29
3	C	138	THR	CA-C-N	-6.79	112.23	123.37
3	C	138	THR	C-N-CA	-6.79	112.23	123.37
3	C	250	GLN	N-CA-C	6.79	119.34	108.41
1	A	60	PRO	CB-CA-C	-6.76	100.40	111.56
2	B	76	LEU	CA-C-N	-6.75	111.40	119.84
2	B	76	LEU	C-N-CA	-6.75	111.40	119.84
1	A	202	HIS	CA-C-N	-6.73	111.26	120.28
1	A	202	HIS	C-N-CA	-6.73	111.26	120.28
1	A	146	TRP	CA-C-N	-6.72	108.47	121.58
1	A	146	TRP	C-N-CA	-6.72	108.47	121.58
2	B	22	MET	CB-CA-C	-6.72	97.05	110.42
1	A	19	ASP	CA-C-N	-6.69	110.78	120.82
1	A	19	ASP	C-N-CA	-6.69	110.78	120.82
1	A	215	LEU	N-CA-C	6.68	129.72	111.00
8	H	22	VAL	CB-CA-C	-6.68	103.42	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	PRO	CA-C-N	-6.67	111.32	120.46
2	B	83	PRO	C-N-CA	-6.67	111.32	120.46
3	C	278	GLN	CA-C-N	-6.67	112.17	121.77
3	C	278	GLN	C-N-CA	-6.67	112.17	121.77
1	A	32	ILE	N-CA-C	6.66	123.19	109.34
2	B	56	VAL	N-CA-C	6.65	117.44	110.72
2	B	125	ARG	CA-CB-CG	-6.65	100.81	114.10
1	A	188	THR	N-CA-CB	6.65	120.42	110.65
3	C	282	VAL	CB-CA-C	-6.64	100.39	111.29
1	A	58	TYR	CA-C-N	-6.62	112.35	122.42
1	A	58	TYR	C-N-CA	-6.62	112.35	122.42
2	B	159	LEU	CA-CB-CG	6.62	139.47	116.30
2	B	72	PRO	N-CA-C	-6.61	101.10	111.34
1	A	200	LEU	N-CA-C	-6.59	104.02	111.14
3	C	256	LYS	CG-CD-CE	6.59	126.47	111.30
4	D	22	LEU	CA-CB-CG	-6.58	93.29	116.30
3	C	257	TRP	N-CA-C	6.57	119.00	111.11
7	G	2	VAL	CB-CA-C	-6.57	100.18	110.69
1	A	21	VAL	N-CA-C	6.57	117.06	110.23
3	C	90	ILE	CB-CA-C	-6.56	104.45	110.88
2	B	10	SER	N-CA-C	6.55	118.50	111.36
6	F	21	GLY	N-CA-C	-6.55	104.39	112.77
4	D	23	ALA	CA-C-N	-6.54	109.81	120.72
4	D	23	ALA	C-N-CA	-6.54	109.81	120.72
3	C	7	GLN	N-CA-C	-6.53	105.45	113.41
1	A	190	VAL	N-CA-C	6.52	116.68	110.42
2	B	92	PRO	CA-C-N	-6.52	114.00	123.00
2	B	92	PRO	C-N-CA	-6.52	114.00	123.00
2	B	45	MET	CB-CG-SD	-6.50	93.20	112.70
3	C	100	ASP	CA-C-N	-6.49	114.72	123.10
3	C	100	ASP	C-N-CA	-6.49	114.72	123.10
5	E	22	ILE	CA-C-N	-6.49	110.29	121.97
5	E	22	ILE	C-N-CA	-6.49	110.29	121.97
1	A	148	VAL	CB-CA-C	6.49	120.93	112.24
2	B	125	ARG	CA-C-N	-6.48	115.39	122.59
2	B	125	ARG	C-N-CA	-6.48	115.39	122.59
5	E	26	ILE	N-CA-C	-6.47	104.34	110.42
8	H	3	ILE	N-CA-C	-6.46	104.22	110.42
1	A	130	SER	CA-CB-OG	-6.45	98.19	111.10
2	B	38	TYR	CA-C-N	-6.44	112.40	121.55
2	B	38	TYR	C-N-CA	-6.44	112.40	121.55
1	A	203	PHE	N-CA-CB	6.43	119.57	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	TYR	N-CA-CB	6.43	116.50	110.39
8	H	27	ASN	CA-C-O	-6.40	114.20	122.14
8	H	14	VAL	N-CA-CB	6.39	117.61	110.51
3	C	102	TYR	N-CA-C	6.37	119.18	109.62
1	A	144	GLY	CA-C-N	-6.37	111.24	122.26
1	A	144	GLY	C-N-CA	-6.37	111.24	122.26
1	A	174	SER	N-CA-C	6.37	118.74	110.53
2	B	40	PHE	CA-C-O	6.35	124.47	118.63
1	A	38	GLY	CA-C-N	-6.34	112.57	120.56
1	A	38	GLY	C-N-CA	-6.34	112.57	120.56
3	C	205	LYS	N-CA-C	6.33	124.28	110.80
4	D	79	VAL	N-CA-C	6.32	117.81	108.45
3	C	124	TYR	N-CA-C	6.32	119.10	109.62
1	A	82	ILE	CA-C-N	-6.32	110.16	120.71
1	A	82	ILE	C-N-CA	-6.32	110.16	120.71
2	B	98	VAL	N-CA-CB	-6.31	103.51	110.51
3	C	154	ASN	N-CA-C	6.31	118.89	108.99
3	C	148	ALA	N-CA-C	6.30	118.66	110.53
4	D	108	CYS	CA-CB-SG	6.28	128.84	114.40
1	A	117	THR	CA-C-N	-6.28	110.22	120.71
1	A	117	THR	C-N-CA	-6.28	110.22	120.71
1	A	25	TYR	CA-C-N	-6.27	115.70	122.85
1	A	25	TYR	C-N-CA	-6.27	115.70	122.85
3	C	43	ASP	CB-CA-C	-6.27	102.96	112.11
1	A	83	ARG	CA-CB-CG	-6.26	101.59	114.10
8	H	14	VAL	CB-CA-C	-6.25	103.88	111.88
1	A	59	LYS	CB-CG-CD	6.24	125.66	111.30
3	C	61	VAL	N-CA-C	6.24	118.62	109.63
2	B	134	LEU	CA-CB-CG	-6.24	94.46	116.30
2	B	90	SER	CB-CA-C	-6.24	102.18	111.72
3	C	245	THR	N-CA-C	6.23	117.33	108.74
1	A	103	ARG	N-CA-C	-6.22	104.50	111.28
1	A	149	LYS	CA-C-N	-6.22	110.77	121.97
1	A	149	LYS	C-N-CA	-6.22	110.77	121.97
3	C	275	LYS	CA-C-N	-6.20	112.38	120.44
3	C	275	LYS	C-N-CA	-6.20	112.38	120.44
4	D	169	ASP	N-CA-C	6.20	119.31	108.52
3	C	108	GLU	CA-C-N	-6.19	112.83	122.86
3	C	108	GLU	C-N-CA	-6.19	112.83	122.86
1	A	103	ARG	CA-C-N	-6.17	110.85	121.97
1	A	103	ARG	C-N-CA	-6.17	110.85	121.97
3	C	256	LYS	CB-CA-C	6.16	120.71	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	244	ASP	N-CA-C	-6.16	99.78	109.50
3	C	127	ILE	CB-CA-C	-6.15	101.20	111.29
1	A	158	ILE	CA-C-N	6.15	127.53	119.84
1	A	158	ILE	C-N-CA	6.15	127.53	119.84
8	H	22	VAL	CA-C-N	-6.14	113.23	120.72
8	H	22	VAL	C-N-CA	-6.14	113.23	120.72
5	E	31	LEU	CA-CB-CG	-6.13	94.83	116.30
2	B	57	LEU	CA-C-N	-6.13	114.88	122.42
2	B	57	LEU	C-N-CA	-6.13	114.88	122.42
4	D	156	GLN	N-CA-C	6.13	118.62	110.53
1	A	100	HIS	N-CA-C	-6.13	104.52	111.14
6	F	15	LEU	CA-CB-CG	-6.12	94.88	116.30
3	C	83	LYS	CA-C-N	-6.12	112.00	121.18
3	C	83	LYS	C-N-CA	-6.12	112.00	121.18
4	D	137	GLY	N-CA-C	-6.10	98.72	113.18
8	H	21	MET	CG-SD-CE	-6.09	87.49	100.90
3	C	8	THR	N-CA-CB	6.09	119.34	110.26
3	C	107	LYS	CA-C-O	-6.09	114.69	121.51
5	E	23	ILE	N-CA-CB	6.08	121.27	111.23
3	C	167	SER	N-CA-C	-6.06	97.89	110.80
2	B	1	MET	CB-CG-SD	-6.05	94.56	112.70
3	C	49	VAL	N-CA-C	6.04	116.57	107.75
4	D	56	ALA	N-CA-C	6.04	119.36	109.76
1	A	26	VAL	CB-CA-C	6.04	118.16	111.04
8	H	23	VAL	CA-CB-CG1	-6.03	100.15	110.40
4	D	161	VAL	N-CA-C	6.03	116.97	108.17
3	C	230	ALA	N-CA-C	6.03	123.64	110.80
2	B	88	LEU	CD1-CG-CD2	6.01	124.01	110.80
6	F	5	MET	CG-SD-CE	5.99	114.08	100.90
1	A	160	VAL	N-CA-C	-5.99	105.23	111.58
6	F	12	SER	O-C-N	5.99	128.25	122.03
3	C	30	LYS	N-CA-C	5.97	117.91	108.23
6	F	24	VAL	CB-CA-C	-5.97	101.50	111.29
2	B	81	LEU	CA-C-N	-5.95	113.22	119.83
2	B	81	LEU	C-N-CA	-5.95	113.22	119.83
5	E	23	ILE	CB-CA-C	-5.95	101.54	111.29
3	C	107	LYS	N-CA-C	-5.93	100.30	109.14
2	B	117	VAL	CA-C-N	-5.93	108.77	121.45
2	B	117	VAL	C-N-CA	-5.93	108.77	121.45
2	B	16	ALA	N-CA-C	-5.92	105.90	113.01
3	C	41	LEU	N-CA-C	5.92	118.72	110.20
2	B	99	LEU	CA-CB-CG	-5.92	95.60	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	29	ILE	CB-CA-C	5.91	120.98	111.29
1	A	148	VAL	N-CA-C	-5.89	104.57	111.00
4	D	43	ILE	N-CA-C	5.89	115.38	108.96
1	A	184	TYR	CB-CA-C	5.88	121.96	110.67
3	C	14	ARG	N-CA-C	5.85	117.95	108.41
3	C	250	GLN	CB-CA-C	-5.85	101.16	110.81
4	D	35	LEU	CA-CB-CG	-5.85	95.83	116.30
1	A	198	PHE	N-CA-C	5.84	118.43	111.71
3	C	82	PHE	N-CA-C	5.83	118.52	110.35
3	C	163	THR	CB-CA-C	-5.83	100.94	110.85
3	C	200	GLN	N-CA-C	5.82	123.19	110.80
1	A	87	ARG	N-CA-C	5.80	117.28	111.07
1	A	51	GLY	CA-C-O	5.79	127.01	121.05
3	C	15	GLU	CA-C-N	5.79	127.07	119.84
3	C	15	GLU	C-N-CA	5.79	127.07	119.84
1	A	10	GLU	O-C-N	5.77	128.26	122.08
7	G	18	LEU	CB-CG-CD2	-5.76	93.41	110.70
1	A	194	LEU	N-CA-CB	5.76	118.53	109.94
7	G	2	VAL	N-CA-C	5.76	118.25	108.86
3	C	1	TYR	CA-C-N	5.76	127.04	119.84
3	C	1	TYR	C-N-CA	5.76	127.04	119.84
1	A	91	SER	CA-CB-OG	-5.76	99.59	111.10
1	A	177	GLN	CA-C-N	-5.76	112.77	120.54
1	A	177	GLN	C-N-CA	-5.76	112.77	120.54
5	E	2	ILE	N-CA-C	-5.75	104.07	110.62
3	C	1	TYR	CB-CA-C	-5.74	99.19	110.10
1	A	185	SER	O-C-N	5.74	128.00	122.03
2	B	146	GLY	CA-C-N	-5.73	111.12	121.14
2	B	146	GLY	C-N-CA	-5.73	111.12	121.14
7	G	9	LEU	CA-CB-CG	-5.72	96.28	116.30
1	A	28	PRO	CA-N-CD	-5.72	104.00	112.00
3	C	104	GLN	N-CA-C	5.71	118.53	109.40
1	A	126	VAL	N-CA-C	5.70	116.35	110.36
3	C	252	PRO	CA-C-N	-5.70	112.07	120.28
3	C	252	PRO	C-N-CA	-5.70	112.07	120.28
4	D	129	HIS	N-CA-C	5.70	122.93	110.80
5	E	15	PHE	O-C-N	5.69	127.93	122.07
1	A	112	LYS	C-N-CD	5.69	148.32	125.00
2	B	20	LYS	N-CA-CB	5.69	118.72	110.47
1	A	10	GLU	CA-C-N	5.66	132.34	121.54
1	A	10	GLU	C-N-CA	5.66	132.34	121.54
1	A	69	VAL	N-CA-C	-5.65	104.82	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	SER	N-CA-C	-5.65	103.25	110.53
6	F	11	LEU	O-C-N	5.64	128.58	122.15
5	E	20	VAL	CB-CA-C	-5.63	102.05	111.29
2	B	94	LYS	N-CA-C	5.63	117.42	111.28
3	C	93	GLU	CB-CA-C	5.62	120.24	110.68
7	G	35	LEU	N-CA-C	5.62	122.77	110.80
1	A	186	ALA	O-C-N	5.60	130.03	122.59
4	D	10	VAL	CA-C-N	-5.59	113.47	120.51
4	D	10	VAL	C-N-CA	-5.59	113.47	120.51
3	C	217	LEU	CA-C-N	-5.59	115.94	122.14
3	C	217	LEU	C-N-CA	-5.59	115.94	122.14
3	C	3	PHE	N-CA-C	5.58	119.60	112.34
2	B	43	VAL	N-CA-C	5.58	116.03	110.23
2	B	77	PRO	CB-CA-C	-5.58	102.35	111.56
7	G	23	TYR	N-CA-C	-5.58	104.58	111.33
1	A	186	ALA	N-CA-CB	-5.54	101.12	110.49
4	D	53	GLY	N-CA-C	5.54	119.38	110.90
1	A	136	TYR	O-C-N	-5.54	115.22	122.59
3	C	117	GLY	N-CA-C	5.54	123.63	112.34
1	A	178	ALA	CA-C-N	-5.53	113.11	120.79
1	A	178	ALA	C-N-CA	-5.53	113.11	120.79
1	A	134	THR	CB-CA-C	-5.51	99.45	110.42
1	A	10	GLU	N-CA-C	-5.49	104.32	111.02
2	B	69	PHE	CA-C-N	-5.47	115.08	123.07
2	B	69	PHE	C-N-CA	-5.47	115.08	123.07
3	C	231	LEU	N-CA-C	5.47	122.44	110.80
3	C	211	ILE	CA-C-N	5.46	126.66	119.84
3	C	211	ILE	C-N-CA	5.46	126.66	119.84
1	A	147	ALA	CA-C-N	-5.46	111.82	120.55
1	A	147	ALA	C-N-CA	-5.46	111.82	120.55
1	A	37	GLY	CA-C-N	5.45	126.03	119.98
1	A	37	GLY	C-N-CA	5.45	126.03	119.98
3	C	285	ALA	N-CA-C	-5.45	106.82	112.93
2	B	29	GLU	N-CA-CB	5.45	118.06	110.11
1	A	33	PHE	N-CA-C	5.45	118.72	111.75
3	C	43	ASP	N-CA-C	5.44	118.63	111.28
7	G	11	LEU	CB-CA-C	-5.44	102.11	110.81
2	B	29	GLU	CB-CA-C	5.43	118.02	109.27
7	G	29	TYR	CB-CA-C	-5.43	99.62	110.42
3	C	89	ARG	CA-CB-CG	-5.41	103.28	114.10
3	C	216	GLU	N-CA-C	-5.40	103.56	110.53
1	A	206	ILE	N-CA-C	5.39	115.60	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	63	ASN	CA-C-N	-5.39	115.91	123.13
4	D	63	ASN	C-N-CA	-5.39	115.91	123.13
1	A	213	GLY	CA-C-N	5.38	126.57	119.84
1	A	213	GLY	C-N-CA	5.38	126.57	119.84
3	C	254	ARG	NE-CZ-NH1	-5.38	116.12	121.50
3	C	44	THR	N-CA-C	5.38	117.59	109.41
1	A	138	LEU	CB-CG-CD2	-5.38	94.56	110.70
1	A	108	GLY	N-CA-C	-5.37	105.64	113.48
3	C	36	VAL	CA-C-N	5.37	126.56	119.84
3	C	36	VAL	C-N-CA	5.37	126.56	119.84
6	F	10	LEU	CA-CB-CG	-5.37	97.50	116.30
4	D	88	PRO	N-CA-C	-5.37	101.41	110.21
3	C	113	VAL	CA-C-N	-5.36	115.44	122.99
3	C	113	VAL	C-N-CA	-5.36	115.44	122.99
1	A	92	MET	CG-SD-CE	-5.35	89.14	100.90
3	C	236	ASN	N-CA-C	5.34	118.06	110.10
1	A	169	LEU	CA-CB-CG	5.34	134.98	116.30
1	A	185	SER	N-CA-CB	5.34	117.70	109.91
1	A	125	ALA	CA-C-N	-5.33	113.72	120.60
1	A	125	ALA	C-N-CA	-5.33	113.72	120.60
6	F	10	LEU	CB-CG-CD1	-5.31	94.76	110.70
2	B	18	LEU	CA-CB-CG	-5.31	97.72	116.30
4	D	107	VAL	N-CA-CB	5.31	116.84	110.31
1	A	126	VAL	N-CA-CB	5.30	116.39	110.51
3	C	146	LYS	CA-CB-CG	5.29	124.68	114.10
2	B	128	VAL	N-CA-C	5.27	115.89	110.36
1	A	34	TYR	N-CA-C	-5.25	106.12	113.37
2	B	15	ARG	NH1-CZ-NH2	5.25	126.12	119.30
4	D	10	VAL	N-CA-C	-5.24	97.56	108.88
1	A	72	ILE	CB-CA-C	-5.23	105.19	112.04
2	B	77	PRO	CA-C-N	-5.23	113.48	121.74
2	B	77	PRO	C-N-CA	-5.23	113.48	121.74
1	A	14	ILE	CA-CB-CG1	-5.23	101.51	110.40
5	E	23	ILE	N-CA-C	-5.22	98.47	109.34
3	C	109	GLY	N-CA-C	5.21	122.01	114.67
2	B	22	MET	N-CA-CB	-5.20	101.70	110.49
1	A	11	ARG	CG-CD-NE	-5.20	100.57	112.00
4	D	110	HIS	N-CA-C	-5.19	99.74	110.80
8	H	28	GLY	O-C-N	-5.19	119.07	123.59
1	A	21	VAL	CB-CA-C	-5.18	105.07	111.70
3	C	119	LEU	CA-C-N	-5.17	113.38	119.84
3	C	119	LEU	C-N-CA	-5.17	113.38	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	PRO	CA-CB-CG	-5.16	94.69	104.50
2	B	121	GLN	N-CA-C	-5.16	104.58	111.24
5	E	3	LEU	CB-CA-C	5.15	119.61	110.85
2	B	43	VAL	N-CA-CB	5.14	116.01	110.62
3	C	137	THR	CB-CA-C	-5.13	99.26	109.99
1	A	168	LEU	CA-CB-CG	-5.12	98.36	116.30
2	B	71	THR	CB-CA-C	-5.12	101.73	109.26
3	C	234	ASN	CB-CA-C	-5.12	105.11	110.33
1	A	122	VAL	CB-CA-C	-5.12	105.15	111.70
7	G	22	PHE	CA-C-N	-5.12	113.37	120.38
7	G	22	PHE	C-N-CA	-5.12	113.37	120.38
2	B	42	VAL	CA-C-N	-5.11	114.07	120.77
2	B	42	VAL	C-N-CA	-5.11	114.07	120.77
1	A	19	ASP	CA-C-O	-5.11	115.45	121.07
1	A	170	ARG	N-CA-C	-5.10	99.93	110.80
1	A	201	LEU	CA-CB-CG	-5.10	98.45	116.30
7	G	18	LEU	CA-CB-CG	-5.10	98.45	116.30
1	A	159	PRO	N-CA-C	5.08	122.93	112.47
3	C	160	ILE	N-CA-C	5.08	119.91	109.34
8	H	21	MET	CB-CG-SD	-5.08	97.47	112.70
4	D	108	CYS	N-CA-CB	5.06	117.32	110.38
7	G	4	PRO	CB-CA-C	-5.06	103.21	111.56
1	A	67	ALA	N-CA-C	5.06	117.57	111.40
4	D	45	PRO	CA-C-O	-5.06	115.81	121.32
3	C	279	VAL	N-CA-C	-5.05	107.00	113.22
1	A	159	PRO	CA-C-N	-5.05	113.16	121.34
1	A	159	PRO	C-N-CA	-5.05	113.16	121.34
3	C	143	HIS	CA-C-O	-5.05	115.45	121.16
2	B	82	TYR	CA-C-N	5.05	126.15	119.84
2	B	82	TYR	C-N-CA	5.05	126.15	119.84
2	B	4	LEU	N-CA-C	5.04	116.58	108.32
4	D	162	LEU	N-CA-C	5.03	117.11	107.75
1	A	38	GLY	N-CA-C	-5.03	106.70	112.73
2	B	87	ILE	CB-CA-C	-5.03	103.05	111.29
3	C	61	VAL	CA-C-N	-5.02	113.09	122.73
3	C	61	VAL	C-N-CA	-5.02	113.09	122.73
1	A	155	PRO	CB-CA-C	-5.02	104.38	112.21
3	C	171	VAL	N-CA-C	5.01	117.04	109.12
3	C	10	PRO	N-CA-C	5.01	116.82	110.70
5	E	1	MET	CB-CG-SD	5.01	127.74	112.70
3	C	67	LYS	N-CA-C	-5.01	100.13	110.80
3	C	173	THR	N-CA-C	5.00	115.92	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	134	ASP	N-CA-C	5.00	121.46	110.80
1	A	119	ILE	N-CA-C	5.00	119.75	109.34

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	PRO	Peptide
1	A	135	GLY	Peptide
1	A	158	ILE	Peptide
1	A	163	VAL	Peptide
1	A	2	ALA	Peptide
1	A	27	PRO	Peptide
2	B	1	MET	Peptide
2	B	2	ALA	Peptide
2	B	21	GLY	Peptide
2	B	32	TRP	Peptide
2	B	33	PRO	Peptide
2	B	64	GLU	Peptide
2	B	91	VAL	Peptide
3	C	100	ASP	Peptide
3	C	124	TYR	Peptide
3	C	125	GLN	Peptide
3	C	141	ASN	Peptide
3	C	150	HIS	Peptide
3	C	20	ILE	Peptide
3	C	22	CYS	Peptide
3	C	28	ALA	Peptide
5	E	12	ILE	Peptide
5	E	24	PHE	Peptide
5	E	28	SER	Peptide
5	E	31	LEU	Peptide
6	F	6	LEU	Peptide
7	G	1	MET	Peptide
7	G	17	THR	Peptide
7	G	29	TYR	Peptide
7	G	33	ASN	Peptide
8	H	2	GLU	Peptide
8	H	27	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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	1711	0	1736	361	0
2	B	1249	0	1308	330	0
3	C	2216	0	2232	425	0
4	D	1260	0	1243	195	0
5	E	248	0	284	81	0
6	F	242	0	260	74	0
7	G	283	0	289	63	0
8	H	230	0	239	80	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	86	0	60	47	0
10	C	43	0	30	23	0
11	A	43	0	31	10	0
12	A	54	0	79	26	0
12	B	54	0	83	11	0
13	A	102	0	123	13	0
13	C	34	0	42	10	0
14	A	21	0	24	7	0
15	B	65	0	72	14	0
16	D	4	0	0	3	0
17	D	54	0	53	11	0
18	G	40	0	52	13	0
19	A	3	0	0	0	0
19	B	2	0	0	0	0
All	All	8046	0	8240	1515	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 93.

All (1515) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:CE	1:A:59:LYS:CD	1.75	1.60
2:B:88:LEU:CG	2:B:88:LEU:CD1	1.75	1.59
6:F:6:LEU:CD2	6:F:6:LEU:CG	1.75	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:29:LEU:CD2	8:H:29:LEU:CG	1.78	1.58
5:E:12:ILE:CD1	5:E:12:ILE:CG1	1.79	1.58
3:C:256:LYS:CG	3:C:256:LYS:CD	1.77	1.57
3:C:225:VAL:CG1	3:C:229:GLU:HG2	1.13	1.57
1:A:61:THR:CG2	1:A:61:THR:CB	1.79	1.54
1:A:92:MET:HG3	12:A:1002:OPC:CCB	1.37	1.50
3:C:25:CYS:SG	10:C:301:HEM:CBC	2.05	1.43
1:A:54:MET:CE	10:A:301:HEM:HBD1	1.48	1.40
3:C:233:ASN:ND2	3:C:234:ASN:N	1.69	1.39
3:C:225:VAL:HG11	3:C:229:GLU:CG	1.49	1.38
3:C:225:VAL:CG1	3:C:229:GLU:CG	2.03	1.37
3:C:233:ASN:ND2	3:C:234:ASN:H	1.19	1.36
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	1.46	1.34
1:A:92:MET:CG	12:A:1002:OPC:HCB1	1.58	1.30
1:A:92:MET:HE3	12:A:1002:OPC:CCB	1.62	1.28
1:A:96:MET:CA	1:A:96:MET:HE2	1.64	1.27
4:D:123:LYS:HE3	4:D:132:GLN:NE2	1.50	1.26
2:B:128:VAL:O	2:B:132:ILE:HD12	1.35	1.24
2:B:101:MET:O	2:B:104:VAL:HG23	1.36	1.24
3:C:119:LEU:HD23	3:C:124:TYR:CD1	1.72	1.24
2:B:95:LEU:CD2	2:B:99:LEU:HD12	1.66	1.23
3:C:199:ILE:O	3:C:200:GLN:HG3	1.06	1.21
6:F:7:TYR:O	6:F:11:LEU:HD12	1.35	1.21
7:G:31:ARG:HH11	7:G:31:ARG:CG	1.56	1.18
3:C:151:LEU:CD1	3:C:152:GLY:H	1.55	1.17
3:C:119:LEU:CD2	3:C:124:TYR:CD1	2.27	1.16
2:B:151:LEU:HD12	2:B:151:LEU:C	1.55	1.16
1:A:47:GLN:NE2	1:A:89:SER:HB3	1.60	1.14
3:C:285:ALA:O	3:C:286:GLU:OE1	1.64	1.14
7:G:31:ARG:NH1	7:G:31:ARG:HG2	1.47	1.13
3:C:107:LYS:CD	3:C:110:GLN:NE2	2.12	1.13
4:D:62:ASN:O	4:D:63:ASN:ND2	1.82	1.12
4:D:78:ARG:HG3	4:D:117:TRP:CD1	1.82	1.12
7:G:30:LYS:HE2	7:G:30:LYS:O	1.48	1.12
4:D:105:ASN:HB3	4:D:149:ALA:HB3	1.29	1.12
2:B:134:LEU:HD13	2:B:134:LEU:N	1.43	1.12
3:C:151:LEU:HD12	3:C:152:GLY:N	1.63	1.11
3:C:25:CYS:SG	10:C:301:HEM:CAC	2.39	1.11
3:C:262:ILE:HG23	8:H:14:VAL:HG13	1.27	1.11
3:C:60:GLN:HE22	3:C:157:ARG:HG3	1.01	1.11
1:A:7:TRP:CE2	1:A:11:ARG:NH2	2.19	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:23:VAL:CG1	8:H:28:GLY:H	1.64	1.10
3:C:194:LYS:O	3:C:195:TYR:C	1.92	1.10
3:C:107:LYS:HD3	3:C:110:GLN:NE2	1.64	1.10
3:C:176:ALA:HB3	3:C:199:ILE:HD12	1.11	1.10
1:A:24:LYS:NZ	13:A:1102:UMQ:O3	1.85	1.09
1:A:93:MET:HE2	1:A:128:THR:CG2	1.81	1.09
1:A:12:LEU:O	1:A:13:GLU:HB2	1.51	1.09
4:D:105:ASN:CB	4:D:149:ALA:HB3	1.81	1.09
1:A:100:HIS:HE1	10:A:302:HEM:C1A	1.70	1.08
3:C:199:ILE:O	3:C:200:GLN:CG	1.99	1.08
1:A:87:ARG:HG3	1:A:87:ARG:HH11	1.00	1.08
1:A:207:ARG:HH12	14:A:501:QNO:C3	1.65	1.08
6:F:29:ILE:O	6:F:29:ILE:CD1	1.99	1.08
2:B:95:LEU:HD21	2:B:99:LEU:HD12	1.24	1.08
3:C:22:CYS:HB2	10:C:301:HEM:CBB	1.83	1.08
4:D:152:HIS:CE1	4:D:165:TRP:CD1	2.41	1.08
1:A:7:TRP:NE1	1:A:11:ARG:NH2	2.03	1.07
2:B:158:GLY:O	2:B:159:LEU:HD23	1.54	1.07
3:C:266:MET:HE1	8:H:13:VAL:CG1	1.84	1.07
10:A:302:HEM:HBC2	10:A:302:HEM:HMC2	1.28	1.07
4:D:25:GLY:HA3	17:D:201:SQD:H341	1.29	1.06
10:A:301:HEM:CBB	10:A:301:HEM:HMB2	1.85	1.06
2:B:151:LEU:C	2:B:151:LEU:CD1	2.26	1.06
1:A:31:ASN:C	1:A:31:ASN:HD22	1.64	1.05
1:A:54:MET:HE3	10:A:301:HEM:HBD1	1.10	1.05
2:B:134:LEU:N	2:B:134:LEU:CD1	2.07	1.05
8:H:3:ILE:HG23	8:H:4:ASP:N	1.67	1.05
2:B:42:VAL:HG13	3:C:269:GLN:HG2	1.35	1.04
2:B:128:VAL:O	2:B:132:ILE:CD1	2.04	1.04
3:C:84:ILE:HD11	3:C:114:LEU:HD13	1.36	1.04
4:D:138:LYS:HA	4:D:147:SER:OG	1.55	1.04
1:A:100:HIS:HE1	10:A:302:HEM:NA	1.56	1.04
6:F:13:PHE:CE2	6:F:17:PHE:HE1	1.76	1.03
1:A:54:MET:HE1	10:A:301:HEM:HBD1	1.34	1.03
3:C:266:MET:HE1	8:H:13:VAL:HG12	1.34	1.02
1:A:92:MET:CE	12:A:1002:OPC:CCB	2.36	1.02
2:B:109:ILE:HG22	2:B:110:LEU:N	1.74	1.02
1:A:96:MET:HA	1:A:96:MET:CE	1.89	1.01
3:C:233:ASN:HD22	3:C:234:ASN:N	1.39	1.01
2:B:118:ASN:ND2	2:B:120:PHE:H	1.57	1.01
8:H:3:ILE:CG2	8:H:4:ASP:H	1.72	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:HD12	2:B:151:LEU:O	1.60	1.01
10:A:301:HEM:HBB2	10:A:301:HEM:HMB2	1.03	1.00
3:C:285:ALA:C	3:C:286:GLU:OE1	2.04	1.00
3:C:225:VAL:HG12	3:C:229:GLU:HG2	1.05	1.00
1:A:207:ARG:HH12	14:A:501:QNO:H3	1.25	1.00
2:B:32:TRP:O	2:B:34:ASN:HB2	1.60	1.00
5:E:22:ILE:HG22	5:E:22:ILE:O	1.59	1.00
2:B:101:MET:HE3	15:B:201:CLA:C9	1.92	0.99
3:C:60:GLN:HE22	3:C:157:ARG:CG	1.75	0.99
1:A:95:LEU:HB2	2:B:79:TRP:HH2	1.26	0.99
3:C:71:ASN:HB2	10:C:301:HEM:O2A	1.63	0.99
3:C:225:VAL:HG11	3:C:229:GLU:HG2	0.99	0.99
2:B:151:LEU:O	2:B:154:THR:HG22	1.63	0.99
1:A:175:VAL:CG1	1:A:176:GLY:N	2.26	0.99
6:F:20:TRP:O	6:F:24:VAL:HG23	1.63	0.99
1:A:66:TYR:CZ	2:B:65:PRO:HD3	1.97	0.98
1:A:92:MET:CE	12:A:1002:OPC:HCB2	1.91	0.98
3:C:151:LEU:HD12	3:C:152:GLY:H	0.84	0.98
1:A:183:TYR:O	1:A:186:ALA:HB3	1.63	0.98
4:D:134:ASP:HB2	4:D:137:GLY:O	1.64	0.98
8:H:23:VAL:HG13	8:H:28:GLY:H	1.25	0.98
6:F:25:LEU:HD23	6:F:29:ILE:HG22	1.43	0.97
6:F:29:ILE:O	6:F:29:ILE:HD13	1.63	0.97
1:A:54:MET:CE	10:A:301:HEM:CBD	2.42	0.97
1:A:92:MET:CG	12:A:1002:OPC:CCB	2.30	0.97
1:A:96:MET:CA	1:A:96:MET:CE	2.42	0.97
2:B:4:LEU:C	2:B:4:LEU:HD23	1.89	0.97
2:B:118:ASN:ND2	2:B:120:PHE:N	2.12	0.97
1:A:96:MET:HE2	1:A:96:MET:HA	1.00	0.97
12:A:1002:OPC:HBC2	12:A:1002:OPC:HAY1	1.47	0.97
3:C:173:THR:O	3:C:231:LEU:HG	1.63	0.97
3:C:60:GLN:NE2	3:C:157:ARG:HG3	1.80	0.96
3:C:225:VAL:HG11	3:C:229:GLU:HG3	1.44	0.96
4:D:129:HIS:HB2	16:D:200:FES:S1	2.06	0.96
10:A:301:HEM:CMB	10:A:301:HEM:CBB	2.38	0.96
6:F:29:ILE:O	6:F:29:ILE:HD12	1.66	0.96
1:A:20:ASP:OD1	13:A:1102:UMQ:O3	1.83	0.95
4:D:59:LYS:HG3	4:D:60:LEU:N	1.81	0.95
2:B:134:LEU:HD13	2:B:134:LEU:H	1.07	0.95
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.28	0.95
1:A:92:MET:HE3	12:A:1002:OPC:HCB2	0.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:LEU:HD22	3:C:252:PRO:HG3	1.48	0.95
3:C:58:LEU:HD12	3:C:59:GLN:N	1.81	0.95
1:A:186:ALA:O	1:A:191:LEU:HD12	1.66	0.95
6:F:4:GLU:O	6:F:6:LEU:N	1.99	0.95
5:E:10:VAL:O	5:E:13:ALA:CB	2.15	0.95
2:B:139:VAL:O	2:B:143:LEU:HD12	1.66	0.95
3:C:107:LYS:HD3	3:C:110:GLN:HE21	1.26	0.95
3:C:12:THR:HG23	3:C:14:ARG:H	1.28	0.94
4:D:109:THR:HG22	4:D:144:ALA:HB1	1.45	0.94
1:A:93:MET:HE2	1:A:128:THR:HG23	1.46	0.94
2:B:17:LYS:HE3	2:B:26:TYR:OH	1.65	0.94
3:C:70:LEU:HD23	3:C:70:LEU:H	1.31	0.94
1:A:92:MET:HG3	12:A:1002:OPC:HCB3	1.49	0.94
8:H:23:VAL:HG13	8:H:28:GLY:N	1.81	0.94
1:A:87:ARG:HH11	1:A:87:ARG:CG	1.81	0.93
1:A:111:LYS:O	1:A:113:PRO:HD2	1.68	0.93
3:C:71:ASN:OD1	3:C:120:PRO:HA	1.67	0.93
3:C:187:GLU:HG3	3:C:187:GLU:O	1.68	0.92
2:B:79:TRP:CD1	2:B:79:TRP:C	2.48	0.92
1:A:212:SER:HB3	10:A:302:HEM:O2D	1.69	0.92
3:C:144:PHE:CZ	3:C:251:ASP:HB2	2.05	0.92
5:E:10:VAL:O	5:E:13:ALA:HB3	1.70	0.92
1:A:39:ILE:HG22	1:A:96:MET:HG3	1.52	0.92
1:A:151:VAL:HG22	1:A:152:SER:N	1.84	0.92
8:H:3:ILE:CG2	8:H:4:ASP:N	2.29	0.92
1:A:161:VAL:HG23	1:A:162:GLY:H	1.33	0.91
1:A:7:TRP:NE1	1:A:11:ARG:HH21	1.62	0.91
6:F:27:LEU:HD11	8:H:27:ASN:HA	1.52	0.91
1:A:87:ARG:HG3	1:A:87:ARG:NH1	1.67	0.91
7:G:26:TYR:O	7:G:28:GLN:N	2.03	0.91
3:C:41:LEU:CD2	3:C:252:PRO:HG3	2.00	0.91
4:D:123:LYS:HE3	4:D:132:GLN:HE21	1.33	0.91
6:F:11:LEU:HB3	6:F:15:LEU:CD1	2.00	0.91
3:C:272:LEU:O	3:C:275:LYS:HB3	1.71	0.90
1:A:93:MET:HE2	1:A:128:THR:HG21	1.52	0.90
1:A:96:MET:HE2	1:A:96:MET:N	1.86	0.90
3:C:119:LEU:HD23	3:C:124:TYR:HD1	1.34	0.90
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.06	0.90
7:G:20:GLY:N	18:G:101:BCR:H363	1.87	0.90
2:B:124:PHE:O	2:B:126:ARG:N	2.06	0.89
5:E:10:VAL:O	5:E:14:LEU:HD12	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:PHE:HE2	6:F:17:PHE:CE1	1.91	0.89
2:B:109:ILE:O	2:B:112:PRO:CD	2.21	0.89
2:B:57:LEU:HD11	8:H:8:TRP:HA	1.54	0.88
4:D:169:ASP:O	4:D:171:ARG:N	2.05	0.88
1:A:106:LEU:HD21	2:B:133:PHE:CE1	2.08	0.88
2:B:74:GLU:O	2:B:74:GLU:HG3	1.72	0.88
1:A:215:LEU:HB2	7:G:28:GLN:OE1	1.73	0.88
1:A:156:GLU:HG2	1:A:163:VAL:HG22	1.53	0.88
1:A:96:MET:CE	1:A:96:MET:N	2.37	0.88
1:A:103:ARG:HH12	1:A:104:VAL:HG23	1.38	0.87
1:A:103:ARG:NH1	1:A:104:VAL:HA	1.89	0.87
1:A:103:ARG:O	1:A:107:THR:HG22	1.73	0.87
1:A:141:ASP:C	2:B:66:ALA:HB2	1.97	0.87
1:A:95:LEU:HB2	2:B:79:TRP:CH2	2.08	0.87
10:C:301:HEM:HHC	10:C:301:HEM:HBB2	1.55	0.87
1:A:103:ARG:HH12	1:A:104:VAL:CG2	1.87	0.87
2:B:61:MET:HB2	3:C:146:LYS:HG2	1.55	0.87
3:C:262:ILE:HG23	8:H:14:VAL:CG1	2.04	0.87
3:C:276:LYS:HE2	8:H:25:GLY:O	1.74	0.87
1:A:54:MET:HE1	10:A:301:HEM:CBD	2.01	0.86
7:G:23:TYR:CE2	7:G:27:GLN:NE2	2.44	0.86
1:A:207:ARG:NH1	14:A:501:QNO:H3	1.89	0.86
3:C:125:GLN:HE21	3:C:125:GLN:HA	1.40	0.86
10:A:302:HEM:HBC2	10:A:302:HEM:CMC	2.01	0.85
4:D:152:HIS:CE1	4:D:165:TRP:NE1	2.44	0.85
1:A:175:VAL:HG12	1:A:176:GLY:N	1.90	0.85
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.56	0.85
1:A:175:VAL:HG13	1:A:176:GLY:H	1.39	0.85
4:D:78:ARG:HG3	4:D:117:TRP:NE1	1.91	0.85
2:B:115:GLU:OE2	2:B:126:ARG:NH1	2.10	0.85
3:C:54:TYR:HE1	3:C:70:LEU:HD21	1.41	0.84
3:C:19:ARG:HG2	3:C:19:ARG:HH11	1.43	0.84
1:A:156:GLU:HG2	1:A:163:VAL:CG2	2.07	0.84
2:B:95:LEU:HD21	2:B:99:LEU:CD1	2.07	0.84
3:C:94:LEU:O	3:C:98:VAL:HG23	1.76	0.84
3:C:98:VAL:HG11	3:C:130:PRO:HD3	1.57	0.84
1:A:54:MET:HE3	10:A:301:HEM:CBD	2.03	0.84
1:A:24:LYS:NZ	13:A:1102:UMQ:HO31	1.75	0.84
3:C:66:SER:O	3:C:67:LYS:HB2	1.77	0.84
6:F:6:LEU:CD2	6:F:6:LEU:HG	2.04	0.84
6:F:7:TYR:O	6:F:11:LEU:CD1	2.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:HG23	8:H:4:ASP:H	1.27	0.84
1:A:207:ARG:HH12	14:A:501:QNO:C4	1.90	0.83
3:C:194:LYS:O	3:C:195:TYR:O	1.96	0.83
2:B:57:LEU:CD1	8:H:8:TRP:CD2	2.60	0.83
4:D:55:THR:O	4:D:57:LYS:HE3	1.79	0.83
4:D:118:ASN:ND2	4:D:121:GLU:HB2	1.92	0.83
2:B:118:ASN:HD21	2:B:120:PHE:H	1.24	0.83
3:C:70:LEU:HD23	3:C:70:LEU:N	1.91	0.83
3:C:184:ALA:O	3:C:185:LYS:HB3	1.79	0.83
4:D:25:GLY:CA	17:D:201:SQD:H341	2.07	0.83
2:B:113:PHE:O	2:B:115:GLU:N	2.13	0.82
3:C:47:LYS:NZ	3:C:97:GLU:OE2	2.12	0.82
5:E:9:ILE:O	5:E:13:ALA:HB2	1.79	0.82
4:D:109:THR:CG2	4:D:144:ALA:HB1	2.08	0.82
2:B:95:LEU:HD23	2:B:99:LEU:HD12	1.59	0.82
3:C:81:GLY:CA	3:C:142:ILE:HD11	2.08	0.82
2:B:88:LEU:CD1	2:B:101:MET:SD	2.68	0.82
3:C:19:ARG:O	3:C:20:ILE:HB	1.78	0.82
7:G:26:TYR:C	7:G:28:GLN:H	1.85	0.82
1:A:110:PHE:CD1	2:B:112:PRO:HB3	2.14	0.82
3:C:211:ILE:O	3:C:211:ILE:HG13	1.80	0.81
4:D:131:SER:HA	4:D:142:GLY:HA3	1.60	0.81
1:A:211:ILE:HD12	1:A:212:SER:H	1.45	0.81
1:A:104:VAL:O	1:A:107:THR:HG22	1.80	0.81
3:C:21:VAL:O	3:C:24:ASN:HB2	1.80	0.81
3:C:259:ILE:HD12	8:H:6:LEU:HD13	1.60	0.81
2:B:109:ILE:O	2:B:112:PRO:HD3	1.80	0.81
1:A:145:TYR:O	1:A:145:TYR:CD1	2.33	0.81
3:C:107:LYS:CD	3:C:110:GLN:HE22	1.91	0.81
6:F:13:PHE:CE2	6:F:17:PHE:CE1	2.64	0.81
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.61	0.81
4:D:59:LYS:O	4:D:61:GLY:N	2.13	0.81
1:A:161:VAL:HG23	1:A:162:GLY:N	1.96	0.81
3:C:54:TYR:CE1	3:C:70:LEU:HD21	2.16	0.81
3:C:2:PRO:HD3	10:C:301:HEM:CHB	2.11	0.80
2:B:101:MET:HE3	15:B:201:CLA:H93	1.62	0.80
3:C:281:LYS:HG2	3:C:282:VAL:N	1.96	0.80
3:C:22:CYS:HB2	10:C:301:HEM:CAB	2.10	0.80
1:A:31:ASN:C	1:A:31:ASN:ND2	2.38	0.80
1:A:100:HIS:CE1	10:A:302:HEM:C1A	2.63	0.80
2:B:57:LEU:HD12	8:H:8:TRP:CD2	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:CG2	1:A:152:SER:N	2.44	0.80
3:C:270:LEU:HG	8:H:21:MET:HE1	1.63	0.80
4:D:116:PRO:HD2	4:D:125:LYS:O	1.81	0.80
6:F:4:GLU:O	6:F:5:MET:C	2.25	0.80
2:B:75:ILE:O	2:B:75:ILE:HG12	1.82	0.80
3:C:159:GLN:NE2	3:C:169:ASN:HB3	1.96	0.80
4:D:78:ARG:CG	4:D:117:TRP:CD1	2.64	0.80
7:G:29:TYR:CG	7:G:29:TYR:O	2.34	0.80
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.17	0.80
6:F:11:LEU:O	6:F:15:LEU:HD12	1.82	0.80
3:C:159:GLN:HE21	3:C:169:ASN:HB3	1.46	0.79
4:D:132:GLN:C	4:D:133:TYR:CD1	2.59	0.79
3:C:196:GLN:O	3:C:197:VAL:CG2	2.31	0.79
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.16	0.79
6:F:25:LEU:HD23	6:F:29:ILE:CG2	2.12	0.79
1:A:134:THR:HG22	1:A:183:TYR:CD2	2.17	0.79
2:B:53:ALA:HA	3:C:258:MET:HE2	1.63	0.79
2:B:79:TRP:CD1	2:B:80:TYR:N	2.51	0.79
2:B:11:ASP:OD1	2:B:13:LYS:HB2	1.82	0.78
3:C:107:LYS:HD2	3:C:110:GLN:HE22	1.46	0.78
1:A:39:ILE:CG2	1:A:96:MET:HG3	2.13	0.78
1:A:103:ARG:HD2	1:A:107:THR:HG21	1.63	0.78
12:A:1002:OPC:HAS1	5:E:4:GLY:HA3	1.66	0.78
1:A:211:ILE:CD1	1:A:212:SER:H	1.96	0.78
4:D:59:LYS:C	4:D:61:GLY:H	1.92	0.78
2:B:88:LEU:HD12	2:B:101:MET:SD	2.23	0.78
2:B:113:PHE:O	2:B:114:ILE:C	2.27	0.78
1:A:81:LEU:C	1:A:81:LEU:HD23	2.09	0.78
3:C:19:ARG:O	3:C:242:GLN:OE1	2.02	0.78
2:B:57:LEU:HD12	8:H:8:TRP:CE3	2.19	0.77
3:C:58:LEU:CD1	3:C:59:GLN:N	2.47	0.77
3:C:261:PHE:O	3:C:265:VAL:HG23	1.84	0.77
1:A:92:MET:HG3	12:A:1002:OPC:HCB1	0.77	0.77
3:C:180:ILE:HG13	3:C:198:SER:O	1.84	0.77
3:C:233:ASN:ND2	3:C:233:ASN:C	2.42	0.77
6:F:13:PHE:HE2	6:F:17:PHE:HE1	1.21	0.77
3:C:44:THR:HG22	3:C:45:VAL:N	2.00	0.77
7:G:15:PHE:O	7:G:17:THR:N	2.18	0.77
7:G:34:GLU:O	7:G:35:LEU:HD12	1.83	0.77
2:B:10:SER:O	2:B:12:PRO:HD3	1.83	0.77
3:C:125:GLN:HA	3:C:125:GLN:NE2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:29:ILE:HD12	6:F:29:ILE:C	2.09	0.77
1:A:207:ARG:NH1	14:A:501:QNO:C3	2.46	0.77
2:B:142:TRP:CZ2	2:B:155:LEU:O	2.37	0.77
4:D:140:ILE:O	4:D:140:ILE:HG13	1.83	0.77
1:A:103:ARG:O	1:A:107:THR:CG2	2.33	0.76
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.49	0.76
2:B:88:LEU:CD1	2:B:88:LEU:HG	2.10	0.76
1:A:7:TRP:CD1	1:A:11:ARG:NH2	2.52	0.76
2:B:33:PRO:HG2	2:B:34:ASN:HD22	1.51	0.76
5:E:16:PHE:CD2	6:F:22:LEU:HD21	2.21	0.76
1:A:161:VAL:O	1:A:163:VAL:N	2.17	0.76
3:C:44:THR:HG22	3:C:45:VAL:H	1.48	0.76
2:B:96:LEU:O	2:B:100:LEU:HB2	1.85	0.76
4:D:77:ASP:OD2	4:D:92:VAL:O	2.03	0.76
2:B:61:MET:HG2	2:B:62:VAL:N	1.99	0.76
4:D:118:ASN:HD22	4:D:121:GLU:HB2	1.47	0.76
3:C:262:ILE:CG2	8:H:14:VAL:HG13	2.14	0.75
4:D:134:ASP:HB3	4:D:136:THR:H	1.51	0.75
1:A:175:VAL:HG13	1:A:176:GLY:N	1.96	0.75
2:B:149:PHE:HB3	2:B:150:PRO:CD	2.17	0.75
7:G:30:LYS:O	7:G:30:LYS:CE	2.32	0.75
12:A:1002:OPC:HBU2	8:H:15:PHE:CD1	2.21	0.75
3:C:173:THR:O	3:C:231:LEU:CG	2.33	0.75
4:D:89:THR:HG22	4:D:105:ASN:HA	1.68	0.75
3:C:176:ALA:HB3	3:C:199:ILE:CD1	2.05	0.75
3:C:146:LYS:HB2	3:C:248:VAL:HG22	1.68	0.75
8:H:23:VAL:HG13	8:H:28:GLY:CA	2.16	0.75
2:B:142:TRP:HZ2	2:B:155:LEU:O	1.70	0.74
4:D:152:HIS:ND1	4:D:165:TRP:NE1	2.33	0.74
5:E:16:PHE:HD2	6:F:22:LEU:HD21	1.52	0.74
1:A:25:TYR:CD2	2:B:30:PRO:HA	2.22	0.74
3:C:188:ASP:O	3:C:190:TYR:N	2.19	0.74
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.49	0.74
10:A:301:HEM:HBB2	10:A:301:HEM:HMB3	1.66	0.74
3:C:225:VAL:HG12	3:C:229:GLU:CG	1.88	0.74
3:C:288:ASN:C	3:C:288:ASN:HD22	1.95	0.74
6:F:29:ILE:CD1	6:F:29:ILE:C	2.60	0.74
6:F:24:VAL:O	6:F:27:LEU:HB2	1.87	0.74
2:B:82:TYR:N	2:B:83:PRO:HD2	2.02	0.74
2:B:109:ILE:O	2:B:112:PRO:HD2	1.87	0.74
3:C:107:LYS:HD2	3:C:110:GLN:NE2	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:VAL:O	5:E:10:VAL:HG23	1.86	0.74
3:C:71:ASN:CB	10:C:301:HEM:O2A	2.36	0.74
2:B:113:PHE:O	2:B:116:ASN:HB2	1.87	0.74
4:D:123:LYS:HE3	4:D:132:GLN:HE22	1.45	0.74
1:A:36:LEU:HB3	1:A:100:HIS:HB2	1.70	0.73
3:C:15:GLU:HB2	3:C:19:ARG:HB3	1.68	0.73
4:D:132:GLN:C	4:D:133:TYR:HD1	1.95	0.73
1:A:163:VAL:O	1:A:166:SER:N	2.21	0.73
13:A:1102:UMQ:H3'1	13:A:1102:UMQ:O5	1.88	0.73
1:A:80:TRP:O	1:A:84:SER:HB2	1.87	0.73
3:C:70:LEU:N	3:C:70:LEU:CD2	2.52	0.73
1:A:111:LYS:HE2	2:B:115:GLU:O	1.87	0.73
3:C:79:PRO:HD2	3:C:82:PHE:CD1	2.24	0.73
1:A:145:TYR:CD1	1:A:145:TYR:C	2.67	0.73
1:A:1:MET:HA	1:A:1:MET:CE	2.19	0.73
2:B:158:GLY:O	2:B:159:LEU:CD2	2.36	0.73
3:C:199:ILE:C	3:C:200:GLN:HG3	2.10	0.73
5:E:2:ILE:HD12	5:E:2:ILE:H	1.53	0.73
1:A:54:MET:HE1	10:A:301:HEM:CGD	2.19	0.73
7:G:31:ARG:HH11	7:G:31:ARG:HG2	0.66	0.73
2:B:118:ASN:HD21	2:B:120:PHE:N	1.79	0.72
4:D:81:VAL:O	4:D:88:PRO:HA	1.88	0.72
1:A:111:LYS:O	1:A:113:PRO:CD	2.38	0.72
4:D:105:ASN:HB3	4:D:149:ALA:CB	2.15	0.72
15:B:201:CLA:HED3	15:B:201:CLA:HBA1	1.70	0.72
6:F:11:LEU:HD23	6:F:15:LEU:HD11	1.71	0.72
1:A:1:MET:HA	1:A:1:MET:HE2	1.71	0.72
3:C:12:THR:HG23	3:C:14:ARG:N	2.04	0.72
2:B:151:LEU:O	2:B:154:THR:CG2	2.38	0.72
1:A:31:ASN:H	1:A:34:TYR:HD2	1.36	0.72
3:C:279:VAL:O	3:C:283:GLN:HB2	1.90	0.72
4:D:25:GLY:HA3	17:D:201:SQD:C34	2.13	0.72
4:D:115:VAL:HG13	4:D:125:LYS:O	1.88	0.72
3:C:193:VAL:HG12	3:C:194:LYS:H	1.54	0.71
2:B:101:MET:O	2:B:104:VAL:CG2	2.29	0.71
7:G:15:PHE:O	7:G:16:ALA:C	2.32	0.71
1:A:61:THR:CG2	1:A:61:THR:HB	2.09	0.71
5:E:12:ILE:CD1	5:E:12:ILE:CB	2.68	0.71
3:C:94:LEU:HD22	3:C:98:VAL:CG2	2.20	0.71
5:E:12:ILE:HG21	5:E:12:ILE:HD13	1.72	0.71
1:A:7:TRP:CD1	1:A:11:ARG:HH21	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:LYS:HE2	4:D:20:ASN:OD1	1.91	0.71
3:C:9:TYR:N	3:C:9:TYR:CD1	2.59	0.71
5:E:14:LEU:O	5:E:18:ILE:HG13	1.91	0.71
1:A:103:ARG:NH1	1:A:104:VAL:HG23	2.05	0.71
4:D:15:ARG:CD	5:E:31:LEU:HD21	2.21	0.71
6:F:25:LEU:O	6:F:26:LEU:C	2.33	0.71
8:H:9:VAL:HA	8:H:12:LEU:HD12	1.73	0.70
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.73	0.70
4:D:152:HIS:ND1	4:D:165:TRP:CD1	2.58	0.70
2:B:126:ARG:O	2:B:129:ALA:HB3	1.91	0.70
2:B:151:LEU:CD1	2:B:154:THR:HG21	2.21	0.70
3:C:266:MET:HE1	8:H:13:VAL:HG11	1.73	0.70
8:H:23:VAL:O	8:H:24:TRP:C	2.32	0.70
1:A:104:VAL:HG12	1:A:105:TYR:N	2.05	0.70
1:A:29:HIS:CG	1:A:214:PRO:HA	2.27	0.70
3:C:98:VAL:CG1	3:C:130:PRO:HD3	2.21	0.70
3:C:119:LEU:CD2	3:C:124:TYR:CG	2.75	0.70
2:B:151:LEU:CD1	2:B:154:THR:CG2	2.69	0.70
3:C:151:LEU:CD1	3:C:152:GLY:N	2.38	0.70
4:D:59:LYS:HG3	4:D:60:LEU:H	1.54	0.70
4:D:138:LYS:O	4:D:139:VAL:O	2.07	0.70
1:A:207:ARG:NH1	14:A:501:QNO:O41	2.24	0.70
2:B:37:LEU:O	2:B:37:LEU:HG	1.90	0.70
3:C:81:GLY:HA2	3:C:142:ILE:HD11	1.72	0.70
1:A:9:GLN:NE2	1:A:13:GLU:HA	2.07	0.69
1:A:43:CYS:HB3	1:A:93:MET:HB2	1.72	0.69
3:C:25:CYS:SG	10:C:301:HEM:HBC2	2.28	0.69
3:C:128:VAL:CG1	3:C:129:PHE:N	2.55	0.69
3:C:176:ALA:CB	3:C:199:ILE:HD12	2.06	0.69
5:E:10:VAL:C	5:E:13:ALA:CB	2.65	0.69
1:A:44:PHE:HB2	1:A:93:MET:SD	2.33	0.69
3:C:54:TYR:HE1	3:C:70:LEU:CD2	2.03	0.69
7:G:17:THR:O	7:G:21:LEU:HB2	1.93	0.69
2:B:88:LEU:CD1	2:B:88:LEU:CB	2.70	0.69
1:A:72:ILE:HA	1:A:76:VAL:HG23	1.74	0.69
3:C:173:THR:O	3:C:231:LEU:CD2	2.40	0.69
4:D:75:ALA:O	4:D:76:GLY:C	2.35	0.69
1:A:3:ASN:HB3	1:A:6:ASP:OD2	1.93	0.69
1:A:12:LEU:O	1:A:13:GLU:CB	2.32	0.69
3:C:273:ILE:CD1	8:H:25:GLY:HA3	2.23	0.69
5:E:2:ILE:O	5:E:5:ALA:HB3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ALA:HB2	3:C:132:LEU:HB2	1.74	0.69
3:C:4:TRP:CD2	3:C:162:PRO:HG3	2.28	0.69
3:C:186:GLU:O	3:C:187:GLU:HB3	1.92	0.69
3:C:263:CYS:O	3:C:264:LEU:C	2.34	0.69
12:B:1001:OPC:HBG2	12:B:1001:OPC:OAI	1.92	0.68
3:C:273:ILE:CD1	8:H:25:GLY:CA	2.71	0.68
5:E:22:ILE:O	5:E:22:ILE:CG2	2.35	0.68
1:A:145:TYR:O	1:A:145:TYR:CG	2.43	0.68
1:A:39:ILE:HD11	18:G:101:BCR:C31	2.24	0.68
1:A:61:THR:HA	1:A:177:GLN:OE1	1.93	0.68
1:A:30:VAL:HG22	1:A:34:TYR:CG	2.28	0.68
12:A:1002:OPC:HBC2	12:A:1002:OPC:CAY	2.23	0.68
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.28	0.68
8:H:24:TRP:O	8:H:24:TRP:CD1	2.47	0.68
1:A:41:LEU:HD23	11:A:303:HEC:HBC2	1.74	0.68
3:C:1:TYR:HA	10:C:301:HEM:NA	2.08	0.68
3:C:2:PRO:HD3	10:C:301:HEM:C1B	2.29	0.68
3:C:40:VAL:HG11	3:C:46:PHE:CD2	2.28	0.68
3:C:251:ASP:OD2	3:C:252:PRO:HD2	1.93	0.68
5:E:23:ILE:O	5:E:27:LYS:N	2.25	0.68
2:B:151:LEU:HD12	2:B:154:THR:HG22	1.74	0.68
4:D:109:THR:HG21	4:D:146:LEU:O	1.95	0.67
5:E:10:VAL:C	5:E:13:ALA:HB2	2.19	0.67
12:A:1002:OPC:HAY1	12:A:1002:OPC:CBC	2.21	0.67
2:B:110:LEU:O	2:B:111:VAL:C	2.32	0.67
3:C:82:PHE:HZ	3:C:249:LEU:HD23	1.60	0.67
4:D:153:ALA:O	4:D:154:THR:O	2.12	0.67
2:B:99:LEU:O	2:B:103:SER:OG	2.12	0.67
4:D:118:ASN:HD22	4:D:121:GLU:CB	2.08	0.67
2:B:118:ASN:HD22	2:B:119:LYS:N	1.93	0.67
2:B:124:PHE:CZ	7:G:26:TYR:HD1	2.13	0.67
1:A:95:LEU:C	1:A:95:LEU:HD23	2.20	0.67
8:H:16:THR:C	8:H:18:SER:H	1.99	0.67
2:B:129:ALA:O	2:B:131:THR:N	2.27	0.66
3:C:60:GLN:OE1	3:C:70:LEU:CB	2.43	0.66
3:C:46:PHE:CZ	3:C:131:VAL:HG22	2.30	0.66
6:F:11:LEU:C	6:F:15:LEU:HD12	2.20	0.66
1:A:7:TRP:O	1:A:11:ARG:HG3	1.95	0.66
1:A:32:ILE:HG23	1:A:33:PHE:N	2.08	0.66
12:A:1002:OPC:HAW	5:E:8:TYR:HD2	1.61	0.66
8:H:5:VAL:O	8:H:6:LEU:C	2.37	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:82:GLN:O	4:D:82:GLN:CG	2.38	0.66
2:B:45:MET:HE1	4:D:27:VAL:HG22	1.77	0.66
3:C:1:TYR:HA	10:C:301:HEM:C4A	2.31	0.66
3:C:4:TRP:CG	3:C:162:PRO:HG3	2.31	0.66
3:C:180:ILE:HG12	3:C:181:THR:N	2.11	0.66
6:F:31:GLY:O	6:F:32:ALA:HB2	1.96	0.66
3:C:174:ALA:HB3	3:C:228:GLY:N	2.10	0.66
3:C:270:LEU:HA	8:H:21:MET:HE2	1.76	0.66
3:C:151:LEU:CG	3:C:152:GLY:N	2.59	0.66
3:C:52:ILE:O	3:C:52:ILE:HG22	1.96	0.66
4:D:59:LYS:C	4:D:61:GLY:N	2.50	0.66
8:H:3:ILE:HG22	8:H:4:ASP:H	1.57	0.66
1:A:96:MET:N	1:A:96:MET:HE3	2.10	0.66
2:B:126:ARG:N	2:B:127:PRO:HD3	2.10	0.65
3:C:279:VAL:HA	3:C:282:VAL:HG23	1.78	0.65
1:A:20:ASP:OD1	1:A:24:LYS:NZ	2.28	0.65
1:A:68:SER:O	1:A:72:ILE:HG13	1.94	0.65
2:B:123:PRO:CD	7:G:25:ALA:HB1	2.25	0.65
1:A:62:VAL:HG22	1:A:177:GLN:OE1	1.96	0.65
3:C:175:SER:HB2	3:C:209:ASP:CG	2.21	0.65
7:G:31:ARG:CG	7:G:31:ARG:NH1	2.27	0.65
1:A:47:GLN:NE2	1:A:89:SER:CB	2.51	0.65
3:C:196:GLN:O	3:C:197:VAL:HG23	1.96	0.65
4:D:34:ALA:O	4:D:37:PRO:HD2	1.97	0.65
4:D:130:GLY:O	4:D:141:ARG:NH2	2.28	0.65
1:A:44:PHE:O	1:A:47:GLN:HB2	1.96	0.65
2:B:132:ILE:HD12	2:B:132:ILE:H	1.62	0.65
10:A:302:HEM:CHA	10:A:302:HEM:HBA1	2.27	0.65
12:A:1002:OPC:HBN1	7:G:5:LEU:CD1	2.27	0.65
3:C:233:ASN:HD22	3:C:234:ASN:H	0.68	0.65
7:G:1:MET:HG2	7:G:2:VAL:N	2.11	0.65
3:C:92:GLU:O	3:C:95:LYS:N	2.29	0.65
5:E:23:ILE:O	5:E:26:ILE:N	2.30	0.65
3:C:257:TRP:O	3:C:260:ALA:HB3	1.97	0.65
1:A:95:LEU:C	1:A:95:LEU:CD2	2.69	0.64
3:C:277:LYS:HE2	8:H:24:TRP:NE1	2.13	0.64
4:D:138:LYS:CA	4:D:147:SER:OG	2.40	0.64
12:A:1002:OPC:CAY	12:A:1002:OPC:CBC	2.74	0.64
3:C:151:LEU:CG	3:C:152:GLY:H	2.09	0.64
3:C:229:GLU:OE2	3:C:230:ALA:N	2.29	0.64
6:F:4:GLU:C	6:F:6:LEU:N	2.54	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:OH	2:B:65:PRO:HD3	1.96	0.64
3:C:270:LEU:HG	8:H:21:MET:CE	2.26	0.64
10:C:301:HEM:HBC2	10:C:301:HEM:CMC	2.27	0.64
1:A:95:LEU:HD23	1:A:95:LEU:O	1.98	0.64
2:B:151:LEU:HD11	2:B:154:THR:HG21	1.79	0.64
4:D:59:LYS:CG	4:D:60:LEU:N	2.58	0.64
1:A:21:VAL:HA	1:A:207:ARG:HH21	1.63	0.64
1:A:32:ILE:CG2	1:A:33:PHE:N	2.60	0.64
2:B:118:ASN:HD22	2:B:120:PHE:N	1.95	0.64
5:E:14:LEU:O	5:E:18:ILE:CG1	2.46	0.64
6:F:25:LEU:CD2	6:F:29:ILE:HG22	2.25	0.64
1:A:103:ARG:HH22	10:A:302:HEM:CBD	2.10	0.64
1:A:211:ILE:HG12	11:A:303:HEC:HAA1	1.79	0.64
2:B:84:VAL:HG13	2:B:101:MET:CG	2.28	0.64
3:C:151:LEU:HD11	3:C:153:ALA:HB2	1.80	0.64
1:A:29:HIS:CD2	1:A:213:GLY:O	2.51	0.64
1:A:72:ILE:HA	1:A:76:VAL:CG2	2.28	0.64
1:A:212:SER:CB	10:A:302:HEM:O2D	2.43	0.64
10:A:302:HEM:HBA1	10:A:302:HEM:HHA	1.80	0.64
1:A:211:ILE:HG23	1:A:212:SER:O	1.98	0.64
3:C:268:ALA:O	3:C:269:GLN:C	2.41	0.64
4:D:115:VAL:HG22	4:D:126:CYS:HA	1.80	0.64
4:D:177:TRP:NE1	4:D:178:TRP:CE3	2.66	0.64
2:B:139:VAL:HG12	2:B:143:LEU:HD11	1.78	0.63
4:D:25:GLY:HA2	17:D:201:SQD:C33	2.29	0.63
2:B:122:ASN:OD1	2:B:123:PRO:CD	2.46	0.63
6:F:11:LEU:HB3	6:F:15:LEU:HD12	1.81	0.63
1:A:14:ILE:HD13	1:A:14:ILE:N	2.13	0.63
1:A:212:SER:HB3	10:A:302:HEM:CGD	2.28	0.63
4:D:127:PRO:O	4:D:129:HIS:N	2.32	0.63
1:A:103:ARG:CA	7:G:21:LEU:HD21	2.27	0.63
1:A:111:LYS:HZ1	2:B:126:ARG:HD3	1.63	0.63
3:C:134:PRO:HB3	3:C:142:ILE:HD12	1.80	0.63
4:D:15:ARG:HD2	5:E:31:LEU:HD21	1.80	0.63
1:A:36:LEU:HD23	1:A:99:LEU:HB3	1.81	0.63
4:D:105:ASN:HB2	4:D:149:ALA:HB3	1.77	0.63
3:C:119:LEU:HD21	3:C:124:TYR:CD1	2.32	0.63
3:C:223:GLN:HB3	3:C:225:VAL:HG23	1.80	0.63
5:E:24:PHE:O	5:E:27:LYS:N	2.32	0.63
2:B:118:ASN:HD21	2:B:120:PHE:HB2	1.64	0.63
3:C:175:SER:HB2	3:C:209:ASP:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ALA:CA	3:C:258:MET:HE2	2.29	0.62
3:C:196:GLN:O	3:C:197:VAL:HG22	1.98	0.62
4:D:99:ILE:HG13	4:D:100:ARG:H	1.63	0.62
1:A:93:MET:CE	1:A:128:THR:HG23	2.27	0.62
5:E:12:ILE:CD1	5:E:12:ILE:HG21	2.28	0.62
1:A:211:ILE:HB	11:A:303:HEC:HBA2	1.80	0.62
2:B:87:ILE:HG12	2:B:143:LEU:HD22	1.82	0.62
3:C:25:CYS:SG	10:C:301:HEM:HBC1	2.29	0.62
3:C:158:GLY:H	10:C:301:HEM:CAD	2.11	0.62
1:A:35:CYS:O	1:A:39:ILE:HD12	2.00	0.62
3:C:84:ILE:CD1	3:C:114:LEU:HD13	2.20	0.62
3:C:270:LEU:HA	8:H:21:MET:CE	2.30	0.62
3:C:279:VAL:HA	3:C:282:VAL:CG2	2.30	0.62
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.35	0.62
2:B:79:TRP:CG	2:B:80:TYR:N	2.68	0.62
3:C:20:ILE:HG22	3:C:20:ILE:O	2.00	0.62
3:C:81:GLY:HA3	3:C:142:ILE:HD11	1.80	0.62
3:C:44:THR:O	3:C:132:LEU:HD12	1.99	0.62
3:C:278:GLN:O	3:C:278:GLN:HG2	2.00	0.62
12:A:1002:OPC:HAW	5:E:8:TYR:CD2	2.34	0.61
2:B:4:LEU:HD23	2:B:4:LEU:O	1.99	0.61
2:B:106:LEU:O	2:B:109:ILE:HB	2.00	0.61
10:A:301:HEM:HMC1	10:A:301:HEM:HBC2	1.80	0.61
3:C:78:LEU:HD12	3:C:78:LEU:H	1.65	0.61
1:A:34:TYR:CE1	1:A:103:ARG:NE	2.67	0.61
1:A:39:ILE:CD1	18:G:101:BCR:C31	2.77	0.61
2:B:95:LEU:CD2	2:B:99:LEU:CD1	2.61	0.61
2:B:113:PHE:O	2:B:116:ASN:N	2.33	0.61
3:C:187:GLU:O	3:C:187:GLU:CG	2.45	0.61
7:G:26:TYR:C	7:G:28:GLN:N	2.48	0.61
3:C:84:ILE:HD12	3:C:103:PHE:CD1	2.36	0.61
3:C:233:ASN:CG	3:C:234:ASN:N	2.55	0.61
3:C:237:VAL:CG2	3:C:237:VAL:O	2.48	0.61
2:B:118:ASN:HD21	2:B:120:PHE:CB	2.14	0.61
3:C:52:ILE:HG12	3:C:153:ALA:HB1	1.82	0.61
3:C:248:VAL:HG12	3:C:248:VAL:O	2.01	0.61
3:C:288:ASN:C	3:C:288:ASN:ND2	2.58	0.61
1:A:121:GLY:HA3	10:A:302:HEM:C3C	2.36	0.61
15:B:201:CLA:HBB1	12:B:1001:OPC:HBP1	1.83	0.61
1:A:7:TRP:NE1	1:A:11:ARG:HH22	1.94	0.61
1:A:19:ASP:O	1:A:20:ASP:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HD11	18:G:101:BCR:H313	1.80	0.61
2:B:74:GLU:C	2:B:75:ILE:HG22	2.25	0.61
3:C:17:THR:OG1	3:C:18:GLY:N	2.34	0.61
2:B:37:LEU:HD21	2:B:38:TYR:CZ	2.36	0.61
5:E:28:SER:O	5:E:29:ILE:HG12	2.01	0.60
1:A:111:LYS:NZ	2:B:120:PHE:O	2.33	0.60
4:D:127:PRO:O	4:D:128:CYS:C	2.42	0.60
2:B:124:PHE:C	2:B:126:ARG:H	2.08	0.60
3:C:185:LYS:O	3:C:186:GLU:O	2.20	0.60
8:H:8:TRP:O	8:H:9:VAL:C	2.45	0.60
1:A:92:MET:CE	12:A:1002:OPC:HCB3	2.28	0.60
1:A:186:ALA:C	1:A:191:LEU:HD12	2.27	0.60
3:C:191:GLY:O	3:C:192:ASN:O	2.19	0.60
5:E:22:ILE:HA	5:E:25:ALA:HB3	1.84	0.60
2:B:89:ARG:HG3	2:B:90:SER:N	2.15	0.60
2:B:150:PRO:O	2:B:151:LEU:O	2.20	0.60
3:C:90:ILE:HG22	3:C:91:PRO:O	2.01	0.60
4:D:59:LYS:CG	4:D:60:LEU:H	2.14	0.60
1:A:62:VAL:HG12	1:A:140:TRP:NE1	2.17	0.60
1:A:92:MET:CB	12:A:1002:OPC:HCB1	2.28	0.60
2:B:82:TYR:O	2:B:85:PHE:HB3	2.01	0.60
3:C:20:ILE:HD12	3:C:152:GLY:HA3	1.83	0.60
3:C:174:ALA:HB2	3:C:231:LEU:HD23	1.83	0.60
2:B:57:LEU:HD11	8:H:8:TRP:CA	2.30	0.60
2:B:96:LEU:HD13	2:B:100:LEU:HD12	1.82	0.60
3:C:71:ASN:OD1	3:C:120:PRO:CA	2.47	0.60
3:C:78:LEU:HB3	3:C:79:PRO:HD3	1.84	0.60
5:E:26:ILE:CG2	5:E:31:LEU:HB3	2.31	0.60
8:H:23:VAL:CG1	8:H:28:GLY:N	2.43	0.60
1:A:103:ARG:NH1	1:A:104:VAL:CG2	2.63	0.59
1:A:142:GLN:OE1	1:A:142:GLN:HA	2.02	0.59
2:B:25:ASN:HD22	2:B:25:ASN:C	2.09	0.59
3:C:71:ASN:CG	3:C:120:PRO:HA	2.27	0.59
4:D:90:TYR:N	4:D:104:ILE:O	2.35	0.59
5:E:8:TYR:OH	5:E:12:ILE:HD11	2.00	0.59
5:E:22:ILE:CG2	5:E:26:ILE:HG12	2.32	0.59
2:B:159:LEU:O	2:B:160:PHE:HB3	2.02	0.59
3:C:98:VAL:HG22	3:C:128:VAL:HG11	1.84	0.59
4:D:78:ARG:HD3	4:D:92:VAL:CG2	2.32	0.59
7:G:6:LEU:O	7:G:9:LEU:CB	2.50	0.59
1:A:47:GLN:HE21	1:A:89:SER:HB3	1.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:277:LYS:HE3	6:F:30:GLN:OE1	2.02	0.59
2:B:71:THR:CG2	2:B:72:PRO:HD2	2.33	0.59
3:C:60:GLN:OE1	3:C:70:LEU:HB3	2.02	0.59
3:C:273:ILE:HG13	8:H:21:MET:HG3	1.83	0.59
4:D:110:HIS:CD2	4:D:143:PRO:HB2	2.37	0.59
8:H:23:VAL:O	8:H:25:GLY:N	2.36	0.59
2:B:141:ILE:O	2:B:145:ILE:HG13	2.02	0.59
2:B:159:LEU:O	2:B:160:PHE:CD2	2.55	0.59
3:C:22:CYS:O	3:C:23:ALA:C	2.45	0.59
3:C:22:CYS:SG	3:C:23:ALA:N	2.75	0.59
3:C:68:VAL:HG13	3:C:68:VAL:O	2.03	0.59
3:C:200:GLN:HG2	3:C:206:THR:HA	1.83	0.59
8:H:29:LEU:CD2	8:H:29:LEU:CD1	2.79	0.59
1:A:36:LEU:CB	1:A:100:HIS:HB2	2.32	0.59
1:A:79:GLY:O	1:A:83:ARG:N	2.30	0.59
1:A:103:ARG:HH11	1:A:104:VAL:CA	2.16	0.59
3:C:232:THR:O	3:C:233:ASN:HB3	2.03	0.59
4:D:123:LYS:CE	4:D:132:GLN:HE21	2.11	0.59
1:A:81:LEU:C	1:A:81:LEU:CD2	2.75	0.59
1:A:111:LYS:CE	2:B:115:GLU:O	2.51	0.59
2:B:57:LEU:CD1	8:H:8:TRP:CE2	2.85	0.59
4:D:127:PRO:C	4:D:129:HIS:N	2.59	0.59
6:F:20:TRP:CD1	6:F:20:TRP:C	2.80	0.58
7:G:22:PHE:O	7:G:23:TYR:C	2.44	0.58
1:A:117:THR:HG22	10:A:302:HEM:C2D	2.38	0.58
7:G:29:TYR:O	7:G:29:TYR:CD2	2.56	0.58
5:E:11:PHE:CD1	8:H:13:VAL:HG21	2.39	0.58
6:F:20:TRP:CZ3	18:G:101:BCR:H19C	2.38	0.58
1:A:8:PHE:HB3	1:A:14:ILE:HG12	1.86	0.58
1:A:36:LEU:CD2	1:A:99:LEU:HB3	2.32	0.58
1:A:104:VAL:HG21	10:A:302:HEM:C2D	2.37	0.58
2:B:23:GLY:O	2:B:26:TYR:HD1	1.86	0.58
2:B:61:MET:CG	2:B:62:VAL:N	2.66	0.58
3:C:58:LEU:HG	3:C:237:VAL:HG21	1.85	0.58
4:D:177:TRP:NE1	4:D:178:TRP:CZ3	2.71	0.58
3:C:134:PRO:HB3	3:C:142:ILE:CD1	2.34	0.58
3:C:196:GLN:NE2	3:C:210:THR:HG22	2.19	0.58
6:F:25:LEU:CD2	6:F:29:ILE:CG2	2.81	0.58
13:A:1103:UMQ:H6'2	13:A:1103:UMQ:O5	2.03	0.58
4:D:134:ASP:CB	4:D:136:THR:H	2.16	0.58
5:E:5:ALA:O	5:E:6:VAL:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:GLN:O	3:C:282:VAL:HG22	2.04	0.58
5:E:22:ILE:O	5:E:23:ILE:C	2.43	0.58
1:A:39:ILE:HD13	18:G:101:BCR:H311	1.86	0.58
1:A:33:PHE:CD1	7:G:21:LEU:HD13	2.39	0.58
3:C:271:MET:HE3	4:D:22:LEU:HD21	1.85	0.58
6:F:16:ILE:HG22	6:F:17:PHE:N	2.13	0.58
7:G:26:TYR:O	7:G:27:GLN:C	2.46	0.58
2:B:41:PRO:O	2:B:45:MET:HB2	2.04	0.57
2:B:109:ILE:HG22	2:B:110:LEU:H	1.66	0.57
3:C:78:LEU:HB3	3:C:79:PRO:CD	2.33	0.57
1:A:68:SER:OG	1:A:69:VAL:N	2.37	0.57
2:B:96:LEU:HD13	2:B:100:LEU:CD1	2.33	0.57
3:C:58:LEU:CD1	3:C:59:GLN:H	2.16	0.57
3:C:271:MET:HE3	4:D:22:LEU:CD2	2.33	0.57
4:D:82:GLN:O	4:D:82:GLN:HG2	2.04	0.57
4:D:84:LEU:O	4:D:85:LYS:HB3	2.02	0.57
1:A:191:LEU:N	1:A:192:PRO:CD	2.68	0.57
3:C:237:VAL:O	3:C:237:VAL:HG23	2.04	0.57
3:C:273:ILE:O	3:C:276:LYS:N	2.38	0.57
1:A:72:ILE:O	1:A:79:GLY:HA3	2.04	0.57
1:A:138:LEU:N	1:A:139:PRO:CD	2.68	0.57
2:B:83:PRO:O	2:B:87:ILE:HG13	2.05	0.57
3:C:8:THR:C	3:C:10:PRO:HD3	2.29	0.57
13:C:1101:UMQ:HL3	4:D:37:PRO:CG	2.33	0.57
6:F:11:LEU:CA	6:F:15:LEU:HD12	2.34	0.57
1:A:113:PRO:HB2	2:B:22:MET:HE2	1.86	0.57
2:B:4:LEU:C	2:B:4:LEU:CD2	2.65	0.57
5:E:12:ILE:CD1	5:E:12:ILE:CG2	2.83	0.57
1:A:9:GLN:OE1	1:A:15:GLN:HB2	2.05	0.57
2:B:151:LEU:CD1	2:B:151:LEU:O	2.42	0.57
3:C:254:ARG:O	3:C:255:VAL:C	2.47	0.57
7:G:7:ASP:O	7:G:8:GLY:C	2.47	0.57
2:B:3:THR:O	2:B:29:GLU:CB	2.53	0.57
3:C:20:ILE:HG21	3:C:240:PHE:HZ	1.69	0.57
3:C:94:LEU:HD22	3:C:98:VAL:HG23	1.85	0.57
8:H:16:THR:C	8:H:18:SER:N	2.60	0.57
1:A:94:VAL:HG21	2:B:80:TYR:CE2	2.40	0.57
2:B:115:GLU:HG3	12:B:1001:OPC:OCC	2.05	0.57
2:B:134:LEU:HD21	7:G:22:PHE:CZ	2.40	0.57
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.87	0.57
3:C:81:GLY:HA3	3:C:142:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:LEU:N	6:F:10:LEU:HD13	1.91	0.57
6:F:20:TRP:HZ3	18:G:101:BCR:H19C	1.69	0.57
1:A:36:LEU:HB3	1:A:100:HIS:CB	2.33	0.57
1:A:113:PRO:HG2	1:A:114:ARG:HE	1.70	0.57
3:C:34:VAL:HG22	3:C:151:LEU:HB2	1.87	0.57
3:C:85:ALA:CB	3:C:132:LEU:HB2	2.34	0.57
13:C:1101:UMQ:HL3	4:D:37:PRO:HG3	1.86	0.57
4:D:90:TYR:OH	4:D:116:PRO:HA	2.04	0.57
1:A:158:ILE:O	1:A:162:GLY:HA3	2.05	0.57
8:H:9:VAL:O	8:H:13:VAL:HG23	2.05	0.57
3:C:28:ALA:HB2	3:C:236:ASN:ND2	2.19	0.56
6:F:13:PHE:CD2	6:F:17:PHE:HE1	2.22	0.56
1:A:88:TRP:CE3	2:B:54:LEU:CD1	2.88	0.56
12:B:1001:OPC:OAI	12:B:1001:OPC:CBG	2.53	0.56
3:C:21:VAL:O	3:C:22:CYS:O	2.23	0.56
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.39	0.56
3:C:162:PRO:HD3	10:C:301:HEM:HAC	1.85	0.56
3:C:281:LYS:C	3:C:283:GLN:N	2.63	0.56
1:A:88:TRP:CZ3	2:B:54:LEU:CD1	2.89	0.56
1:A:143:VAL:HG13	1:A:143:VAL:O	2.03	0.56
1:A:168:LEU:O	1:A:182:ARG:NH1	2.38	0.56
2:B:45:MET:HG2	4:D:30:VAL:HG11	1.87	0.56
2:B:80:TYR:CD1	2:B:81:LEU:HD23	2.40	0.56
4:D:15:ARG:CG	5:E:31:LEU:HD21	2.35	0.56
4:D:70:LEU:C	4:D:72:SER:H	2.11	0.56
5:E:24:PHE:O	5:E:25:ALA:C	2.48	0.56
1:A:14:ILE:HG23	13:A:1103:UMQ:HF2	1.88	0.56
1:A:83:ARG:NH1	10:A:301:HEM:O2A	2.38	0.56
2:B:44:ILE:HG22	2:B:45:MET:N	2.21	0.56
2:B:150:PRO:O	2:B:151:LEU:C	2.46	0.56
3:C:77:MET:HG2	3:C:150:HIS:O	2.05	0.56
12:A:1002:OPC:HAX1	12:A:1002:OPC:HBC1	1.85	0.56
3:C:226:LYS:O	3:C:229:GLU:HB3	2.05	0.56
2:B:10:SER:O	2:B:12:PRO:CD	2.53	0.56
2:B:32:TRP:CG	2:B:33:PRO:N	2.74	0.56
3:C:9:TYR:O	3:C:106:TYR:OH	2.21	0.56
3:C:146:LYS:HE2	3:C:246:GLU:HG2	1.87	0.56
7:G:1:MET:HG2	7:G:2:VAL:H	1.69	0.56
2:B:142:TRP:O	2:B:143:LEU:C	2.48	0.56
4:D:177:TRP:CD1	4:D:178:TRP:CE3	2.94	0.56
1:A:4:VAL:O	1:A:5:TYR:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LYS:O	2:B:20:LYS:N	2.39	0.56
2:B:118:ASN:ND2	2:B:118:ASN:C	2.64	0.56
3:C:98:VAL:HG11	3:C:130:PRO:CD	2.33	0.56
3:C:119:LEU:CD2	3:C:124:TYR:CE1	2.85	0.56
2:B:6:LYS:O	2:B:7:PRO:O	2.24	0.56
2:B:124:PHE:C	2:B:126:ARG:N	2.64	0.56
1:A:7:TRP:CG	1:A:11:ARG:HH21	2.24	0.55
1:A:41:LEU:HD23	11:A:303:HEC:CBC	2.37	0.55
3:C:92:GLU:O	3:C:93:GLU:C	2.49	0.55
1:A:103:ARG:O	1:A:104:VAL:C	2.44	0.55
1:A:122:VAL:O	1:A:123:ILE:C	2.47	0.55
1:A:178:ALA:O	1:A:179:THR:C	2.45	0.55
4:D:13:MET:O	4:D:15:ARG:N	2.29	0.55
4:D:70:LEU:C	4:D:72:SER:N	2.63	0.55
8:H:26:ARG:C	8:H:27:ASN:ND2	2.63	0.55
3:C:173:THR:OG1	3:C:174:ALA:N	2.32	0.55
2:B:151:LEU:HD12	2:B:154:THR:CG2	2.36	0.55
3:C:19:ARG:HG2	3:C:19:ARG:NH1	2.18	0.55
3:C:196:GLN:C	3:C:197:VAL:HG23	2.31	0.55
8:H:1:MET:C	8:H:2:GLU:HG3	2.31	0.55
1:A:32:ILE:HG22	1:A:33:PHE:CD2	2.42	0.55
2:B:80:TYR:CD1	2:B:80:TYR:C	2.85	0.55
2:B:93:ASN:OD1	2:B:96:LEU:HB2	2.05	0.55
2:B:139:VAL:HG12	2:B:143:LEU:CD1	2.36	0.55
3:C:28:ALA:HB3	3:C:239:GLY:HA3	1.87	0.55
4:D:25:GLY:CA	17:D:201:SQD:C34	2.81	0.55
6:F:11:LEU:CB	6:F:15:LEU:HD12	2.37	0.55
2:B:57:LEU:HD12	8:H:8:TRP:CE2	2.41	0.55
2:B:84:VAL:O	2:B:84:VAL:HG12	2.06	0.55
2:B:142:TRP:C	2:B:144:GLY:N	2.60	0.55
3:C:26:HIS:ND1	3:C:154:ASN:ND2	2.54	0.55
3:C:174:ALA:HB3	3:C:229:GLU:H	1.71	0.55
3:C:265:VAL:O	3:C:266:MET:C	2.49	0.55
5:E:22:ILE:O	5:E:23:ILE:O	2.25	0.55
3:C:81:GLY:CA	3:C:142:ILE:CD1	2.82	0.55
2:B:36:LEU:O	2:B:40:PHE:HB2	2.06	0.55
3:C:193:VAL:HB	3:C:213:ALA:HB2	1.89	0.55
2:B:54:LEU:HD23	8:H:11:LEU:HD22	1.88	0.55
2:B:37:LEU:CD2	2:B:38:TYR:CE1	2.89	0.55
3:C:36:VAL:HG12	3:C:48:ALA:HB1	1.89	0.55
3:C:47:LYS:NZ	3:C:97:GLU:CD	2.64	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD2	10:A:301:HEM:O1D	2.08	0.54
2:B:136:GLY:HA2	15:B:201:CLA:HBC2	1.88	0.54
2:B:138:LEU:O	2:B:139:VAL:C	2.48	0.54
1:A:39:ILE:CD1	18:G:101:BCR:H311	2.37	0.54
1:A:102:PHE:CD2	1:A:102:PHE:N	2.74	0.54
3:C:117:GLY:HA2	3:C:118:PRO:C	2.33	0.54
3:C:139:ASP:O	3:C:141:ASN:N	2.40	0.54
3:C:180:ILE:CG2	3:C:223:GLN:N	2.70	0.54
3:C:225:VAL:HG12	3:C:229:GLU:CB	2.38	0.54
4:D:25:GLY:HA2	17:D:201:SQD:C32	2.37	0.54
4:D:62:ASN:O	4:D:63:ASN:CG	2.50	0.54
4:D:163:THR:O	4:D:164:PRO:O	2.24	0.54
4:D:77:ASP:CG	4:D:92:VAL:O	2.50	0.54
6:F:13:PHE:CD2	6:F:13:PHE:C	2.85	0.54
1:A:84:SER:HA	2:B:60:ALA:HB2	1.90	0.54
2:B:74:GLU:O	2:B:74:GLU:CG	2.50	0.54
6:F:4:GLU:C	6:F:6:LEU:H	2.16	0.54
2:B:129:ALA:O	2:B:130:THR:C	2.50	0.54
3:C:60:GLN:OE1	3:C:70:LEU:HB2	2.07	0.54
4:D:116:PRO:CD	4:D:125:LYS:O	2.52	0.54
1:A:93:MET:O	1:A:94:VAL:C	2.49	0.54
2:B:82:TYR:N	2:B:83:PRO:CD	2.70	0.54
3:C:20:ILE:O	3:C:23:ALA:HB3	2.07	0.54
3:C:66:SER:O	3:C:67:LYS:CB	2.52	0.54
3:C:128:VAL:HG12	3:C:129:PHE:N	2.18	0.54
5:E:2:ILE:O	5:E:6:VAL:HG23	2.06	0.54
6:F:20:TRP:O	6:F:20:TRP:HD1	1.91	0.54
1:A:47:GLN:O	1:A:51:GLY:N	2.39	0.54
1:A:88:TRP:CZ2	2:B:54:LEU:HD13	2.42	0.54
1:A:99:LEU:O	1:A:102:PHE:HB2	2.08	0.54
1:A:103:ARG:CD	1:A:107:THR:HG21	2.37	0.54
4:D:108:CYS:HB3	4:D:115:VAL:HG23	1.90	0.54
4:D:142:GLY:O	4:D:144:ALA:N	2.40	0.54
5:E:26:ILE:HG22	5:E:32:ILE:HD12	1.90	0.54
1:A:111:LYS:NZ	2:B:126:ARG:HD3	2.23	0.54
1:A:183:TYR:O	1:A:186:ALA:CB	2.46	0.54
2:B:100:LEU:CD2	12:B:1001:OPC:CBX	2.86	0.54
2:B:159:LEU:O	2:B:160:PHE:CB	2.56	0.54
7:G:33:ASN:O	7:G:34:GLU:O	2.26	0.53
1:A:94:VAL:HG11	2:B:80:TYR:CD2	2.43	0.53
1:A:95:LEU:HD22	1:A:96:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LYS:C	2:B:19:ALA:N	2.64	0.53
3:C:61:VAL:HG11	3:C:168:ASN:ND2	2.23	0.53
3:C:171:VAL:HB	3:C:233:ASN:O	2.07	0.53
3:C:276:LYS:O	3:C:279:VAL:N	2.38	0.53
6:F:12:SER:OG	7:G:12:GLY:HA3	2.08	0.53
1:A:103:ARG:HH22	10:A:302:HEM:HBD1	1.72	0.53
2:B:37:LEU:CD2	2:B:38:TYR:CZ	2.92	0.53
3:C:79:PRO:HD2	3:C:82:PHE:CG	2.43	0.53
6:F:18:VAL:O	6:F:22:LEU:HB2	2.09	0.53
2:B:100:LEU:CD2	12:B:1001:OPC:HBX2	2.39	0.53
1:A:91:SER:O	1:A:92:MET:C	2.50	0.53
12:A:1002:OPC:HBU2	8:H:15:PHE:CG	2.43	0.53
3:C:154:ASN:HB2	3:C:240:PHE:HD1	1.74	0.53
4:D:139:VAL:O	4:D:140:ILE:HG22	2.09	0.53
1:A:26:VAL:O	2:B:28:GLY:HA3	2.09	0.53
1:A:211:ILE:HD13	10:A:302:HEM:O1D	2.09	0.53
2:B:25:ASN:O	2:B:25:ASN:ND2	2.39	0.53
2:B:145:ILE:O	2:B:148:THR:N	2.40	0.53
3:C:120:PRO:HD2	3:C:124:TYR:HD1	1.72	0.53
1:A:110:PHE:HE1	2:B:112:PRO:HA	1.73	0.53
2:B:69:PHE:N	2:B:69:PHE:CD2	2.76	0.53
7:G:20:GLY:H	18:G:101:BCR:H363	1.70	0.53
2:B:82:TYR:O	2:B:85:PHE:N	2.42	0.53
6:F:6:LEU:O	6:F:7:TYR:C	2.52	0.53
2:B:123:PRO:HD2	7:G:25:ALA:CB	2.33	0.53
2:B:129:ALA:C	2:B:131:THR:N	2.65	0.53
4:D:107:VAL:HG12	4:D:112:GLY:HA2	1.91	0.53
1:A:19:ASP:N	1:A:19:ASP:OD1	2.41	0.52
1:A:30:VAL:HA	1:A:34:TYR:CD2	2.43	0.52
2:B:57:LEU:HD12	8:H:8:TRP:CZ3	2.44	0.52
2:B:156:THR:C	2:B:158:GLY:H	2.17	0.52
3:C:119:LEU:HD22	3:C:124:TYR:CG	2.43	0.52
4:D:70:LEU:O	4:D:72:SER:N	2.42	0.52
1:A:78:PHE:O	1:A:79:GLY:C	2.51	0.52
2:B:71:THR:HG22	2:B:72:PRO:O	2.10	0.52
4:D:25:GLY:CA	17:D:201:SQD:C33	2.87	0.52
4:D:132:GLN:O	4:D:133:TYR:CD1	2.62	0.52
2:B:84:VAL:HG13	2:B:101:MET:HG3	1.92	0.52
2:B:118:ASN:ND2	2:B:120:PHE:CB	2.72	0.52
3:C:21:VAL:HG23	3:C:22:CYS:N	2.23	0.52
13:A:1104:UMQ:HL2	17:D:201:SQD:C13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:THR:O	2:B:140:THR:HB	2.10	0.52
3:C:103:PHE:CE1	3:C:130:PRO:HD2	2.44	0.52
2:B:51:ILE:O	2:B:52:VAL:C	2.52	0.52
3:C:61:VAL:CG1	3:C:168:ASN:ND2	2.73	0.52
1:A:206:ILE:O	1:A:207:ARG:C	2.53	0.52
2:B:104:VAL:O	2:B:108:LEU:HB2	2.09	0.52
2:B:156:THR:C	2:B:158:GLY:N	2.63	0.52
3:C:28:ALA:HB3	3:C:239:GLY:CA	2.40	0.52
3:C:174:ALA:HB3	3:C:228:GLY:H	1.75	0.52
4:D:25:GLY:HA2	17:D:201:SQD:H332	1.90	0.52
2:B:71:THR:HG22	2:B:72:PRO:HD2	1.92	0.52
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.92	0.52
2:B:102:ALA:O	2:B:105:PRO:HD2	2.10	0.52
3:C:251:ASP:OD2	3:C:252:PRO:CD	2.58	0.52
3:C:276:LYS:CE	8:H:25:GLY:O	2.54	0.52
4:D:15:ARG:HD2	5:E:31:LEU:CD2	2.40	0.52
5:E:3:LEU:O	5:E:7:PHE:HB2	2.09	0.52
3:C:184:ALA:O	3:C:185:LYS:CB	2.54	0.52
2:B:121:GLN:O	2:B:126:ARG:NH2	2.43	0.52
1:A:86:HIS:CD2	10:A:301:HEM:NA	2.77	0.52
1:A:88:TRP:CE2	2:B:54:LEU:HD13	2.45	0.52
1:A:133:VAL:O	1:A:136:TYR:HB3	2.10	0.52
1:A:194:LEU:O	1:A:195:ILE:C	2.52	0.52
2:B:40:PHE:N	2:B:41:PRO:CD	2.72	0.52
6:F:17:PHE:O	6:F:18:VAL:C	2.53	0.52
6:F:31:GLY:O	6:F:32:ALA:CB	2.58	0.52
2:B:40:PHE:HB2	2:B:41:PRO:HD3	1.93	0.51
3:C:13:PRO:HB3	3:C:106:TYR:HE1	1.72	0.51
3:C:43:ASP:HA	3:C:133:SER:O	2.10	0.51
3:C:70:LEU:H	3:C:70:LEU:CD2	2.10	0.51
3:C:161:TYR:C	3:C:163:THR:N	2.68	0.51
1:A:29:HIS:NE2	1:A:213:GLY:O	2.43	0.51
1:A:51:GLY:O	1:A:55:THR:HG23	2.09	0.51
1:A:70:GLN:HA	1:A:73:MET:HB2	1.91	0.51
1:A:103:ARG:NH1	1:A:104:VAL:CA	2.68	0.51
3:C:161:TYR:O	3:C:163:THR:N	2.43	0.51
3:C:193:VAL:O	3:C:194:LYS:HG3	2.11	0.51
4:D:58:ASP:OD1	4:D:62:ASN:HB2	2.09	0.51
5:E:21:GLY:O	5:E:25:ALA:HB2	2.10	0.51
2:B:3:THR:O	2:B:29:GLU:HA	2.10	0.51
2:B:136:GLY:HA2	15:B:201:CLA:CBC	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:GLN:HB3	3:C:170:ASN:HD22	1.75	0.51
5:E:3:LEU:O	5:E:4:GLY:C	2.53	0.51
1:A:88:TRP:CH2	2:B:54:LEU:HD13	2.44	0.51
1:A:147:ALA:O	1:A:151:VAL:HG13	2.11	0.51
3:C:20:ILE:CD1	3:C:152:GLY:HA3	2.40	0.51
3:C:54:TYR:HE1	3:C:70:LEU:CG	2.23	0.51
4:D:133:TYR:CD1	4:D:133:TYR:N	2.78	0.51
1:A:110:PHE:CE1	2:B:112:PRO:HA	2.45	0.51
2:B:54:LEU:HD23	8:H:11:LEU:CD2	2.40	0.51
3:C:177:THR:HG23	3:C:226:LYS:HG2	1.91	0.51
1:A:110:PHE:H	1:A:110:PHE:HD2	1.58	0.51
4:D:59:LYS:O	4:D:60:LEU:C	2.54	0.51
8:H:12:LEU:O	8:H:13:VAL:C	2.52	0.51
13:A:1102:UMQ:HB2	13:A:1102:UMQ:O2'	2.10	0.51
2:B:83:PRO:O	2:B:84:VAL:C	2.52	0.51
3:C:36:VAL:HG23	3:C:37:PRO:O	2.11	0.51
3:C:53:PRO:O	3:C:54:TYR:HB3	2.10	0.51
7:G:7:ASP:OD2	7:G:7:ASP:N	2.40	0.51
1:A:213:GLY:HA2	2:B:24:HIS:CD2	2.46	0.51
2:B:125:ARG:C	2:B:127:PRO:HD3	2.36	0.51
3:C:3:PHE:O	3:C:6:GLN:HB3	2.10	0.51
5:E:1:MET:O	5:E:2:ILE:C	2.52	0.51
1:A:9:GLN:OE1	1:A:15:GLN:CB	2.59	0.51
13:A:1102:UMQ:O5	13:A:1102:UMQ:C3'	2.58	0.51
3:C:274:LEU:O	3:C:277:LYS:HB2	2.11	0.51
10:C:301:HEM:HBC2	10:C:301:HEM:HMC1	1.93	0.51
1:A:180:LEU:O	1:A:181:THR:C	2.54	0.51
10:A:302:HEM:HBB2	10:A:302:HEM:HMB1	1.92	0.51
2:B:124:PHE:CE1	7:G:26:TYR:HD1	2.29	0.51
1:A:208:LYS:HD2	1:A:208:LYS:C	2.35	0.50
1:A:215:LEU:CB	7:G:28:GLN:OE1	2.54	0.50
2:B:17:LYS:C	2:B:19:ALA:H	2.17	0.50
2:B:121:GLN:O	2:B:126:ARG:NE	2.41	0.50
2:B:149:PHE:HB3	2:B:150:PRO:HD2	1.93	0.50
3:C:208:VAL:HG12	3:C:209:ASP:N	2.25	0.50
3:C:263:CYS:O	3:C:265:VAL:N	2.44	0.50
2:B:32:TRP:CB	2:B:33:PRO:CD	2.89	0.50
2:B:122:ASN:OD1	2:B:123:PRO:HD2	2.11	0.50
3:C:21:VAL:O	3:C:22:CYS:C	2.54	0.50
3:C:22:CYS:SG	3:C:240:PHE:CE1	3.00	0.50
3:C:61:VAL:HG11	3:C:168:ASN:HD22	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:LYS:O	4:D:68:LYS:HD3	2.12	0.50
15:B:201:CLA:HBB1	15:B:201:CLA:CHC	2.41	0.50
6:F:11:LEU:HD12	6:F:11:LEU:H	1.76	0.50
3:C:23:ALA:O	3:C:25:CYS:N	2.45	0.50
3:C:46:PHE:CZ	3:C:131:VAL:CG2	2.94	0.50
5:E:21:GLY:O	5:E:25:ALA:CB	2.59	0.50
2:B:32:TRP:HB3	2:B:33:PRO:CD	2.42	0.50
2:B:129:ALA:O	2:B:132:ILE:N	2.45	0.50
3:C:65:GLY:O	3:C:66:SER:O	2.29	0.50
3:C:119:LEU:HD21	3:C:124:TYR:CE1	2.47	0.50
5:E:16:PHE:CD1	5:E:16:PHE:C	2.90	0.50
1:A:44:PHE:C	1:A:44:PHE:CD2	2.89	0.50
1:A:59:LYS:CD	1:A:59:LYS:HE2	2.18	0.50
3:C:101:VAL:HG11	3:C:103:PHE:CE2	2.47	0.50
3:C:144:PHE:CD2	3:C:251:ASP:N	2.79	0.50
13:C:1101:UMQ:HA1	13:C:1101:UMQ:C5'	2.42	0.50
1:A:110:PHE:CD2	1:A:110:PHE:N	2.80	0.50
2:B:123:PRO:O	2:B:130:THR:OG1	2.30	0.50
2:B:71:THR:HG22	2:B:72:PRO:N	2.26	0.49
15:B:201:CLA:CBB	15:B:201:CLA:HHC	2.42	0.49
3:C:281:LYS:C	3:C:283:GLN:H	2.20	0.49
1:A:25:TYR:CE2	2:B:30:PRO:HA	2.46	0.49
2:B:45:MET:CG	4:D:30:VAL:HG11	2.42	0.49
2:B:149:PHE:CB	2:B:150:PRO:CD	2.82	0.49
3:C:229:GLU:O	3:C:231:LEU:N	2.45	0.49
4:D:74:ASN:O	4:D:75:ALA:O	2.30	0.49
4:D:133:TYR:HD1	4:D:133:TYR:N	2.09	0.49
8:H:24:TRP:C	8:H:24:TRP:CD1	2.85	0.49
3:C:159:GLN:CG	3:C:170:ASN:HD22	2.25	0.49
3:C:262:ILE:N	3:C:262:ILE:HD13	2.26	0.49
6:F:11:LEU:CB	6:F:15:LEU:CD1	2.82	0.49
8:H:19:ILE:O	8:H:20:ALA:C	2.55	0.49
1:A:53:ALA:HB1	4:D:41:TYR:CE2	2.47	0.49
5:E:26:ILE:HG23	5:E:31:LEU:HB3	1.94	0.49
1:A:148:VAL:O	1:A:149:LYS:C	2.55	0.49
2:B:95:LEU:HD23	2:B:95:LEU:C	2.37	0.49
3:C:107:LYS:CG	3:C:110:GLN:NE2	2.76	0.49
3:C:206:THR:CG2	3:C:206:THR:O	2.60	0.49
3:C:231:LEU:C	3:C:232:THR:OG1	2.56	0.49
3:C:268:ALA:HB2	4:D:26:THR:HB	1.93	0.49
4:D:178:TRP:O	4:D:179:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.93	0.49
2:B:82:TYR:O	2:B:83:PRO:C	2.56	0.49
4:D:152:HIS:CE1	4:D:165:TRP:HD1	2.18	0.49
3:C:60:GLN:HG2	3:C:70:LEU:HB3	1.95	0.49
3:C:273:ILE:CD1	8:H:25:GLY:HA2	2.42	0.49
4:D:71:GLU:O	4:D:71:GLU:HG2	2.12	0.49
4:D:123:LYS:CE	4:D:132:GLN:NE2	2.46	0.49
6:F:13:PHE:C	6:F:13:PHE:HD2	2.20	0.49
10:A:301:HEM:HHA	10:A:301:HEM:O2D	2.13	0.49
2:B:74:GLU:N	2:B:75:ILE:HG22	2.27	0.49
3:C:149:ILE:O	3:C:149:ILE:HG22	2.13	0.49
3:C:155:ARG:NH1	3:C:239:GLY:O	2.39	0.49
10:C:301:HEM:CBC	10:C:301:HEM:HMC1	2.43	0.49
5:E:20:VAL:O	5:E:21:GLY:C	2.55	0.49
6:F:21:GLY:O	6:F:22:LEU:C	2.55	0.49
1:A:18:ALA:HB1	13:A:1104:UMQ:HB1	1.95	0.48
1:A:32:ILE:CD1	8:H:22:VAL:HG11	2.43	0.48
2:B:45:MET:CE	4:D:27:VAL:HG13	2.42	0.48
2:B:118:ASN:HD21	2:B:120:PHE:CA	2.26	0.48
3:C:26:HIS:HD1	3:C:154:ASN:HD21	1.60	0.48
3:C:273:ILE:HD11	8:H:25:GLY:HA3	1.95	0.48
5:E:16:PHE:HE1	5:E:20:VAL:HG21	1.78	0.48
6:F:28:LYS:O	6:F:30:GLN:N	2.46	0.48
7:G:34:GLU:O	7:G:36:GLY:N	2.41	0.48
1:A:1:MET:O	1:A:2:ALA:CB	2.61	0.48
1:A:81:LEU:O	1:A:82:ILE:C	2.55	0.48
1:A:88:TRP:CZ3	2:B:54:LEU:HD13	2.48	0.48
1:A:134:THR:HA	1:A:183:TYR:HD2	1.78	0.48
2:B:32:TRP:HB3	2:B:33:PRO:HD2	1.94	0.48
2:B:57:LEU:CD1	8:H:8:TRP:CE3	2.92	0.48
2:B:87:ILE:O	2:B:88:LEU:C	2.49	0.48
4:D:105:ASN:O	4:D:148:LEU:HD22	2.13	0.48
4:D:154:THR:C	4:D:155:VAL:HG22	2.38	0.48
7:G:17:THR:O	7:G:18:LEU:C	2.55	0.48
1:A:59:LYS:CD	1:A:59:LYS:HE3	2.18	0.48
2:B:115:GLU:CG	12:B:1001:OPC:OCC	2.61	0.48
2:B:118:ASN:ND2	2:B:120:PHE:CD1	2.81	0.48
3:C:58:LEU:HD13	3:C:59:GLN:H	1.78	0.48
3:C:139:ASP:O	3:C:140:LYS:C	2.56	0.48
3:C:271:MET:HB3	4:D:23:ALA:HA	1.95	0.48
4:D:103:GLY:N	4:D:151:CYS:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:ILE:HG23	5:E:26:ILE:HG12	1.95	0.48
2:B:100:LEU:CD2	12:B:1001:OPC:HBX1	2.44	0.48
4:D:44:PRO:HA	4:D:45:PRO:HD2	1.57	0.48
4:D:103:GLY:O	4:D:150:LEU:HA	2.12	0.48
8:H:23:VAL:C	8:H:25:GLY:N	2.71	0.48
1:A:22:THR:O	1:A:23:SER:HB3	2.12	0.48
10:A:301:HEM:CGD	10:A:301:HEM:HHA	2.43	0.48
2:B:71:THR:HG22	2:B:72:PRO:CD	2.43	0.48
2:B:141:ILE:O	2:B:141:ILE:HG22	2.12	0.48
1:A:57:TYR:CE1	1:A:76:VAL:HG11	2.49	0.48
1:A:102:PHE:O	1:A:103:ARG:C	2.55	0.48
2:B:32:TRP:CD1	2:B:33:PRO:CD	2.92	0.48
3:C:82:PHE:CZ	3:C:249:LEU:HD23	2.43	0.48
3:C:263:CYS:C	3:C:265:VAL:N	2.72	0.48
4:D:81:VAL:HG21	4:D:91:ILE:HG13	1.96	0.48
3:C:36:VAL:HG11	3:C:149:ILE:HD13	1.95	0.48
4:D:78:ARG:HD3	4:D:92:VAL:HG21	1.94	0.48
4:D:156:GLN:O	4:D:157:ASP:C	2.56	0.48
3:C:128:VAL:HG13	3:C:129:PHE:N	2.27	0.48
3:C:262:ILE:O	3:C:266:MET:HG2	2.13	0.48
7:G:28:GLN:C	7:G:30:LYS:H	2.22	0.48
7:G:28:GLN:C	7:G:30:LYS:N	2.70	0.48
2:B:40:PHE:CB	2:B:41:PRO:HD3	2.44	0.48
2:B:90:SER:O	2:B:91:VAL:HG23	2.13	0.48
1:A:134:THR:HA	1:A:183:TYR:CD2	2.49	0.48
3:C:133:SER:HA	3:C:134:PRO:HD2	1.62	0.48
4:D:36:TYR:C	4:D:36:TYR:CD2	2.91	0.48
1:A:54:MET:HE1	10:A:301:HEM:O1D	2.14	0.47
2:B:1:MET:HB3	2:B:2:ALA:H	1.32	0.47
2:B:6:LYS:C	2:B:7:PRO:O	2.57	0.47
2:B:53:ALA:CB	3:C:258:MET:HE2	2.43	0.47
15:B:201:CLA:C4	15:B:201:CLA:O2A	2.62	0.47
3:C:104:GLN:HA	3:C:105:PRO:HD3	1.41	0.47
4:D:149:ALA:C	4:D:150:LEU:HD23	2.38	0.47
11:A:303:HEC:C1C	2:B:40:PHE:CE2	2.97	0.47
2:B:37:LEU:HD21	2:B:38:TYR:CE2	2.50	0.47
4:D:127:PRO:C	4:D:129:HIS:H	2.21	0.47
5:E:16:PHE:C	5:E:16:PHE:HD1	2.22	0.47
6:F:17:PHE:O	6:F:20:TRP:HB3	2.14	0.47
5:E:26:ILE:HG22	5:E:31:LEU:HB3	1.96	0.47
1:A:24:LYS:HZ3	13:A:1102:UMQ:HO31	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:LYS:O	3:C:196:GLN:N	2.44	0.47
4:D:43:ILE:HG23	4:D:44:PRO:HD2	1.95	0.47
4:D:89:THR:HG23	4:D:105:ASN:OD1	2.15	0.47
1:A:66:TYR:OH	2:B:63:GLY:O	2.24	0.47
1:A:215:LEU:CD2	2:B:121:GLN:HB2	2.44	0.47
2:B:100:LEU:HD22	12:B:1001:OPC:HBX1	1.95	0.47
3:C:144:PHE:CE2	3:C:251:ASP:CA	2.98	0.47
4:D:81:VAL:HB	4:D:89:THR:O	2.15	0.47
4:D:177:TRP:CD1	4:D:177:TRP:H	2.32	0.47
5:E:24:PHE:O	5:E:28:SER:N	2.46	0.47
2:B:14:LEU:HD12	2:B:14:LEU:HA	1.30	0.47
2:B:51:ILE:HD12	2:B:51:ILE:HG21	1.60	0.47
2:B:123:PRO:CD	7:G:25:ALA:CB	2.91	0.47
3:C:211:ILE:O	3:C:211:ILE:CG1	2.58	0.47
8:H:16:THR:O	8:H:18:SER:N	2.48	0.47
1:A:86:HIS:HE1	10:A:301:HEM:C1C	2.32	0.47
1:A:120:SER:O	1:A:124:LEU:N	2.46	0.47
1:A:142:GLN:N	2:B:66:ALA:HA	2.30	0.47
10:A:302:HEM:CMC	10:A:302:HEM:CBC	2.83	0.47
2:B:15:ARG:C	2:B:17:LYS:N	2.71	0.47
2:B:17:LYS:O	2:B:19:ALA:N	2.48	0.47
2:B:159:LEU:O	2:B:160:PHE:HD2	1.97	0.47
3:C:20:ILE:HG21	3:C:240:PHE:CZ	2.50	0.47
3:C:144:PHE:CE2	3:C:251:ASP:HB2	2.50	0.47
3:C:157:ARG:HB3	10:C:301:HEM:HAD2	1.94	0.47
3:C:161:TYR:C	3:C:163:THR:H	2.22	0.47
3:C:203:SER:HB2	3:C:205:LYS:HD2	1.97	0.47
3:C:232:THR:O	3:C:232:THR:HG22	2.14	0.47
4:D:35:LEU:O	4:D:39:VAL:HG23	2.15	0.47
4:D:78:ARG:CB	4:D:117:TRP:CD1	2.97	0.47
5:E:3:LEU:HD11	5:E:7:PHE:CE1	2.49	0.47
1:A:202:HIS:HE1	10:A:302:HEM:C4C	2.32	0.47
1:A:204:LEU:O	1:A:205:MET:C	2.57	0.47
2:B:15:ARG:O	2:B:18:LEU:HB2	2.14	0.47
2:B:94:LYS:O	2:B:98:VAL:HG23	2.15	0.47
2:B:106:LEU:O	2:B:107:GLY:C	2.58	0.47
3:C:169:ASN:O	3:C:235:PRO:HB2	2.15	0.47
3:C:275:LYS:O	3:C:276:LYS:C	2.57	0.47
1:A:114:ARG:CZ	1:A:212:SER:HA	2.44	0.47
2:B:8:ASP:H	2:B:14:LEU:HD23	1.80	0.47
2:B:101:MET:HB3	2:B:101:MET:HE2	1.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:HD13	2:B:151:LEU:HA	1.48	0.47
3:C:41:LEU:O	3:C:42:PRO:C	2.57	0.47
3:C:94:LEU:O	3:C:94:LEU:HD22	2.15	0.47
3:C:175:SER:HB2	3:C:209:ASP:OD2	2.15	0.47
4:D:58:ASP:O	4:D:61:GLY:N	2.45	0.47
5:E:4:GLY:O	5:E:7:PHE:HB2	2.15	0.47
1:A:176:GLY:O	1:A:179:THR:N	2.48	0.47
2:B:57:LEU:HD23	3:C:258:MET:HE3	1.97	0.47
2:B:57:LEU:HD13	8:H:8:TRP:CE2	2.50	0.47
2:B:82:TYR:H	2:B:83:PRO:HD2	1.78	0.47
3:C:234:ASN:HA	3:C:235:PRO:HD3	1.71	0.47
3:C:271:MET:O	3:C:272:LEU:C	2.57	0.47
4:D:109:THR:HG23	4:D:145:PRO:HD2	1.97	0.47
4:D:153:ALA:C	4:D:154:THR:O	2.57	0.47
8:H:6:LEU:O	8:H:9:VAL:HB	2.15	0.47
1:A:188:THR:HG22	10:A:301:HEM:CAC	2.45	0.46
3:C:14:ARG:HA	3:C:20:ILE:HA	1.96	0.46
3:C:73:GLY:C	10:C:301:HEM:HMB2	2.40	0.46
3:C:78:LEU:CB	3:C:79:PRO:CD	2.93	0.46
3:C:245:THR:OG1	3:C:246:GLU:N	2.45	0.46
1:A:27:PRO:HA	1:A:28:PRO:HD2	1.75	0.46
1:A:134:THR:HG21	1:A:186:ALA:HB1	1.96	0.46
2:B:27:TYR:N	2:B:27:TYR:CD2	2.83	0.46
5:E:6:VAL:HG12	5:E:10:VAL:CG2	2.45	0.46
6:F:11:LEU:HB3	6:F:15:LEU:HD11	1.90	0.46
3:C:257:TRP:CD1	13:C:1101:UMQ:HB1	2.51	0.46
4:D:177:TRP:NE1	4:D:178:TRP:HE3	2.14	0.46
2:B:37:LEU:HD23	2:B:37:LEU:C	2.41	0.46
4:D:154:THR:O	4:D:155:VAL:HG22	2.15	0.46
5:E:9:ILE:H	5:E:9:ILE:HG12	1.51	0.46
1:A:103:ARG:HH11	1:A:104:VAL:N	2.14	0.46
2:B:44:ILE:O	2:B:47:THR:N	2.49	0.46
3:C:58:LEU:HD12	3:C:58:LEU:C	2.41	0.46
3:C:231:LEU:HD12	3:C:231:LEU:O	2.15	0.46
10:C:301:HEM:HBB2	10:C:301:HEM:CHC	2.14	0.46
6:F:25:LEU:C	6:F:27:LEU:N	2.73	0.46
1:A:34:TYR:CD1	1:A:103:ARG:NE	2.66	0.46
3:C:81:GLY:HA2	3:C:142:ILE:CD1	2.43	0.46
1:A:120:SER:O	1:A:123:ILE:N	2.49	0.46
1:A:201:LEU:HA	1:A:201:LEU:HD23	1.57	0.46
12:A:1002:OPC:HBC1	12:A:1002:OPC:CAX	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TRP:CG	2:B:33:PRO:CD	2.99	0.46
2:B:101:MET:HE3	15:B:201:CLA:H91	1.91	0.46
3:C:278:GLN:O	3:C:282:VAL:CG2	2.64	0.46
4:D:117:TRP:HA	4:D:117:TRP:CE3	2.51	0.46
8:H:3:ILE:HA	8:H:3:ILE:HD12	1.73	0.46
1:A:133:VAL:O	1:A:134:THR:C	2.59	0.46
2:B:71:THR:CG2	2:B:72:PRO:CD	2.94	0.46
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.46	0.46
4:D:133:TYR:CD2	4:D:148:LEU:HG	2.51	0.46
1:A:54:MET:HA	4:D:41:TYR:OH	2.16	0.46
1:A:110:PHE:CD1	1:A:110:PHE:O	2.69	0.46
1:A:148:VAL:HG11	1:A:179:THR:HG21	1.97	0.46
1:A:208:LYS:HD2	1:A:208:LYS:O	2.16	0.46
1:A:155:PRO:HB2	1:A:166:SER:OG	2.16	0.45
1:A:186:ALA:HB3	1:A:187:HIS:H	1.12	0.45
2:B:57:LEU:CD2	3:C:258:MET:HE3	2.46	0.45
7:G:11:LEU:O	7:G:12:GLY:C	2.59	0.45
8:H:29:LEU:CD2	8:H:29:LEU:HG	2.20	0.45
1:A:94:VAL:HG21	2:B:80:TYR:CD2	2.51	0.45
1:A:103:ARG:HH12	1:A:104:VAL:HG22	1.75	0.45
3:C:2:PRO:O	3:C:3:PHE:C	2.59	0.45
3:C:151:LEU:HG	3:C:152:GLY:N	2.30	0.45
3:C:273:ILE:HD13	8:H:25:GLY:CA	2.46	0.45
4:D:23:ALA:O	4:D:24:PHE:C	2.55	0.45
4:D:32:LEU:O	4:D:33:GLY:C	2.59	0.45
4:D:79:VAL:HG12	4:D:80:LEU:N	2.30	0.45
1:A:9:GLN:HE22	1:A:13:GLU:HA	1.81	0.45
1:A:88:TRP:CD2	2:B:54:LEU:HD13	2.51	0.45
1:A:103:ARG:HH21	1:A:211:ILE:HD11	1.80	0.45
1:A:116:LEU:HB3	1:A:205:MET:SD	2.56	0.45
1:A:141:ASP:CA	2:B:66:ALA:HB2	2.45	0.45
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.72	0.45
2:B:38:TYR:CE2	3:C:275:LYS:CG	2.99	0.45
3:C:146:LYS:HB2	3:C:248:VAL:CG2	2.43	0.45
3:C:180:ILE:CG1	3:C:198:SER:O	2.62	0.45
4:D:25:GLY:CA	17:D:201:SQD:H332	2.46	0.45
18:G:101:BCR:HC42	18:G:101:BCR:H312	1.98	0.45
1:A:112:LYS:O	1:A:113:PRO:C	2.50	0.45
12:A:1002:OPC:HBS	6:F:12:SER:HA	1.98	0.45
2:B:80:TYR:CE1	2:B:81:LEU:HD23	2.51	0.45
2:B:134:LEU:CD2	7:G:22:PHE:CZ	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:PRO:HA	3:C:142:ILE:HG22	1.98	0.45
3:C:180:ILE:HG22	3:C:223:GLN:N	2.31	0.45
3:C:251:ASP:HA	3:C:252:PRO:HD3	1.64	0.45
4:D:177:TRP:CD1	4:D:178:TRP:HE3	2.32	0.45
1:A:4:VAL:HG12	1:A:5:TYR:N	2.31	0.45
3:C:159:GLN:HG3	3:C:170:ASN:ND2	2.32	0.45
7:G:31:ARG:CG	7:G:31:ARG:O	2.62	0.45
1:A:88:TRP:CE3	2:B:54:LEU:HD13	2.51	0.45
1:A:177:GLN:O	1:A:178:ALA:C	2.56	0.45
3:C:254:ARG:HA	13:C:1101:UMQ:HB2	1.98	0.45
13:C:1101:UMQ:C5'	13:C:1101:UMQ:CA	2.94	0.45
4:D:172:THR:HG22	4:D:174:GLU:H	1.82	0.45
2:B:37:LEU:HD23	2:B:38:TYR:CD1	2.52	0.45
2:B:61:MET:HG2	2:B:62:VAL:H	1.78	0.45
2:B:124:PHE:O	2:B:127:PRO:HD3	2.17	0.45
3:C:77:MET:HG2	3:C:77:MET:H	1.63	0.45
3:C:79:PRO:O	3:C:82:PHE:HD1	2.00	0.45
13:C:1101:UMQ:CL	4:D:37:PRO:CG	2.94	0.45
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.99	0.45
5:E:15:PHE:HA	5:E:18:ILE:HG13	1.98	0.45
7:G:6:LEU:O	7:G:9:LEU:HB2	2.17	0.45
8:H:23:VAL:HG13	8:H:28:GLY:HA3	1.98	0.45
3:C:159:GLN:HA	3:C:167:SER:OG	2.17	0.45
3:C:161:TYR:HA	3:C:162:PRO:HD2	1.61	0.45
3:C:266:MET:CE	8:H:13:VAL:HG11	2.46	0.45
1:A:33:PHE:C	1:A:35:CYS:N	2.75	0.45
1:A:33:PHE:CG	7:G:21:LEU:CD1	3.00	0.45
1:A:126:VAL:O	1:A:130:SER:OG	2.35	0.45
1:A:128:THR:O	1:A:129:VAL:C	2.58	0.45
1:A:138:LEU:N	1:A:139:PRO:HD3	2.31	0.45
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.34	0.45
2:B:73:LEU:H	2:B:73:LEU:HG	1.74	0.45
3:C:158:GLY:H	10:C:301:HEM:HAD2	1.82	0.45
3:C:221:GLU:OE1	3:C:222:GLY:N	2.48	0.45
5:E:22:ILE:HA	5:E:25:ALA:CB	2.47	0.45
7:G:16:ALA:O	18:G:101:BCR:H16C	2.17	0.45
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.51	0.45
1:A:215:LEU:HD21	2:B:121:GLN:HB2	1.98	0.45
3:C:26:HIS:HD1	3:C:154:ASN:ND2	2.13	0.45
3:C:59:GLN:HB3	3:C:68:VAL:O	2.17	0.45
3:C:60:GLN:NE2	3:C:157:ARG:CG	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:GLN:CD	3:C:159:GLN:N	2.74	0.45
3:C:180:ILE:HG22	3:C:223:GLN:O	2.17	0.45
5:E:22:ILE:CG2	5:E:26:ILE:CG1	2.94	0.45
1:A:31:ASN:HD21	1:A:33:PHE:HD2	1.64	0.44
1:A:202:HIS:CE1	10:A:302:HEM:C4C	3.04	0.44
2:B:13:LYS:O	2:B:14:LEU:C	2.60	0.44
2:B:32:TRP:HD1	2:B:33:PRO:HD3	1.75	0.44
2:B:158:GLY:O	2:B:159:LEU:CB	2.65	0.44
3:C:6:GLN:OE1	3:C:106:TYR:O	2.36	0.44
3:C:257:TRP:CB	13:C:1101:UMQ:HD1	2.47	0.44
3:C:278:GLN:NE2	4:D:16:ARG:HA	2.33	0.44
5:E:3:LEU:O	5:E:4:GLY:O	2.34	0.44
5:E:14:LEU:O	5:E:18:ILE:HG12	2.17	0.44
8:H:18:SER:O	8:H:19:ILE:C	2.60	0.44
2:B:118:ASN:ND2	2:B:119:LYS:N	2.63	0.44
3:C:159:GLN:CB	3:C:170:ASN:HD22	2.31	0.44
4:D:13:MET:C	4:D:15:ARG:H	2.24	0.44
4:D:177:TRP:CD1	4:D:178:TRP:CZ3	3.05	0.44
1:A:30:VAL:HG22	1:A:34:TYR:CD1	2.52	0.44
3:C:12:THR:O	3:C:12:THR:HG22	2.17	0.44
3:C:15:GLU:HB2	3:C:19:ARG:CB	2.42	0.44
1:A:98:ILE:O	1:A:99:LEU:C	2.58	0.44
2:B:69:PHE:N	2:B:69:PHE:HD2	2.13	0.44
3:C:74:ALA:CB	3:C:153:ALA:HA	2.48	0.44
4:D:58:ASP:O	4:D:61:GLY:HA2	2.17	0.44
3:C:101:VAL:CG1	3:C:103:PHE:CE2	3.01	0.44
5:E:16:PHE:O	5:E:19:ALA:HB3	2.18	0.44
2:B:145:ILE:O	2:B:146:GLY:C	2.59	0.44
3:C:54:TYR:OH	3:C:121:GLY:HA3	2.17	0.44
3:C:58:LEU:HD12	3:C:59:GLN:CA	2.46	0.44
3:C:82:PHE:CD1	3:C:82:PHE:N	2.84	0.44
7:G:34:GLU:C	7:G:35:LEU:HD12	2.41	0.44
8:H:6:LEU:HA	8:H:6:LEU:HD23	1.50	0.44
2:B:3:THR:O	2:B:29:GLU:HB3	2.16	0.44
2:B:118:ASN:ND2	2:B:120:PHE:HB2	2.29	0.44
15:B:201:CLA:CHC	15:B:201:CLA:CBB	2.96	0.44
3:C:4:TRP:CD2	3:C:162:PRO:CG	2.99	0.44
3:C:34:VAL:CG2	3:C:243:ASP:HB3	2.48	0.44
3:C:278:GLN:HE22	4:D:16:ARG:HA	1.82	0.44
4:D:46:SER:O	4:D:48:GLY:N	2.51	0.44
4:D:146:LEU:O	4:D:147:SER:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:CYS:SG	11:A:303:HEC:HMB3	2.58	0.44
1:A:99:LEU:HD13	7:G:17:THR:OG1	2.18	0.44
3:C:27:LEU:CD2	3:C:27:LEU:H	2.31	0.44
3:C:115:LEU:O	3:C:116:VAL:HG23	2.18	0.44
3:C:121:GLY:O	3:C:122:GLU:C	2.57	0.44
3:C:208:VAL:HG12	3:C:209:ASP:H	1.83	0.44
4:D:89:THR:HG22	4:D:105:ASN:CA	2.42	0.44
5:E:3:LEU:CD1	5:E:7:PHE:CE1	3.00	0.44
1:A:33:PHE:C	1:A:35:CYS:H	2.26	0.44
2:B:105:PRO:HG2	15:B:201:CLA:H102	2.00	0.44
3:C:15:GLU:H	3:C:20:ILE:H	1.66	0.44
3:C:101:VAL:HG11	3:C:103:PHE:CZ	2.52	0.44
4:D:18:PHE:O	4:D:19:MET:C	2.61	0.44
4:D:60:LEU:HD12	4:D:62:ASN:HD21	1.83	0.44
4:D:79:VAL:CG1	4:D:80:LEU:N	2.79	0.44
1:A:42:THR:O	1:A:43:CYS:C	2.61	0.43
1:A:97:MET:O	1:A:98:ILE:C	2.61	0.43
1:A:125:ALA:HB2	10:A:302:HEM:HMC1	2.01	0.43
1:A:131:PHE:HE1	1:A:195:ILE:HD12	1.83	0.43
1:A:176:GLY:O	1:A:177:GLN:C	2.61	0.43
1:A:207:ARG:NH1	14:A:501:QNO:C4	2.71	0.43
3:C:272:LEU:HD23	3:C:272:LEU:HA	1.86	0.43
6:F:3:GLU:O	6:F:7:TYR:HB2	2.18	0.43
1:A:11:ARG:HB2	1:A:12:LEU:H	1.52	0.43
1:A:103:ARG:HD2	1:A:103:ARG:C	2.43	0.43
1:A:165:ILE:O	1:A:169:LEU:HG	2.18	0.43
2:B:80:TYR:HD1	2:B:81:LEU:HD23	1.82	0.43
2:B:124:PHE:HE1	7:G:26:TYR:N	2.15	0.43
2:B:135:PHE:O	2:B:136:GLY:C	2.61	0.43
15:B:201:CLA:HBB1	15:B:201:CLA:HHC	2.00	0.43
15:B:201:CLA:H61	15:B:201:CLA:H2	1.39	0.43
3:C:196:GLN:CD	3:C:210:THR:HG22	2.42	0.43
3:C:211:ILE:HA	3:C:212:PRO:HD2	1.94	0.43
4:D:160:ILE:HG22	4:D:161:VAL:N	2.33	0.43
4:D:170:PHE:O	4:D:171:ARG:HB2	2.17	0.43
17:D:201:SQD:H241	17:D:201:SQD:O49	2.18	0.43
2:B:38:TYR:CE2	3:C:275:LYS:HG3	2.53	0.43
6:F:24:VAL:O	6:F:27:LEU:CB	2.60	0.43
7:G:29:TYR:HB3	7:G:30:LYS:HB2	2.00	0.43
1:A:13:GLU:C	1:A:15:GLN:N	2.72	0.43
1:A:42:THR:HG23	2:B:44:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:SD	12:A:1002:OPC:CCB	3.06	0.43
1:A:129:VAL:O	1:A:130:SER:C	2.60	0.43
1:A:142:GLN:N	2:B:66:ALA:CA	2.81	0.43
2:B:90:SER:O	2:B:90:SER:OG	2.35	0.43
3:C:270:LEU:HD12	8:H:17:TRP:HZ2	1.82	0.43
4:D:115:VAL:HG22	4:D:126:CYS:CA	2.47	0.43
4:D:154:THR:C	4:D:155:VAL:CG2	2.91	0.43
5:E:6:VAL:C	5:E:10:VAL:HG23	2.43	0.43
5:E:13:ALA:O	5:E:16:PHE:HB3	2.19	0.43
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.78	0.43
2:B:71:THR:C	2:B:72:PRO:O	2.54	0.43
3:C:72:VAL:H	3:C:72:VAL:HG13	1.56	0.43
3:C:270:LEU:O	3:C:271:MET:C	2.60	0.43
4:D:80:LEU:HG	4:D:90:TYR:CE2	2.54	0.43
6:F:20:TRP:O	6:F:20:TRP:CD1	2.71	0.43
1:A:215:LEU:HD13	2:B:122:ASN:HA	2.01	0.43
2:B:71:THR:HG23	2:B:72:PRO:HD2	2.00	0.43
2:B:149:PHE:CB	2:B:150:PRO:HD3	2.48	0.43
3:C:61:VAL:HG13	3:C:65:GLY:HA2	2.00	0.43
4:D:21:LEU:O	4:D:22:LEU:C	2.60	0.43
2:B:95:LEU:HD23	2:B:95:LEU:O	2.18	0.43
2:B:140:THR:O	2:B:141:ILE:C	2.61	0.43
3:C:135:ASN:O	3:C:136:PRO:C	2.61	0.43
3:C:262:ILE:HA	3:C:262:ILE:HD12	1.57	0.43
3:C:270:LEU:HD23	3:C:274:LEU:HG	2.01	0.43
4:D:115:VAL:CG1	4:D:124:PHE:HB3	2.49	0.43
1:A:80:TRP:CZ3	1:A:81:LEU:HG	2.54	0.43
1:A:86:HIS:HE1	10:A:301:HEM:NC	2.08	0.43
2:B:124:PHE:O	2:B:125:ARG:C	2.50	0.43
2:B:151:LEU:O	2:B:154:THR:CB	2.66	0.43
3:C:84:ILE:HD12	3:C:103:PHE:CG	2.54	0.43
3:C:180:ILE:HA	3:C:199:ILE:HA	2.00	0.43
6:F:9:ALA:O	6:F:10:LEU:C	2.60	0.43
8:H:8:TRP:O	8:H:11:LEU:N	2.52	0.43
1:A:30:VAL:HG21	11:A:303:HEC:CMA	2.49	0.43
1:A:197:VAL:HG12	1:A:198:PHE:N	2.32	0.43
3:C:257:TRP:HB2	13:C:1101:UMQ:HD1	2.00	0.43
3:C:278:GLN:OE1	4:D:16:ARG:HA	2.19	0.43
4:D:59:LYS:HB2	4:D:59:LYS:NZ	2.34	0.43
2:B:48:PHE:HB3	2:B:49:ALA:H	1.68	0.43
3:C:9:TYR:CG	3:C:21:VAL:HG11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:ALA:O	3:C:63:ALA:C	2.62	0.43
3:C:267:LEU:HD23	5:E:15:PHE:HE2	1.84	0.43
5:E:8:TYR:O	5:E:11:PHE:N	2.52	0.43
7:G:19:GLY:C	18:G:101:BCR:H363	2.44	0.43
2:B:138:LEU:C	2:B:140:THR:N	2.75	0.42
4:D:126:CYS:HA	4:D:127:PRO:HD3	1.74	0.42
4:D:169:ASP:OD1	4:D:176:PRO:HB3	2.19	0.42
8:H:7:GLY:O	8:H:8:TRP:C	2.59	0.42
1:A:88:TRP:CE3	2:B:54:LEU:HD12	2.53	0.42
1:A:158:ILE:HG23	1:A:159:PRO:HD3	2.00	0.42
3:C:44:THR:CG2	3:C:45:VAL:N	2.71	0.42
3:C:180:ILE:CG2	3:C:222:GLY:C	2.92	0.42
13:C:1101:UMQ:CL	4:D:37:PRO:HG3	2.49	0.42
4:D:139:VAL:HG12	4:D:140:ILE:H	1.84	0.42
5:E:8:TYR:O	5:E:9:ILE:C	2.62	0.42
7:G:31:ARG:HG2	7:G:31:ARG:O	2.18	0.42
1:A:106:LEU:CD2	2:B:133:PHE:CE1	2.91	0.42
1:A:207:ARG:HG2	13:A:1102:UMQ:H41	2.01	0.42
2:B:61:MET:CG	2:B:62:VAL:H	2.31	0.42
2:B:124:PHE:HE1	7:G:26:TYR:CA	2.32	0.42
3:C:68:VAL:HG22	3:C:69:GLY:N	2.33	0.42
6:F:7:TYR:C	6:F:11:LEU:HD12	2.31	0.42
6:F:20:TRP:CD1	6:F:24:VAL:CG2	3.02	0.42
7:G:3:GLU:HA	7:G:4:PRO:HD2	1.70	0.42
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.49	0.42
2:B:126:ARG:HB3	12:B:1001:OPC:OBH	2.19	0.42
3:C:59:GLN:HB3	3:C:68:VAL:C	2.45	0.42
3:C:250:GLN:HG3	3:C:251:ASP:O	2.19	0.42
5:E:10:VAL:O	5:E:14:LEU:CD1	2.56	0.42
6:F:8:ALA:O	6:F:11:LEU:N	2.53	0.42
1:A:80:TRP:CG	1:A:81:LEU:N	2.88	0.42
1:A:191:LEU:O	1:A:192:PRO:C	2.63	0.42
4:D:15:ARG:CD	5:E:31:LEU:CD2	2.96	0.42
4:D:168:THR:HG22	4:D:175:LYS:HA	2.01	0.42
1:A:43:CYS:O	1:A:46:ILE:HB	2.20	0.42
3:C:146:LYS:NZ	7:G:3:GLU:OE1	2.34	0.42
3:C:281:LYS:O	3:C:283:GLN:N	2.52	0.42
4:D:29:GLY:O	4:D:30:VAL:C	2.62	0.42
4:D:66:VAL:HG21	4:D:155:VAL:CG1	2.49	0.42
6:F:17:PHE:HA	6:F:20:TRP:HB3	2.01	0.42
8:H:14:VAL:O	8:H:18:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG22	10:A:302:HEM:HBD2	2.00	0.42
2:B:33:PRO:HB2	2:B:38:TYR:HE1	1.85	0.42
2:B:38:TYR:CE2	3:C:275:LYS:HG2	2.55	0.42
2:B:107:GLY:O	2:B:108:LEU:C	2.63	0.42
2:B:110:LEU:HB3	2:B:114:ILE:HD12	2.01	0.42
2:B:135:PHE:O	2:B:139:VAL:HG23	2.18	0.42
4:D:46:SER:O	4:D:46:SER:OG	2.32	0.42
1:A:14:ILE:HD12	1:A:14:ILE:HA	1.26	0.42
1:A:20:ASP:OD1	13:A:1102:UMQ:C3	2.65	0.42
1:A:119:ILE:O	1:A:120:SER:C	2.62	0.42
1:A:130:SER:HB2	1:A:191:LEU:CD2	2.50	0.42
2:B:124:PHE:CE1	7:G:26:TYR:CD1	3.08	0.42
3:C:85:ALA:HA	3:C:86:PRO:HD2	1.51	0.42
3:C:104:GLN:HG3	3:C:115:LEU:HB2	2.02	0.42
3:C:115:LEU:HA	3:C:115:LEU:HD23	1.17	0.42
1:A:47:GLN:NE2	1:A:47:GLN:HA	2.33	0.42
1:A:80:TRP:CD2	1:A:81:LEU:N	2.88	0.42
12:A:1002:OPC:HAS1	5:E:4:GLY:CA	2.44	0.42
2:B:13:LYS:O	2:B:16:ALA:N	2.53	0.42
2:B:76:LEU:HD12	2:B:76:LEU:HA	1.71	0.42
2:B:100:LEU:HD21	12:B:1001:OPC:HBX2	2.01	0.42
2:B:106:LEU:HD23	2:B:106:LEU:HA	1.63	0.42
3:C:85:ALA:HB2	3:C:132:LEU:CB	2.45	0.42
3:C:255:VAL:H	3:C:255:VAL:HG23	1.49	0.42
5:E:16:PHE:CD2	6:F:22:LEU:CD2	2.97	0.42
1:A:78:PHE:CE1	4:D:37:PRO:HA	2.55	0.42
3:C:273:ILE:O	3:C:274:LEU:C	2.63	0.42
4:D:111:LEU:N	16:D:200:FES:S2	2.93	0.42
4:D:144:ALA:HA	4:D:145:PRO:HD3	1.89	0.42
6:F:26:LEU:HD13	6:F:26:LEU:HA	1.65	0.42
1:A:50:THR:H	1:A:50:THR:HG23	1.62	0.41
2:B:104:VAL:CB	2:B:105:PRO:CD	2.98	0.41
3:C:192:ASN:HB3	3:C:193:VAL:H	1.67	0.41
4:D:131:SER:CA	4:D:142:GLY:HA3	2.43	0.41
6:F:8:ALA:O	6:F:9:ALA:C	2.62	0.41
2:B:122:ASN:HA	2:B:123:PRO:HD3	1.92	0.41
3:C:47:LYS:HZ2	3:C:97:GLU:CD	2.28	0.41
1:A:29:HIS:CD2	1:A:214:PRO:CA	2.95	0.41
1:A:29:HIS:NE2	1:A:213:GLY:C	2.78	0.41
1:A:95:LEU:C	1:A:95:LEU:HD22	2.45	0.41
2:B:106:LEU:O	2:B:109:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:ASN:O	3:C:254:ARG:C	2.60	0.41
4:D:117:TRP:HA	4:D:117:TRP:HE3	1.85	0.41
1:A:37:GLY:HA3	10:A:302:HEM:C3A	2.55	0.41
1:A:150:ILE:O	1:A:151:VAL:C	2.63	0.41
3:C:159:GLN:HG3	3:C:170:ASN:HD22	1.85	0.41
4:D:43:ILE:HG22	4:D:44:PRO:O	2.20	0.41
5:E:10:VAL:C	5:E:13:ALA:HB3	2.41	0.41
6:F:25:LEU:O	6:F:27:LEU:N	2.53	0.41
1:A:34:TYR:O	11:A:303:HEC:C1B	2.69	0.41
2:B:153:LYS:HB3	2:B:153:LYS:HE3	1.71	0.41
3:C:273:ILE:HD13	8:H:25:GLY:HA2	2.02	0.41
6:F:10:LEU:O	6:F:11:LEU:C	2.61	0.41
7:G:34:GLU:HB3	7:G:35:LEU:H	1.64	0.41
2:B:79:TRP:CE3	7:G:6:LEU:HD11	2.56	0.41
3:C:21:VAL:CG2	3:C:22:CYS:N	2.83	0.41
3:C:77:MET:CG	3:C:150:HIS:O	2.67	0.41
4:D:60:LEU:HD12	4:D:62:ASN:ND2	2.35	0.41
6:F:21:GLY:C	6:F:23:GLY:N	2.78	0.41
1:A:111:LYS:O	1:A:113:PRO:N	2.53	0.41
1:A:155:PRO:O	1:A:156:GLU:C	2.63	0.41
1:A:161:VAL:C	1:A:163:VAL:H	2.18	0.41
1:A:184:TYR:O	1:A:188:THR:N	2.48	0.41
2:B:3:THR:O	2:B:29:GLU:CA	2.68	0.41
7:G:20:GLY:HA2	7:G:23:TYR:HB3	2.02	0.41
1:A:54:MET:C	1:A:56:PHE:N	2.78	0.41
1:A:107:THR:O	2:B:121:GLN:HB3	2.19	0.41
3:C:98:VAL:HA	3:C:128:VAL:HB	2.01	0.41
4:D:89:THR:CG2	4:D:105:ASN:OD1	2.69	0.41
1:A:35:CYS:O	1:A:36:LEU:C	2.61	0.41
1:A:62:VAL:HG12	1:A:140:TRP:CD1	2.55	0.41
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.43	0.41
1:A:148:VAL:C	1:A:150:ILE:N	2.73	0.41
2:B:84:VAL:CG1	2:B:101:MET:CG	2.97	0.41
3:C:45:VAL:HG22	3:C:85:ALA:CB	2.51	0.41
3:C:139:ASP:OD1	3:C:141:ASN:ND2	2.54	0.41
4:D:40:LYS:O	4:D:41:TYR:C	2.63	0.41
4:D:137:GLY:HA2	4:D:148:LEU:HB2	2.02	0.41
4:D:139:VAL:HG22	4:D:147:SER:N	2.36	0.41
5:E:2:ILE:H	5:E:2:ILE:CD1	2.28	0.41
5:E:18:ILE:O	5:E:22:ILE:HG13	2.21	0.41
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:23:GLY:O	6:F:26:LEU:HB2	2.20	0.41
6:F:30:GLN:HG3	6:F:31:GLY:N	2.34	0.41
2:B:17:LYS:HE3	2:B:26:TYR:HH	1.80	0.41
3:C:25:CYS:SG	10:C:301:HEM:C3C	3.10	0.41
3:C:78:LEU:HD12	3:C:78:LEU:N	2.33	0.41
3:C:144:PHE:HB3	3:C:145:GLY:H	1.71	0.41
3:C:218:ILE:CG2	3:C:233:ASN:HB2	2.51	0.41
1:A:95:LEU:HD22	1:A:96:MET:HE1	2.03	0.40
1:A:103:ARG:HD2	1:A:107:THR:CG2	2.44	0.40
1:A:196:ALA:O	1:A:197:VAL:C	2.62	0.40
2:B:76:LEU:HG	2:B:82:TYR:CE2	2.56	0.40
5:E:12:ILE:O	5:E:13:ALA:C	2.64	0.40
1:A:32:ILE:HD12	8:H:22:VAL:HG11	2.04	0.40
11:A:303:HEC:HMA3	11:A:303:HEC:HBB	1.79	0.40
2:B:11:ASP:HA	2:B:12:PRO:HD3	1.69	0.40
3:C:27:LEU:H	3:C:27:LEU:HD23	1.86	0.40
3:C:176:ALA:O	3:C:227:ALA:HA	2.21	0.40
4:D:38:LEU:HD12	4:D:38:LEU:HA	1.82	0.40
4:D:80:LEU:HA	4:D:80:LEU:HD23	1.40	0.40
4:D:142:GLY:C	4:D:144:ALA:H	2.30	0.40
18:G:101:BCR:H20C	18:G:101:BCR:H361	1.11	0.40
1:A:142:GLN:HG3	2:B:72:PRO:HG3	2.03	0.40
11:A:303:HEC:HAD2	11:A:303:HEC:HMD1	1.79	0.40
3:C:266:MET:CE	8:H:13:VAL:CG1	2.77	0.40
3:C:273:ILE:HD12	8:H:25:GLY:CA	2.51	0.40
3:C:255:VAL:O	3:C:256:LYS:C	2.64	0.40
4:D:68:LYS:O	4:D:68:LYS:CD	2.69	0.40
4:D:152:HIS:O	4:D:162:LEU:HD23	2.21	0.40
1:A:7:TRP:CZ2	1:A:11:ARG:NH2	2.84	0.40
1:A:100:HIS:CE1	10:A:302:HEM:C4A	2.97	0.40
1:A:179:THR:O	1:A:180:LEU:C	2.62	0.40
2:B:128:VAL:H	2:B:128:VAL:HG23	1.42	0.40
3:C:183:ILE:HD11	3:C:220:SER:O	2.22	0.40
3:C:254:ARG:HH11	3:C:254:ARG:HD2	1.60	0.40
4:D:129:HIS:CB	16:D:200:FES:S1	2.95	0.40
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.64	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	142 (67%)	53 (25%)	18 (8%)	0	7
2	B	158/160 (99%)	91 (58%)	36 (23%)	31 (20%)	0	1
3	C	286/289 (99%)	195 (68%)	50 (18%)	41 (14%)	0	3
4	D	162/179 (90%)	93 (57%)	39 (24%)	30 (18%)	0	1
5	E	30/32 (94%)	9 (30%)	10 (33%)	11 (37%)	0	0
6	F	30/35 (86%)	14 (47%)	8 (27%)	8 (27%)	0	0
7	G	35/37 (95%)	13 (37%)	9 (26%)	13 (37%)	0	0
8	H	27/29 (93%)	14 (52%)	6 (22%)	7 (26%)	0	0
All	All	941/976 (96%)	571 (61%)	211 (22%)	159 (17%)	0	2

All (159) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	23	SER
1	A	28	PRO
1	A	112	LYS
1	A	136	TYR
1	A	162	GLY
1	A	164	LEU
1	A	186	ALA
2	B	7	PRO
2	B	22	MET
2	B	33	PRO
2	B	34	ASN
2	B	75	ILE
2	B	87	ILE
2	B	109	ILE
2	B	110	LEU
2	B	114	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	117	VAL
2	B	125	ARG
2	B	129	ALA
2	B	130	THR
2	B	151	LEU
2	B	159	LEU
3	C	22	CYS
3	C	23	ALA
3	C	24	ASN
3	C	27	LEU
3	C	63	ALA
3	C	66	SER
3	C	67	LYS
3	C	144	PHE
3	C	185	LYS
3	C	186	GLU
3	C	187	GLU
3	C	189	GLU
3	C	192	ASN
3	C	201	THR
3	C	205	LYS
3	C	212	PRO
3	C	230	ALA
4	D	47	GLY
4	D	59	LYS
4	D	60	LEU
4	D	63	ASN
4	D	75	ALA
4	D	77	ASP
4	D	139	VAL
4	D	140	ILE
4	D	147	SER
4	D	154	THR
4	D	157	ASP
4	D	164	PRO
4	D	170	PHE
4	D	171	ARG
5	E	8	TYR
5	E	9	ILE
5	E	25	ALA
6	F	5	MET
6	F	7	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	8	ALA
6	F	9	ALA
7	G	16	ALA
7	G	30	LYS
7	G	34	GLU
7	G	35	LEU
1	A	3	ASN
1	A	13	GLU
1	A	32	ILE
1	A	43	CYS
1	A	132	GLY
1	A	134	THR
1	A	170	ARG
2	B	2	ALA
2	B	18	LEU
2	B	65	PRO
2	B	103	SER
2	B	113	PHE
2	B	124	PHE
2	B	158	GLY
3	C	134	PRO
3	C	162	PRO
3	C	193	VAL
3	C	194	LYS
3	C	195	TYR
3	C	200	GLN
3	C	232	THR
3	C	274	LEU
3	C	282	VAL
4	D	51	GLY
4	D	72	SER
4	D	76	GLY
4	D	101	ASP
4	D	138	LYS
4	D	155	VAL
5	E	13	ALA
5	E	21	GLY
7	G	15	PHE
7	G	18	LEU
7	G	19	GLY
7	G	27	GLN
7	G	29	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	2	GLU
8	H	6	LEU
8	H	20	ALA
8	H	24	TRP
2	B	44	ILE
2	B	108	LEU
3	C	184	ALA
4	D	33	GLY
4	D	50	VAL
5	E	24	PHE
6	F	13	PHE
6	F	24	VAL
7	G	4	PRO
7	G	20	GLY
8	H	4	ASP
8	H	19	ILE
2	B	32	TRP
2	B	86	GLN
2	B	111	VAL
2	B	146	GLY
3	C	19	ARG
3	C	20	ILE
3	C	28	ALA
3	C	110	GLN
3	C	272	LEU
3	C	275	LYS
4	D	71	GLU
4	D	143	PRO
2	B	134	LEU
3	C	86	PRO
3	C	100	ASP
4	D	18	PHE
4	D	74	ASN
4	D	127	PRO
5	E	14	LEU
5	E	19	ALA
2	B	144	GLY
3	C	2	PRO
3	C	37	PRO
3	C	91	PRO
3	C	152	GLY
4	D	14	GLY

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Mol	Chain	Res	Type
5	E	4	GLY
5	E	6	VAL
5	E	20	VAL
6	F	26	LEU
6	F	29	ILE
3	C	69	GLY
8	H	7	GLY
1	A	82	ILE
1	A	197	VAL
2	B	139	VAL
3	C	11	PRO
4	D	142	GLY
4	D	145	PRO
7	G	12	GLY
1	A	210	GLY
7	G	36	GLY

### 5.3.2 Protein sidechains [i](#)

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	184/184 (100%)	132 (72%)	52 (28%)	0	3
2	B	137/137 (100%)	90 (66%)	47 (34%)	0	2
3	C	242/243 (100%)	142 (59%)	100 (41%)	0	0
4	D	134/146 (92%)	93 (69%)	41 (31%)	0	2
5	E	25/25 (100%)	17 (68%)	8 (32%)	0	2
6	F	24/27 (89%)	12 (50%)	12 (50%)	0	0
7	G	28/28 (100%)	19 (68%)	9 (32%)	0	2
8	H	24/24 (100%)	14 (58%)	10 (42%)	0	0
All	All	798/814 (98%)	519 (65%)	279 (35%)	0	1

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ARG
1	A	12	LEU
1	A	13	GLU
1	A	14	ILE
1	A	17	LEU
1	A	28	PRO
1	A	30	VAL
1	A	31	ASN
1	A	32	ILE
1	A	36	LEU
1	A	40	THR
1	A	46	ILE
1	A	59	LYS
1	A	62	VAL
1	A	63	THR
1	A	70	GLN
1	A	72	ILE
1	A	81	LEU
1	A	84	SER
1	A	87	ARG
1	A	92	MET
1	A	95	LEU
1	A	96	MET
1	A	98	ILE
1	A	99	LEU
1	A	100	HIS
1	A	103	ARG
1	A	104	VAL
1	A	106	LEU
1	A	112	LYS
1	A	115	GLU
1	A	122	VAL
1	A	130	SER
1	A	136	TYR
1	A	139	PRO
1	A	143	VAL
1	A	148	VAL
1	A	150	ILE
1	A	151	VAL
1	A	163	VAL
1	A	165	ILE
1	A	167	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	169	LEU
1	A	170	ARG
1	A	173	SER
1	A	175	VAL
1	A	182	ARG
1	A	192	PRO
1	A	200	LEU
1	A	211	ILE
1	A	215	LEU
2	B	1	MET
2	B	3	THR
2	B	4	LEU
2	B	6	LYS
2	B	7	PRO
2	B	22	MET
2	B	25	ASN
2	B	37	LEU
2	B	39	VAL
2	B	44	ILE
2	B	51	ILE
2	B	54	LEU
2	B	64	GLU
2	B	65	PRO
2	B	73	LEU
2	B	74	GLU
2	B	75	ILE
2	B	78	GLU
2	B	79	TRP
2	B	81	LEU
2	B	87	ILE
2	B	88	LEU
2	B	89	ARG
2	B	93	ASN
2	B	94	LYS
2	B	96	LEU
2	B	99	LEU
2	B	100	LEU
2	B	101	MET
2	B	103	SER
2	B	104	VAL
2	B	109	ILE
2	B	115	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	117	VAL
2	B	118	ASN
2	B	119	LYS
2	B	126	ARG
2	B	127	PRO
2	B	134	LEU
2	B	141	ILE
2	B	145	ILE
2	B	151	LEU
2	B	152	ASP
2	B	153	LYS
2	B	155	LEU
2	B	156	THR
2	B	159	LEU
3	C	2	PRO
3	C	6	GLN
3	C	7	GLN
3	C	8	THR
3	C	9	TYR
3	C	10	PRO
3	C	12	THR
3	C	19	ARG
3	C	20	ILE
3	C	27	LEU
3	C	34	VAL
3	C	37	PRO
3	C	39	SER
3	C	44	THR
3	C	54	TYR
3	C	56	THR
3	C	58	LEU
3	C	60	GLN
3	C	61	VAL
3	C	67	LYS
3	C	70	LEU
3	C	72	VAL
3	C	75	VAL
3	C	77	MET
3	C	84	ILE
3	C	86	PRO
3	C	88	GLU
3	C	89	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	93	GLU
3	C	94	LEU
3	C	101	VAL
3	C	107	LYS
3	C	111	ASP
3	C	116	VAL
3	C	119	LEU
3	C	122	GLU
3	C	123	GLN
3	C	125	GLN
3	C	126	GLU
3	C	127	ILE
3	C	131	VAL
3	C	137	THR
3	C	138	THR
3	C	140	LYS
3	C	141	ASN
3	C	142	ILE
3	C	146	LYS
3	C	149	ILE
3	C	151	LEU
3	C	154	ASN
3	C	157	ARG
3	C	160	ILE
3	C	163	THR
3	C	165	GLU
3	C	171	VAL
3	C	173	THR
3	C	179	THR
3	C	180	ILE
3	C	182	LYS
3	C	185	LYS
3	C	186	GLU
3	C	187	GLU
3	C	189	GLU
3	C	193	VAL
3	C	198	SER
3	C	205	LYS
3	C	206	THR
3	C	207	VAL
3	C	211	ILE
3	C	216	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	218	ILE
3	C	219	VAL
3	C	220	SER
3	C	225	VAL
3	C	229	GLU
3	C	233	ASN
3	C	237	VAL
3	C	245	THR
3	C	247	ILE
3	C	248	VAL
3	C	249	LEU
3	C	251	ASP
3	C	254	ARG
3	C	256	LYS
3	C	258	MET
3	C	259	ILE
3	C	262	ILE
3	C	264	LEU
3	C	267	LEU
3	C	270	LEU
3	C	271	MET
3	C	273	ILE
3	C	274	LEU
3	C	276	LYS
3	C	277	LYS
3	C	281	LYS
3	C	282	VAL
3	C	283	GLN
3	C	286	GLU
3	C	288	ASN
4	D	10	VAL
4	D	12	ASP
4	D	15	ARG
4	D	16	ARG
4	D	21	LEU
4	D	26	THR
4	D	35	LEU
4	D	40	LYS
4	D	45	PRO
4	D	54	THR
4	D	59	LYS
4	D	64	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	68	LYS
4	D	73	HIS
4	D	77	ASP
4	D	81	VAL
4	D	84	LEU
4	D	89	THR
4	D	99	ILE
4	D	107	VAL
4	D	108	CYS
4	D	113	CYS
4	D	115	VAL
4	D	121	GLU
4	D	131	SER
4	D	133	TYR
4	D	135	GLU
4	D	139	VAL
4	D	141	ARG
4	D	146	LEU
4	D	147	SER
4	D	150	LEU
4	D	154	THR
4	D	155	VAL
4	D	158	ASP
4	D	161	VAL
4	D	165	TRP
4	D	168	THR
4	D	169	ASP
4	D	174	GLU
4	D	175	LYS
5	E	3	LEU
5	E	9	ILE
5	E	14	LEU
5	E	16	PHE
5	E	18	ILE
5	E	22	ILE
5	E	23	ILE
5	E	29	ILE
6	F	1	MET
6	F	3	GLU
6	F	5	MET
6	F	6	LEU
6	F	7	TYR

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Mol	Chain	Res	Type
6	F	10	LEU
6	F	15	LEU
6	F	16	ILE
6	F	22	LEU
6	F	26	LEU
6	F	29	ILE
6	F	30	GLN
7	G	1	MET
7	G	6	LEU
7	G	7	ASP
7	G	9	LEU
7	G	21	LEU
7	G	30	LYS
7	G	31	ARG
7	G	33	ASN
7	G	35	LEU
8	H	1	MET
8	H	2	GLU
8	H	6	LEU
8	H	12	LEU
8	H	13	VAL
8	H	18	SER
8	H	21	MET
8	H	22	VAL
8	H	27	ASN
8	H	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
2	B	34	ASN
2	B	118	ASN
3	C	6	GLN
3	C	59	GLN
3	C	110	GLN
3	C	125	GLN
3	C	141	ASN
3	C	154	ASN
3	C	159	GLN
3	C	168	ASN

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Mol	Chain	Res	Type
3	C	170	ASN
3	C	233	ASN
3	C	242	GLN
3	C	283	GLN
3	C	288	ASN
4	D	62	ASN
4	D	82	GLN
4	D	110	HIS
4	D	118	ASN
4	D	132	GLN
8	H	27	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	HEM	A	302	1	50,50,50	2.25	21 (42%)	67,82,82	3.08	27 (40%)
11	HEC	A	303	1,19,14	46,50,50	2.21	14 (30%)	58,82,82	2.74	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	FES	D	200	4	0,4,4	-	-	-		
17	SQD	D	201	-	52,54,54	2.69	25 (48%)	62,65,65	4.75	35 (56%)
13	UMQ	C	1101	-	35,35,35	1.83	8 (22%)	46,46,46	3.42	20 (43%)
14	QNO	A	501	11	21,22,22	2.50	5 (23%)	22,28,28	2.20	6 (27%)
13	UMQ	A	1104	-	35,35,35	1.60	3 (8%)	46,46,46	2.82	12 (26%)
13	UMQ	A	1102	-	35,35,35	2.04	7 (20%)	46,46,46	3.07	20 (43%)
12	OPC	B	1001	-	53,53,54	2.20	19 (35%)	59,61,64	2.53	26 (44%)
13	UMQ	A	1103	-	35,35,35	1.72	5 (14%)	46,46,46	2.96	16 (34%)
12	OPC	A	1002	-	53,53,54	2.16	14 (26%)	59,61,64	2.84	27 (45%)
10	HEM	A	301	1	50,50,50	2.31	19 (38%)	67,82,82	3.02	31 (46%)
15	CLA	B	201	19	69,73,73	1.98	17 (24%)	82,113,113	3.79	44 (53%)
10	HEM	C	301	3	50,50,50	2.27	22 (44%)	67,82,82	2.60	23 (34%)
18	BCR	G	101	-	41,41,41	3.55	19 (46%)	56,56,56	6.93	36 (64%)

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
10	HEM	A	302	1	-	3/14/54/54	-
11	HEC	A	303	1,19,14	-	13/14/54/54	-
16	FES	D	200	4	-	-	0/1/1/1
17	SQD	D	201	-	3/3/9/9	25/49/69/69	0/1/1/1
10	HEM	A	301	1	-	3/14/54/54	-
13	UMQ	C	1101	-	2/2/10/10	9/20/60/60	0/2/2/2
13	UMQ	A	1104	-	2/2/10/10	16/20/60/60	0/2/2/2
13	UMQ	A	1102	-	2/2/10/10	12/20/60/60	0/2/2/2
12	OPC	B	1001	-	-	22/57/57/60	-
13	UMQ	A	1103	-	2/2/10/10	12/20/60/60	0/2/2/2
12	OPC	A	1002	-	-	23/57/57/60	-
14	QNO	A	501	11	1/1/0/0	4/9/9/9	0/2/2/2
15	CLA	B	201	19	2/2/15/20	12/39/115/115	-
10	HEM	C	301	3	-	3/14/54/54	-
18	BCR	G	101	-	-	10/29/63/63	0/2/2/2

All (198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	101	BCR	C8-C9	-11.24	1.21	1.46
14	A	501	QNO	C2-N1	7.73	1.51	1.36
13	A	1102	UMQ	O1'-C1'	6.59	1.51	1.40
18	G	101	BCR	C23-C22	-6.55	1.31	1.46
15	B	201	CLA	OBD-CAD	6.50	1.33	1.22
18	G	101	BCR	C8-C7	-6.28	1.14	1.33
17	D	201	SQD	C17-C16	-6.23	1.20	1.51
18	G	101	BCR	C26-C25	6.10	1.44	1.34
10	C	301	HEM	C3D-C2D	5.94	1.49	1.36
12	A	1002	OPC	OAN-CAO	5.92	1.51	1.34
10	A	301	HEM	CMC-C2C	5.90	1.62	1.50
13	A	1103	UMQ	C1'-C2'	-5.88	1.35	1.52
11	A	303	HEC	CAB-C3B	5.70	1.53	1.35
10	A	302	HEM	C3D-C2D	5.52	1.48	1.36
10	A	302	HEM	C4C-NC	-5.52	1.29	1.39
13	A	1103	UMQ	O1'-C1'	5.38	1.49	1.40
18	G	101	BCR	C7-C6	-5.36	1.26	1.45
13	A	1104	UMQ	O1'-C1'	5.33	1.49	1.40
13	C	1101	UMQ	C4'-C5'	5.32	1.67	1.52
10	A	302	HEM	CHD-C4C	-5.30	1.27	1.38
17	D	201	SQD	C12-C11	-5.25	1.25	1.51
11	A	303	HEC	CAC-C3C	5.23	1.52	1.35
18	G	101	BCR	C19-C18	-5.17	1.34	1.46
12	B	1001	OPC	CAG-CAH	-5.07	1.35	1.51
12	A	1002	OPC	OBJ-CBK	5.07	1.48	1.33
13	A	1102	UMQ	C1'-C2'	-5.05	1.37	1.52
12	A	1002	OPC	CAG-CAH	-4.99	1.36	1.51
18	G	101	BCR	C12-C13	-4.94	1.35	1.46
12	A	1002	OPC	CBP-CBQ	-4.93	1.31	1.52
17	D	201	SQD	O47-C7	4.89	1.48	1.34
15	B	201	CLA	O2A-CGA	4.88	1.47	1.33
10	A	301	HEM	C3D-C2D	4.87	1.47	1.36
17	D	201	SQD	C16-C15	-4.83	1.27	1.51
13	C	1101	UMQ	C1'-C2'	-4.81	1.38	1.52
10	C	301	HEM	FE-NB	4.76	2.09	1.94
15	B	201	CLA	C3C-C2C	4.74	1.47	1.36
17	D	201	SQD	O6-C1	4.72	1.48	1.40
17	D	201	SQD	C18-C17	-4.70	1.28	1.51
17	D	201	SQD	O48-C23	4.68	1.47	1.33
13	A	1104	UMQ	C1'-C2'	-4.66	1.38	1.52
12	B	1001	OPC	OBJ-CBK	4.62	1.46	1.33
18	G	101	BCR	C24-C23	-4.62	1.19	1.33
12	B	1001	OPC	CAG-NAF	-4.50	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	101	BCR	C30-C25	4.50	1.59	1.53
18	G	101	BCR	C38-C26	4.48	1.58	1.50
12	B	1001	OPC	CAV-CAW	4.46	1.57	1.31
17	D	201	SQD	C11-C10	-4.45	1.29	1.51
10	A	301	HEM	CMB-C2B	4.42	1.59	1.50
17	D	201	SQD	C13-C12	-4.39	1.30	1.51
11	A	303	HEC	CBB-CAB	-4.36	1.33	1.49
12	A	1002	OPC	CBP-CBO	-4.31	1.30	1.51
18	G	101	BCR	C21-C22	4.29	1.45	1.35
18	G	101	BCR	C24-C25	-4.28	1.30	1.45
14	A	501	QNO	O41-C4	-4.28	1.23	1.36
10	A	301	HEM	FE-NB	-4.26	1.81	1.94
11	A	303	HEC	CBC-CAC	-4.26	1.33	1.49
12	B	1001	OPC	CAQ-CAP	-4.20	1.36	1.52
15	B	201	CLA	O2D-CGD	4.18	1.43	1.33
12	A	1002	OPC	CAQ-CAP	-4.16	1.37	1.52
11	A	303	HEC	C3C-C2C	-4.09	1.27	1.41
10	C	301	HEM	FE-NA	-4.06	1.81	1.95
10	A	301	HEM	C4C-NC	-4.05	1.32	1.39
12	A	1002	OPC	CAV-CAW	4.05	1.54	1.31
11	A	303	HEC	C3D-C2D	3.96	1.49	1.38
18	G	101	BCR	C1-C6	-3.92	1.48	1.53
10	A	302	HEM	CHC-C1C	-3.87	1.30	1.38
11	A	303	HEC	C3B-C2B	-3.86	1.28	1.41
15	B	201	CLA	C1B-C2B	3.85	1.52	1.43
10	A	301	HEM	FE-NA	-3.83	1.82	1.95
10	A	301	HEM	CHB-C1B	-3.75	1.31	1.38
17	D	201	SQD	C21-C20	-3.69	1.28	1.51
12	B	1001	OPC	OAN-CAO	3.63	1.44	1.34
13	C	1101	UMQ	C3'-C4'	3.63	1.62	1.52
10	C	301	HEM	CHD-C4C	-3.60	1.31	1.38
17	D	201	SQD	C36-C35	-3.57	1.34	1.51
10	C	301	HEM	C3C-C4C	-3.56	1.39	1.46
10	A	301	HEM	FE-NC	3.55	2.06	1.95
14	A	501	QNO	C21-C2	3.55	1.60	1.50
15	B	201	CLA	C1D-ND	-3.50	1.33	1.37
15	B	201	CLA	C3D-C4D	-3.47	1.36	1.44
10	C	301	HEM	C4A-NA	-3.43	1.33	1.39
15	B	201	CLA	CHC-C1C	3.42	1.45	1.38
10	A	302	HEM	CHD-C1D	-3.40	1.31	1.39
13	A	1103	UMQ	O2'-C2'	-3.39	1.34	1.43
15	B	201	CLA	CHB-C1B	3.38	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	302	HEM	CAB-C3B	3.36	1.56	1.47
17	D	201	SQD	C15-C14	-3.35	1.35	1.51
13	C	1101	UMQ	O5'-C1'	3.35	1.50	1.41
10	C	301	HEM	CHD-C1D	-3.34	1.31	1.39
10	A	302	HEM	O1A-CGA	3.26	1.32	1.22
17	D	201	SQD	C22-C21	-3.22	1.27	1.50
12	A	1002	OPC	CAQ-CAR	-3.20	1.35	1.51
15	B	201	CLA	C3D-C2D	3.20	1.47	1.39
18	G	101	BCR	C37-C22	3.20	1.57	1.50
12	B	1001	OPC	CAE-NAF	-3.19	1.40	1.50
12	B	1001	OPC	CBL-CBK	3.18	1.59	1.50
13	A	1102	UMQ	O5'-C1'	3.14	1.49	1.41
12	A	1002	OPC	CAR-CAS	-3.14	1.36	1.51
10	A	301	HEM	CHA-C4D	-3.11	1.32	1.38
17	D	201	SQD	C20-C19	-3.10	1.36	1.51
17	D	201	SQD	C14-C13	-3.09	1.36	1.51
17	D	201	SQD	C19-C18	-3.07	1.36	1.51
10	A	302	HEM	CBA-CGA	3.06	1.57	1.50
13	A	1104	UMQ	O2'-C2'	-3.05	1.35	1.43
12	A	1002	OPC	CBT-CBS	-3.05	1.33	1.50
12	B	1001	OPC	CBP-CBQ	-3.05	1.39	1.52
13	A	1102	UMQ	O2'-C2'	-3.04	1.35	1.43
10	A	301	HEM	CHB-C4A	-3.04	1.32	1.39
10	A	301	HEM	C2A-C3A	-3.03	1.31	1.38
10	C	301	HEM	CMA-C3A	2.97	1.56	1.50
10	A	302	HEM	CHC-C4B	-2.97	1.32	1.39
15	B	201	CLA	MG-NA	-2.97	1.99	2.06
13	C	1101	UMQ	O1'-C1'	2.96	1.45	1.40
10	C	301	HEM	C3B-C4B	2.95	1.50	1.44
10	C	301	HEM	C2A-C3A	-2.94	1.31	1.38
10	C	301	HEM	CMB-C2B	2.93	1.56	1.50
17	D	201	SQD	C37-C36	-2.91	1.33	1.51
11	A	303	HEC	CAD-C3D	2.91	1.58	1.51
15	B	201	CLA	CHD-C4C	2.88	1.45	1.39
10	A	302	HEM	CMC-C2C	2.87	1.56	1.50
18	G	101	BCR	C27-C26	2.87	1.56	1.51
10	C	301	HEM	CHC-C1C	2.86	1.44	1.38
10	A	302	HEM	CHB-C4A	-2.86	1.33	1.39
12	B	1001	OPC	CBB-CBC	-2.84	1.37	1.51
17	D	201	SQD	C35-C34	-2.83	1.37	1.51
10	A	301	HEM	CAC-C3C	2.81	1.54	1.47
14	A	501	QNO	OH-N1	2.80	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1001	OPC	CAQ-CAR	-2.80	1.37	1.51
10	C	301	HEM	CHB-C4A	-2.77	1.33	1.39
12	B	1001	OPC	CAR-CAS	-2.76	1.38	1.51
12	B	1001	OPC	CBC-CBD	-2.71	1.38	1.51
10	A	302	HEM	CMB-C2B	2.68	1.56	1.50
12	A	1002	OPC	CBQ-CBR	-2.66	1.35	1.50
11	A	303	HEC	C1B-NB	-2.62	1.34	1.39
10	A	301	HEM	C1C-C2C	2.62	1.50	1.45
10	A	301	HEM	C4D-C3D	-2.61	1.40	1.45
10	A	301	HEM	FE-ND	2.61	2.02	1.94
12	A	1002	OPC	CAG-NAF	-2.60	1.43	1.51
18	G	101	BCR	C40-C30	2.60	1.58	1.53
10	C	301	HEM	CHB-C1B	-2.57	1.33	1.38
14	A	501	QNO	C5-C6	-2.56	1.38	1.42
10	A	302	HEM	C1B-C2B	2.54	1.49	1.44
17	D	201	SQD	C32-C31	-2.54	1.39	1.51
17	D	201	SQD	C34-C33	-2.53	1.39	1.51
15	B	201	CLA	CHC-C4B	2.50	1.45	1.39
12	A	1002	OPC	CBC-CBD	-2.49	1.39	1.51
17	D	201	SQD	C4-C3	-2.49	1.45	1.52
15	B	201	CLA	CAA-C2A	-2.48	1.49	1.54
12	B	1001	OPC	OCC-CBK	2.46	1.29	1.22
10	A	302	HEM	C4D-C3D	2.45	1.49	1.45
10	C	301	HEM	CAB-C3B	2.44	1.53	1.47
12	B	1001	OPC	CBQ-CBR	-2.43	1.36	1.50
18	G	101	BCR	C11-C10	-2.42	1.35	1.43
17	D	201	SQD	C38-C37	-2.41	1.33	1.50
11	A	303	HEC	C4A-C3A	-2.39	1.40	1.45
15	B	201	CLA	CHD-C1D	2.38	1.43	1.38
10	A	301	HEM	CHA-C1A	-2.37	1.34	1.39
10	A	301	HEM	C1B-NB	-2.36	1.36	1.40
17	D	201	SQD	C1-C2	2.36	1.59	1.52
13	A	1103	UMQ	O5'-C1'	2.35	1.47	1.41
10	A	302	HEM	O1D-CGD	2.35	1.29	1.22
18	G	101	BCR	C35-C13	2.31	1.55	1.50
10	C	301	HEM	CAC-C3C	2.31	1.53	1.47
10	C	301	HEM	C3C-C2C	-2.31	1.32	1.37
12	B	1001	OPC	CBT-CBS	-2.30	1.37	1.50
11	A	303	HEC	C4B-NB	-2.29	1.35	1.39
12	A	1002	OPC	CBB-CBC	-2.27	1.40	1.51
13	A	1102	UMQ	C3-C4	2.25	1.58	1.52
11	A	303	HEC	CAA-C2A	2.25	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	301	HEM	C1B-NB	-2.25	1.36	1.40
10	A	302	HEM	C3B-C2B	-2.24	1.32	1.37
18	G	101	BCR	C15-C14	-2.23	1.36	1.43
10	A	302	HEM	CBA-CAA	2.23	1.59	1.51
11	A	303	HEC	CHB-C1B	-2.23	1.34	1.39
13	A	1103	UMQ	O5-C1	2.19	1.47	1.41
12	B	1001	OPC	CBZ-CBY	2.17	1.62	1.51
10	C	301	HEM	CMC-C2C	2.16	1.55	1.50
10	A	302	HEM	CAC-C3C	2.16	1.53	1.47
11	A	303	HEC	O1D-CGD	2.15	1.29	1.22
10	A	301	HEM	C4A-NA	-2.15	1.35	1.39
10	C	301	HEM	CAA-C2A	2.15	1.56	1.51
13	C	1101	UMQ	O5-C1	2.14	1.47	1.41
17	D	201	SQD	C33-C32	-2.12	1.41	1.51
13	A	1102	UMQ	C4-C5	2.12	1.57	1.53
10	A	301	HEM	CHD-C4C	-2.11	1.34	1.38
10	C	301	HEM	C1A-NA	-2.11	1.35	1.39
13	C	1101	UMQ	C6'-C5'	2.11	1.58	1.51
15	B	201	CLA	C1D-C2D	2.11	1.49	1.45
12	B	1001	OPC	CBP-CBO	-2.10	1.41	1.51
13	A	1102	UMQ	C4'-C5'	2.08	1.58	1.52
10	A	302	HEM	CMD-C2D	2.07	1.55	1.50
17	D	201	SQD	O7-S	2.04	1.50	1.45
10	C	301	HEM	C1C-C2C	2.04	1.49	1.45
15	B	201	CLA	C1C-NC	-2.03	1.34	1.37
12	B	1001	OPC	CBY-CBX	2.03	1.61	1.51
10	A	302	HEM	C1C-NC	-2.02	1.35	1.39
13	C	1101	UMQ	O3'-C3'	2.01	1.47	1.43
10	A	302	HEM	C3C-C4C	-2.01	1.42	1.46

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	101	BCR	C7-C8-C9	29.43	169.77	126.23
18	G	101	BCR	C24-C23-C22	26.06	164.79	126.23
18	G	101	BCR	C8-C7-C6	17.00	172.42	127.00
18	G	101	BCR	C23-C24-C25	15.39	168.11	127.00
15	B	201	CLA	CMB-C2B-C1B	13.36	145.75	125.42
17	D	201	SQD	O4-C4-C3	13.14	141.36	110.38
13	A	1104	UMQ	O1'-C1'-C2'	12.46	127.19	108.27
17	D	201	SQD	O3-C3-C4	-12.18	81.67	110.38
17	D	201	SQD	C18-C17-C16	12.13	175.67	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	201	SQD	C17-C16-C15	11.17	170.85	114.37
15	B	201	CLA	C4A-NA-C1A	11.10	111.74	106.68
13	A	1102	UMQ	CA-O1'-C1'	10.23	131.15	113.68
10	A	302	HEM	C3C-C2C-C1C	-10.05	97.53	107.05
18	G	101	BCR	C33-C5-C6	-10.00	113.57	124.48
17	D	201	SQD	C12-C11-C10	9.89	164.35	114.37
13	C	1101	UMQ	C1'-O5'-C5'	-9.45	95.27	113.72
13	A	1103	UMQ	CA-O1'-C1'	9.36	129.66	113.68
10	A	301	HEM	C3C-C2C-C1C	-9.34	98.21	107.05
17	D	201	SQD	C22-C21-C20	9.27	175.99	113.36
17	D	201	SQD	O7-S-C6	9.16	120.43	106.76
12	A	1002	OPC	CAA-NAF-CAE	-9.01	85.31	108.98
13	C	1101	UMQ	O1'-C1'-C2'	8.93	121.84	108.27
10	C	301	HEM	CHD-C4C-NC	8.91	134.16	124.45
13	A	1102	UMQ	O1'-C1'-C2'	8.77	121.59	108.27
17	D	201	SQD	C13-C12-C11	8.73	158.51	114.37
11	A	303	HEC	CAD-C3D-C4D	8.35	141.26	124.94
10	A	301	HEM	C3B-C2B-C1B	-8.35	100.14	106.41
10	A	302	HEM	CAD-C3D-C4D	8.35	139.25	124.70
15	B	201	CLA	C1D-ND-C4D	-8.25	100.52	106.31
10	A	302	HEM	CHC-C1C-NC	-7.98	115.76	124.45
12	A	1002	OPC	CAA-NAF-CBG	-7.72	88.70	108.98
17	D	201	SQD	O6-C1-C2	7.56	119.76	108.27
17	D	201	SQD	O47-C7-C8	7.38	127.44	111.48
11	A	303	HEC	CBD-CAD-C3D	7.28	132.67	112.53
10	A	301	HEM	CHC-C1C-NC	-7.16	116.66	124.45
13	A	1104	UMQ	O2'-C2'-C1'	7.16	127.13	110.08
18	G	101	BCR	C3-C4-C5	-7.04	101.50	114.06
11	A	303	HEC	CBC-CAC-C3C	-7.00	113.45	127.43
13	A	1103	UMQ	O1-C4'-C3'	-6.97	89.51	107.23
11	A	303	HEC	CHB-C4A-NA	6.96	132.03	124.45
13	C	1101	UMQ	O5'-C1'-C2'	6.92	124.59	110.37
13	C	1101	UMQ	O2'-C2'-C1'	6.81	126.31	110.08
15	B	201	CLA	CMD-C2D-C1D	6.77	136.65	124.73
10	C	301	HEM	CHD-C4C-C3C	-6.71	113.90	125.21
13	A	1102	UMQ	C1'-C2'-C3'	6.64	123.98	110.01
18	G	101	BCR	C32-C1-C6	-6.63	99.84	110.24
15	B	201	CLA	C2D-C1D-ND	6.57	116.62	110.13
18	G	101	BCR	C15-C14-C13	-6.55	118.09	127.28
10	A	301	HEM	C4C-C3C-C2C	6.52	112.47	106.81
13	A	1103	UMQ	O1'-C1'-C2'	6.44	118.05	108.27
15	B	201	CLA	CED-O2D-CGD	-6.34	101.54	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	201	CLA	CBC-CAC-C3C	-6.22	95.55	112.42
18	G	101	BCR	C1-C6-C5	-6.21	114.15	122.64
13	A	1104	UMQ	C1'-C2'-C3'	5.98	122.60	110.01
13	C	1101	UMQ	O2'-C2'-C3'	5.98	124.48	110.38
10	A	302	HEM	CAD-C3D-C2D	-5.94	116.74	127.87
15	B	201	CLA	CHD-C1D-ND	-5.93	116.46	124.80
12	A	1002	OPC	CAA-NAF-CAG	-5.90	86.46	109.91
17	D	201	SQD	O9-S-C6	5.89	115.55	106.76
15	B	201	CLA	O2D-CGD-CBD	5.88	121.51	111.23
10	C	301	HEM	CHC-C4B-NB	-5.85	118.12	124.42
15	B	201	CLA	CAA-CBA-CGA	-5.72	96.95	113.21
15	B	201	CLA	C3B-C2B-C1B	-5.71	100.44	107.17
10	A	301	HEM	C4B-C3B-C2B	5.70	112.52	107.28
12	B	1001	OPC	OAN-CAO-CAP	5.69	123.79	111.48
10	A	302	HEM	CHA-C4D-ND	-5.62	117.41	124.37
14	A	501	QNO	C21-C2-C3	-5.58	110.04	121.06
10	A	302	HEM	C4C-C3C-C2C	5.58	111.65	106.81
15	B	201	CLA	CHB-C4A-NA	5.58	132.45	124.40
13	A	1104	UMQ	CA-O1'-C1'	5.56	123.18	113.68
13	C	1101	UMQ	C6'-C5'-C4'	5.47	128.78	113.38
13	A	1103	UMQ	C1-O5-C5	5.46	124.39	113.72
15	B	201	CLA	CMB-C2B-C3B	-5.42	113.80	126.55
15	B	201	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
15	B	201	CLA	C4-C3-C5	5.40	124.60	115.23
10	A	302	HEM	CMC-C2C-C1C	5.25	133.97	124.73
18	G	101	BCR	C20-C19-C18	-5.23	112.01	126.36
12	B	1001	OPC	OAN-CAO-OAD	-5.23	111.48	123.70
18	G	101	BCR	C16-C15-C14	5.22	134.21	123.52
12	B	1001	OPC	CAA-NAF-CBG	5.21	122.65	108.98
18	G	101	BCR	C37-C22-C23	5.19	126.02	118.09
14	A	501	QNO	O41-C4-C5	5.18	125.29	116.42
10	A	301	HEM	C2B-C1B-NB	5.11	115.72	109.84
10	A	302	HEM	C3B-C4B-NB	5.10	113.13	109.47
10	A	302	HEM	CHC-C4B-NB	5.07	129.88	124.42
12	B	1001	OPC	CBU-CBT-CBS	5.06	140.96	112.60
13	A	1103	UMQ	O5'-C1'-O1'	4.95	121.75	110.04
15	B	201	CLA	C3D-C4D-ND	4.94	118.03	109.99
12	A	1002	OPC	CBI-CAM-CAL	-4.94	100.28	111.78
10	A	302	HEM	CAA-CBA-CGA	4.93	126.74	113.67
13	C	1101	UMQ	C4-C3-C2	-4.91	102.21	110.83
12	A	1002	OPC	CAQ-CAR-CAS	4.89	139.10	114.37
15	B	201	CLA	C2C-C1C-NC	4.88	115.11	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	301	HEM	CBB-CAB-C3B	-4.88	103.13	127.53
12	A	1002	OPC	OAN-CAO-CAP	4.88	122.03	111.48
10	C	301	HEM	CMD-C2D-C1D	4.79	132.52	125.03
13	A	1103	UMQ	O5'-C1'-C2'	4.78	120.19	110.37
10	C	301	HEM	CAD-C3D-C4D	4.78	133.02	124.70
15	B	201	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
18	G	101	BCR	C31-C1-C6	-4.71	102.86	110.24
17	D	201	SQD	O47-C7-O49	-4.68	112.77	123.70
10	A	302	HEM	CBA-CAA-C2A	-4.67	99.62	112.53
17	D	201	SQD	O2-C2-C1	4.66	121.17	110.08
17	D	201	SQD	O5-C5-C4	4.63	118.05	109.70
13	C	1101	UMQ	C2'-C3'-C4'	-4.62	99.18	109.68
10	A	301	HEM	CMC-C2C-C1C	4.60	132.84	124.73
13	C	1101	UMQ	O2-C2-C3	4.59	121.20	110.38
13	A	1102	UMQ	O1-C1-C2	4.58	119.36	108.09
15	B	201	CLA	C3C-C4C-NC	4.57	116.29	110.43
13	A	1103	UMQ	C1'-C2'-C3'	4.55	119.58	110.01
15	B	201	CLA	O2A-CGA-CBA	4.54	125.68	111.83
18	G	101	BCR	C11-C10-C9	4.54	133.64	127.28
17	D	201	SQD	C14-C13-C12	4.49	137.08	114.37
17	D	201	SQD	O5-C1-O6	4.48	120.63	110.04
10	A	301	HEM	CMD-C2D-C1D	4.42	131.93	125.03
10	A	301	HEM	CMB-C2B-C1B	4.41	131.93	125.03
11	A	303	HEC	CBB-CAB-C3B	-4.40	118.64	127.43
13	C	1101	UMQ	C3'-C4'-C5'	4.39	120.65	110.93
15	B	201	CLA	CHB-C1B-NB	-4.38	117.48	124.05
10	A	301	HEM	CBB-CAB-C3B	-4.37	105.67	127.53
15	B	201	CLA	C2B-C1B-NB	4.37	114.86	110.33
12	B	1001	OPC	CAA-NAF-CAE	-4.37	97.49	108.98
13	A	1103	UMQ	O2'-C2'-C1'	4.29	120.31	110.08
13	A	1103	UMQ	O1-C4'-C5'	4.29	120.73	109.48
11	A	303	HEC	CAD-C3D-C2D	-4.28	117.46	127.07
18	G	101	BCR	C33-C5-C4	4.22	122.59	113.60
13	A	1102	UMQ	O5'-C1'-O1'	4.21	120.00	110.04
13	A	1104	UMQ	O5'-C1'-C2'	4.21	119.01	110.37
12	B	1001	OPC	CAQ-CAP-CAO	4.16	128.93	113.69
17	D	201	SQD	C15-C14-C13	4.15	135.36	114.37
10	A	302	HEM	CHA-C4D-C3D	4.12	132.83	125.23
13	A	1103	UMQ	O2'-C2'-C3'	4.12	120.09	110.38
18	G	101	BCR	C20-C21-C22	4.10	133.03	127.28
10	C	301	HEM	CHC-C4B-C3B	4.08	133.22	125.07
12	A	1002	OPC	OAI-CAH-CAG	4.07	129.26	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	302	HEM	CHC-C4B-C3B	-4.06	116.98	125.07
12	A	1002	OPC	CAR-CAS-CAT	4.02	134.68	114.37
12	A	1002	OPC	CBG-NAF-CAE	4.01	119.52	108.98
11	A	303	HEC	CMD-C2D-C1D	4.00	131.51	125.42
10	C	301	HEM	C2D-C1D-ND	4.00	114.52	109.90
13	A	1102	UMQ	O2'-C2'-C1'	3.99	119.59	110.08
12	B	1001	OPC	CBM-CBL-CBK	3.97	128.25	113.69
11	A	303	HEC	C4D-C3D-C2D	-3.95	100.75	106.87
10	A	301	HEM	C1A-CHA-C4D	-3.94	116.98	126.25
12	B	1001	OPC	CAM-OAN-CAO	3.93	127.20	117.80
15	B	201	CLA	CBB-CAB-C3B	-3.93	107.90	127.53
10	A	302	HEM	C2C-C1C-NC	3.92	116.89	109.64
12	A	1002	OPC	CAQ-CAP-CAO	3.90	127.98	113.69
10	C	301	HEM	C1D-C2D-C3D	-3.89	102.89	106.98
13	A	1102	UMQ	O5'-C1'-C2'	3.85	118.29	110.37
12	B	1001	OPC	CAE-NAF-CAG	3.83	125.11	109.91
13	C	1101	UMQ	C1-O5-C5	3.82	121.18	113.72
10	C	301	HEM	CHC-C1C-NC	3.82	128.61	124.45
10	C	301	HEM	C4C-CHD-C1D	-3.79	117.97	126.02
17	D	201	SQD	O8-S-C6	-3.74	98.75	105.97
10	A	301	HEM	CAD-C3D-C4D	3.70	131.15	124.70
17	D	201	SQD	O8-S-O9	-3.70	102.15	111.40
12	A	1002	OPC	CAH-CAG-NAF	3.69	127.66	115.82
11	A	303	HEC	CHB-C4A-C3A	-3.69	117.82	125.49
12	B	1001	OPC	CBO-CBP-CBQ	3.66	131.47	113.86
15	B	201	CLA	C1-O2A-CGA	-3.66	107.80	116.65
17	D	201	SQD	O6-C44-C45	3.64	119.68	110.82
10	C	301	HEM	O1D-CGD-CBD	-3.64	111.55	123.09
18	G	101	BCR	C12-C13-C14	-3.63	113.30	119.01
18	G	101	BCR	C27-C26-C25	-3.63	117.80	122.70
13	A	1102	UMQ	O3-C3-C4	3.63	118.93	110.38
13	C	1101	UMQ	C3-C4-C5	-3.61	103.69	110.23
12	A	1002	OPC	OAN-CAM-CBI	3.60	121.25	108.34
13	A	1103	UMQ	O3'-C3'-C2'	3.59	118.84	110.38
15	B	201	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
14	A	501	QNO	C61-C6-C5	3.55	123.81	119.43
10	A	301	HEM	C3D-C4D-ND	3.55	114.06	110.17
12	B	1001	OPC	OBJ-CBK-OCC	-3.55	114.75	123.63
17	D	201	SQD	C44-O6-C1	-3.51	106.28	113.80
10	A	301	HEM	CHB-C4A-NA	3.50	130.22	123.86
10	A	301	HEM	O2A-CGA-CBA	3.50	125.06	114.00
17	D	201	SQD	C35-C34-C33	3.49	132.03	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1102	UMQ	O3-C3-C2	-3.47	102.20	110.38
17	D	201	SQD	C16-C15-C14	3.44	131.75	114.37
12	B	1001	OPC	CBA-CBB-CBC	3.41	131.62	114.37
12	A	1002	OPC	CBA-CBB-CBC	3.41	131.59	114.37
10	A	301	HEM	CHB-C4A-C3A	-3.40	117.54	127.43
12	B	1001	OPC	CBP-CBO-CBN	3.38	131.45	114.37
17	D	201	SQD	C33-C32-C31	3.36	131.34	114.37
15	B	201	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
15	B	201	CLA	CAA-C2A-C3A	-3.33	104.00	113.00
12	A	1002	OPC	CBP-CBQ-CBR	3.33	131.25	112.60
10	A	302	HEM	CHD-C1D-ND	3.31	127.99	124.42
18	G	101	BCR	C34-C9-C10	-3.31	117.45	122.82
10	C	301	HEM	CHD-C1D-ND	-3.31	120.86	124.42
13	A	1102	UMQ	C3-C4-C5	3.30	116.22	110.23
15	B	201	CLA	C3B-C4B-NB	3.30	113.47	110.53
13	A	1102	UMQ	O1-C4'-C5'	3.26	118.04	109.48
13	C	1101	UMQ	O3-C3-C2	3.26	118.06	110.38
15	B	201	CLA	C16-C15-C13	-3.25	105.16	115.97
17	D	201	SQD	C34-C33-C32	3.23	130.72	114.37
18	G	101	BCR	C21-C20-C19	3.23	132.55	123.20
10	C	301	HEM	CAD-C3D-C2D	-3.22	121.83	127.87
13	C	1101	UMQ	O3'-C3'-C4'	3.20	118.15	109.94
11	A	303	HEC	CHD-C4C-C3C	3.18	130.57	125.21
13	A	1102	UMQ	O1'-CA-CB	3.17	120.13	109.37
13	A	1102	UMQ	C1-C2-C3	3.17	116.68	110.01
12	B	1001	OPC	CAQ-CAR-CAS	3.16	130.36	114.37
17	D	201	SQD	C32-C31-C30	3.16	130.35	114.37
11	A	303	HEC	CMD-C2D-C3D	-3.16	118.93	125.62
10	A	301	HEM	CBA-CAA-C2A	-3.15	103.82	112.53
10	A	302	HEM	CBC-CAC-C3C	-3.15	111.78	127.53
18	G	101	BCR	C39-C30-C25	3.15	115.18	110.24
10	A	302	HEM	C4D-ND-C1D	3.14	108.93	105.21
10	A	301	HEM	CHC-C4B-NB	3.14	127.81	124.42
12	A	1002	OPC	CBV-CBU-CBT	-3.11	98.89	113.86
10	C	301	HEM	O2D-CGD-CBD	3.11	123.83	114.00
17	D	201	SQD	C1-O5-C5	-3.11	107.65	113.72
11	A	303	HEC	CHD-C4C-NC	-3.09	121.09	124.45
15	B	201	CLA	O2A-C1-C2	3.06	119.89	108.11
13	A	1102	UMQ	O5-C5-C4	3.04	115.18	109.70
10	A	301	HEM	C4C-CHD-C1D	3.02	132.44	126.02
13	A	1104	UMQ	O1'-CA-CB	3.01	119.59	109.37
13	A	1102	UMQ	CI-CH-CG	3.01	129.58	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1001	OPC	CBO-CBN-CBM	3.00	129.55	114.37
14	A	501	QNO	O41-C4-C3	-2.99	112.40	121.38
10	A	302	HEM	CHA-C1A-NA	2.99	129.28	123.86
13	C	1101	UMQ	O3-C3-C4	2.98	117.40	110.38
15	B	201	CLA	O1A-CGA-CBA	-2.97	112.16	123.78
12	A	1002	OPC	CAM-OAN-CAO	2.97	124.91	117.80
10	A	301	HEM	O2A-CGA-O1A	-2.97	115.70	123.33
12	B	1001	OPC	CAA-NAF-CAG	-2.94	98.22	109.91
17	D	201	SQD	C4-C3-C2	-2.94	105.67	110.83
12	B	1001	OPC	CAR-CAQ-CAP	2.93	123.90	113.13
12	B	1001	OPC	CBI-CAM-CAL	-2.93	104.96	111.78
13	A	1103	UMQ	O5-C5-C4	2.92	114.96	109.70
13	C	1101	UMQ	C1-C2-C3	-2.89	103.92	110.01
12	A	1002	OPC	CBN-CBM-CBL	-2.89	102.51	113.13
11	A	303	HEC	CMC-C2C-C1C	2.88	129.81	125.42
12	A	1002	OPC	CBY-CBX-CBW	-2.88	99.80	114.37
12	B	1001	OPC	CAH-CAG-NAF	2.88	125.07	115.82
18	G	101	BCR	C36-C18-C19	-2.87	113.71	118.09
10	A	301	HEM	C4D-C3D-C2D	-2.85	102.75	106.89
18	G	101	BCR	C2-C1-C6	2.84	114.56	110.44
11	A	303	HEC	O1A-CGA-CBA	-2.82	114.14	123.09
12	B	1001	OPC	OAI-CAH-CAG	2.82	123.23	109.65
18	G	101	BCR	C32-C1-C2	2.82	119.77	108.95
10	A	302	HEM	CHD-C1D-C2D	-2.82	120.58	125.03
15	B	201	CLA	CAC-C3C-C2C	2.82	132.73	127.56
18	G	101	BCR	C34-C9-C8	2.82	122.39	118.09
14	A	501	QNO	C4-C3-C2	2.80	120.56	118.45
17	D	201	SQD	O48-C23-C24	2.79	120.33	111.83
13	C	1101	UMQ	O1-C4'-C5'	2.78	116.78	109.48
10	C	301	HEM	CMC-C2C-C3C	-2.74	121.80	128.43
18	G	101	BCR	C10-C11-C12	-2.71	115.36	123.20
15	B	201	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
15	B	201	CLA	CBA-CAA-C2A	-2.66	105.87	113.79
18	G	101	BCR	C29-C30-C25	-2.66	106.58	110.44
10	A	301	HEM	C2C-C1C-NC	2.66	114.56	109.64
10	C	301	HEM	CMC-C2C-C1C	2.65	129.40	124.73
18	G	101	BCR	C36-C18-C17	2.65	127.11	122.82
15	B	201	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
13	A	1102	UMQ	O2-C2-C1	2.64	116.37	110.08
10	A	301	HEM	CBD-CAD-C3D	-2.62	105.28	112.53
10	A	302	HEM	C4C-NC-C1C	-2.61	101.57	105.82
11	A	303	HEC	CAD-CBD-CGD	2.61	120.58	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1102	UMQ	C2'-C3'-C4'	2.60	115.57	109.68
10	A	302	HEM	C3B-C2B-C1B	2.59	108.36	106.41
13	A	1104	UMQ	C1-O1-C4'	2.59	124.11	117.98
15	B	201	CLA	C14-C13-C12	2.58	120.48	111.27
18	G	101	BCR	C16-C17-C18	-2.58	123.66	127.28
10	C	301	HEM	CBD-CAD-C3D	-2.57	105.42	112.53
15	B	201	CLA	CMA-C3A-C4A	-2.56	104.89	111.77
17	D	201	SQD	C46-O48-C23	2.56	126.47	117.12
12	B	1001	OPC	CBG-NAF-CAE	-2.55	102.27	108.98
12	A	1002	OPC	CAZ-CAY-CAX	2.54	126.09	113.86
13	A	1102	UMQ	O2'-C2'-C3'	2.54	116.35	110.38
10	A	301	HEM	CHB-C1B-NB	-2.54	121.23	124.37
10	A	301	HEM	CHD-C1D-ND	2.52	127.14	124.42
10	C	301	HEM	CBC-CAC-C3C	-2.52	114.94	127.53
13	A	1103	UMQ	O5-C1-C2	2.51	115.52	110.37
11	A	303	HEC	CHD-C1D-ND	2.50	128.39	123.86
12	A	1002	OPC	CBG-NAF-CAG	2.50	119.83	109.91
15	B	201	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
10	C	301	HEM	CAB-C3B-C2B	-2.48	120.35	128.43
15	B	201	CLA	CGD-CBD-CAD	-2.48	102.83	110.85
12	A	1002	OPC	CAE-NAF-CAG	2.47	119.74	109.91
10	C	301	HEM	C2C-C1C-NC	-2.47	105.06	109.64
15	B	201	CLA	C12-C11-C10	2.47	124.35	113.28
18	G	101	BCR	C37-C22-C21	-2.47	118.81	122.82
10	A	302	HEM	C2B-C1B-NB	-2.46	107.02	109.84
13	A	1103	UMQ	O2-C2-C1	2.45	115.91	110.08
18	G	101	BCR	C23-C22-C21	-2.44	115.17	119.01
12	B	1001	OPC	CBP-CBQ-CBR	2.42	126.14	112.60
10	A	301	HEM	CAC-C3C-C4C	-2.42	119.05	124.82
18	G	101	BCR	C2-C3-C4	2.40	116.55	111.28
11	A	303	HEC	CMA-C3A-C4A	-2.40	120.51	124.73
12	B	1001	OPC	CBZ-CBY-CBX	2.38	126.42	114.37
10	A	302	HEM	C4A-CHB-C1B	-2.38	120.64	126.25
13	A	1103	UMQ	O3'-C3'-C4'	-2.37	103.85	109.94
17	D	201	SQD	O48-C23-O10	-2.37	117.71	123.63
10	A	301	HEM	CAB-C3B-C2B	-2.37	120.74	128.43
15	B	201	CLA	C4D-C3D-CAD	2.36	110.67	108.11
18	G	101	BCR	C24-C25-C26	-2.36	116.12	121.56
12	A	1002	OPC	CBB-CBC-CBD	2.35	126.26	114.37
13	A	1103	UMQ	O4-C4-C3	2.35	115.92	110.38
10	A	302	HEM	CBD-CAD-C3D	-2.34	106.05	112.53
12	B	1001	OPC	OBJ-CBI-CAM	2.33	115.11	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1102	UMQ	O5'-C5'-C4'	2.31	114.50	109.72
13	C	1101	UMQ	O5-C5-C6	2.31	112.17	106.44
18	G	101	BCR	C35-C13-C12	2.30	121.61	118.09
11	A	303	HEC	C3D-C4D-ND	2.30	112.70	110.15
10	C	301	HEM	C2B-C1B-NB	2.29	112.47	109.84
11	A	303	HEC	C1D-C2D-C3D	2.28	109.43	106.82
10	A	301	HEM	CHA-C4D-C3D	-2.28	121.03	125.23
12	A	1002	OPC	OBJ-CBK-CBL	2.27	118.77	111.83
13	C	1101	UMQ	O1-C1-C2	2.27	113.67	108.09
18	G	101	BCR	C11-C12-C13	2.26	132.56	126.36
12	A	1002	OPC	OAD-CAO-CAP	-2.26	114.96	123.78
12	B	1001	OPC	CBW-CBV-CBU	2.25	125.74	114.37
13	A	1104	UMQ	O3'-C3'-C4'	2.24	115.67	109.94
13	A	1104	UMQ	C1-O5-C5	2.24	118.09	113.72
10	A	301	HEM	C4A-NA-C1A	-2.22	102.20	105.82
15	B	201	CLA	OBD-CAD-C3D	2.22	133.60	128.42
17	D	201	SQD	C45-O47-C7	2.20	123.07	117.80
10	A	302	HEM	CMB-C2B-C1B	2.19	128.45	125.03
11	A	303	HEC	CHC-C4B-NB	-2.18	122.08	124.45
11	A	303	HEC	C4D-ND-C1D	2.18	109.37	105.82
17	D	201	SQD	C36-C35-C34	2.17	125.32	114.37
11	A	303	HEC	O2A-CGA-CBA	2.16	120.84	114.00
10	A	302	HEM	CMB-C2B-C3B	-2.16	123.19	128.43
12	A	1002	OPC	CBQ-CBR-CBS	-2.15	108.72	124.83
17	D	201	SQD	O9-S-O7	-2.14	106.86	113.82
10	A	301	HEM	CAA-C2A-C1A	2.14	129.12	124.94
15	B	201	CLA	C7-C6-C5	2.13	118.93	113.26
10	C	301	HEM	O2A-CGA-CBA	2.12	120.71	114.00
18	G	101	BCR	C1-C6-C7	2.11	121.37	115.65
17	D	201	SQD	C19-C18-C17	2.09	124.91	114.37
12	A	1002	OPC	CBM-CBL-CBK	-2.08	106.06	113.69
14	A	501	QNO	C3-C2-N1	-2.08	116.66	118.94
10	A	301	HEM	C2A-C1A-NA	2.07	112.45	110.15
12	B	1001	OPC	CAT-CAU-CAV	2.06	124.15	112.60
13	A	1104	UMQ	C1-C2-C3	2.06	114.34	110.01
15	B	201	CLA	C3A-C2A-C1A	2.06	104.42	101.34
12	A	1002	OPC	OBJ-CBI-CAM	2.05	114.30	108.40
13	A	1102	UMQ	O5'-C5'-C6'	2.02	111.45	106.44
13	C	1101	UMQ	O4-C4-C3	2.02	115.14	110.38
13	A	1104	UMQ	O5-C5-C4	2.02	113.33	109.70
13	A	1104	UMQ	O4-C4-C5	2.01	114.28	109.32
10	A	302	HEM	CMA-C3A-C4A	2.01	128.48	125.42

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1102	UMQ	C2'
13	A	1102	UMQ	C1'
13	A	1103	UMQ	C2'
13	A	1103	UMQ	C1'
13	A	1104	UMQ	C2'
13	A	1104	UMQ	C1'
13	C	1101	UMQ	C2'
13	C	1101	UMQ	C1'
14	A	501	QNO	C2
15	B	201	CLA	C8
15	B	201	CLA	ND
17	D	201	SQD	C3
17	D	201	SQD	C5
17	D	201	SQD	C4

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	303	HEC	C2B-C3B-CAB-CBB
11	A	303	HEC	C4B-C3B-CAB-CBB
11	A	303	HEC	C2C-C3C-CAC-CBC
11	A	303	HEC	C4C-C3C-CAC-CBC
12	A	1002	OPC	NAF-CAG-CAH-OAI
12	A	1002	OPC	CBO-CBP-CBQ-CBR
12	B	1001	OPC	CAH-OAI-PAJ-OAK
12	B	1001	OPC	CAH-OAI-PAJ-OBH
12	B	1001	OPC	CAH-OAI-PAJ-OAB
12	B	1001	OPC	NAF-CAG-CAH-OAI
12	B	1001	OPC	CBO-CBP-CBQ-CBR
13	A	1102	UMQ	C3'-C4'-O1-C1
13	A	1102	UMQ	O5'-C1'-O1'-CA
13	A	1103	UMQ	O5'-C1'-O1'-CA
13	A	1103	UMQ	CB-CA-O1'-C1'
13	C	1101	UMQ	O5'-C1'-O1'-CA
15	B	201	CLA	C1A-C2A-CAA-CBA
15	B	201	CLA	C3A-C2A-CAA-CBA
15	B	201	CLA	O2A-C1-C2-C3
17	D	201	SQD	O5-C1-O6-C44
17	D	201	SQD	O49-C7-O47-C45
17	D	201	SQD	C8-C7-O47-C45
17	D	201	SQD	O5-C5-C6-S
18	G	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
15	B	201	CLA	CBD-CGD-O2D-CED
15	B	201	CLA	O1D-CGD-O2D-CED
13	A	1104	UMQ	O5-C1-O1-C4'
12	B	1001	OPC	OAD-CAO-OAN-CAM
17	D	201	SQD	C24-C23-O48-C46
12	B	1001	OPC	CAP-CAO-OAN-CAM
13	A	1103	UMQ	O5-C5-C6-O6
17	D	201	SQD	O10-C23-O48-C46
17	D	201	SQD	C31-C32-C33-C34
17	D	201	SQD	C33-C34-C35-C36
13	A	1104	UMQ	O5'-C5'-C6'-O6'
17	D	201	SQD	C13-C14-C15-C16
17	D	201	SQD	C12-C13-C14-C15
15	B	201	CLA	C3-C5-C6-C7
13	A	1102	UMQ	O5'-C5'-C6'-O6'
12	A	1002	OPC	CAQ-CAR-CAS-CAT
11	A	303	HEC	C2A-CAA-CBA-CGA
13	A	1104	UMQ	C4'-C5'-C6'-O6'
13	A	1104	UMQ	O5'-C1'-O1'-CA
12	A	1002	OPC	CAZ-CBA-CBB-CBC
13	A	1104	UMQ	O5-C5-C6-O6
13	C	1101	UMQ	O5'-C5'-C6'-O6'
13	A	1103	UMQ	C4-C5-C6-O6
14	A	501	QNO	C2-C21-C22-C23
12	B	1001	OPC	CAU-CAV-CAW-CAX
13	A	1104	UMQ	CH-CI-CJ-CK
13	A	1104	UMQ	C4-C5-C6-O6
12	A	1002	OPC	CAY-CAZ-CBA-CBB
12	B	1001	OPC	CAH-CAG-NAF-CBG
13	A	1102	UMQ	C2'-C1'-O1'-CA
18	G	101	BCR	C37-C22-C23-C24
18	G	101	BCR	C7-C8-C9-C10
18	G	101	BCR	C21-C22-C23-C24
11	A	303	HEC	C3D-CAD-CBD-CGD
15	B	201	CLA	C13-C15-C16-C17
12	B	1001	OPC	CBK-CBL-CBM-CBN
13	C	1101	UMQ	C4'-C5'-C6'-O6'
12	A	1002	OPC	CAH-CAG-NAF-CAA
13	A	1102	UMQ	C4'-C5'-C6'-O6'
17	D	201	SQD	C44-C45-O47-C7
15	B	201	CLA	C16-C17-C18-C20
13	A	1102	UMQ	CA-CB-CC-CD

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Mol	Chain	Res	Type	Atoms
12	B	1001	OPC	CAH-CAG-NAF-CAA
13	A	1103	UMQ	CH-CI-CJ-CK
13	A	1104	UMQ	CB-CC-CD-CF
13	A	1104	UMQ	CB-CA-O1'-C1'
13	C	1101	UMQ	CB-CA-O1'-C1'
12	B	1001	OPC	CBM-CBN-CBO-CBP
17	D	201	SQD	C29-C30-C31-C32
11	A	303	HEC	C2D-C3D-CAD-CBD
17	D	201	SQD	C15-C16-C17-C18
13	A	1103	UMQ	C3'-C4'-O1-C1
13	A	1103	UMQ	CF-CG-CH-CI
12	A	1002	OPC	CBK-CBL-CBM-CBN
18	G	101	BCR	C1-C6-C7-C8
18	G	101	BCR	C5-C6-C7-C8
18	G	101	BCR	C23-C24-C25-C26
17	D	201	SQD	C16-C17-C18-C19
12	A	1002	OPC	CBY-CBZ-CCA-CCB
12	A	1002	OPC	CBL-CBM-CBN-CBO
13	A	1104	UMQ	CG-CH-CI-CJ
17	D	201	SQD	C10-C11-C12-C13
13	A	1102	UMQ	CB-CC-CD-CF
17	D	201	SQD	C2-C1-O6-C44
13	C	1101	UMQ	CH-CI-CJ-CK
15	B	201	CLA	C16-C17-C18-C19
12	A	1002	OPC	CAX-CAY-CAZ-CBA
13	C	1101	UMQ	CD-CF-CG-CH
12	B	1001	OPC	CAH-CAG-NAF-CAE
12	B	1001	OPC	CAZ-CBA-CBB-CBC
17	D	201	SQD	C27-C28-C29-C30
13	A	1104	UMQ	CC-CD-CF-CG
17	D	201	SQD	C23-C24-C25-C26
13	A	1104	UMQ	C2'-C1'-O1'-CA
17	D	201	SQD	C28-C29-C30-C31
13	A	1102	UMQ	O5-C5-C6-O6
12	B	1001	OPC	CAR-CAS-CAT-CAU
14	A	501	QNO	C22-C23-C24-C25
12	A	1002	OPC	CBV-CBW-CBX-CBY
12	B	1001	OPC	CBT-CBU-CBV-CBW
13	A	1102	UMQ	CI-CJ-CK-CL
13	A	1104	UMQ	CI-CJ-CK-CL
13	A	1102	UMQ	CB-CA-O1'-C1'
14	A	501	QNO	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	B	201	CLA	C11-C10-C8-C7
15	B	201	CLA	C8-C10-C11-C12
13	A	1103	UMQ	O5-C1-O1-C4'
17	D	201	SQD	C19-C20-C21-C22
13	C	1101	UMQ	CC-CD-CF-CG
10	A	302	HEM	C1A-C2A-CAA-CBA
17	D	201	SQD	O6-C44-C45-O47
13	A	1104	UMQ	CD-CF-CG-CH
15	B	201	CLA	C5-C6-C7-C8
13	A	1103	UMQ	CB-CC-CD-CF
13	A	1103	UMQ	C5'-C4'-O1-C1
12	B	1001	OPC	OAK-CAL-CAM-OAN
12	A	1002	OPC	CAL-CAM-CBI-OBJ
10	C	301	HEM	C4B-C3B-CAB-CBB
12	A	1002	OPC	OAN-CAM-CBI-OBJ
12	B	1001	OPC	CBU-CBV-CBW-CBX
13	A	1103	UMQ	CI-CJ-CK-CL
13	A	1104	UMQ	CF-CG-CH-CI
12	B	1001	OPC	OAK-CAL-CAM-CBI
12	A	1002	OPC	OAK-CAL-CAM-OAN
13	A	1104	UMQ	O1'-CA-CB-CC
12	A	1002	OPC	CAH-CAG-NAF-CAE
17	D	201	SQD	O6-C44-C45-C46
12	A	1002	OPC	CBP-CBQ-CBR-CBS
12	B	1001	OPC	CBP-CBQ-CBR-CBS
18	G	101	BCR	C23-C24-C25-C30
11	A	303	HEC	C4D-C3D-CAD-CBD
12	A	1002	OPC	OAN-CAO-CAP-CAQ
13	C	1101	UMQ	CF-CG-CH-CI
17	D	201	SQD	C25-C26-C27-C28
18	G	101	BCR	C11-C10-C9-C34
10	A	301	HEM	C3D-CAD-CBD-CGD
12	B	1001	OPC	CAS-CAT-CAU-CAV
18	G	101	BCR	C11-C10-C9-C8
10	C	301	HEM	CAD-CBD-CGD-O1D
12	A	1002	OPC	CAM-CAL-OAK-PAJ
11	A	303	HEC	CAA-CBA-CGA-O2A
10	A	301	HEM	CAA-CBA-CGA-O1A
10	A	302	HEM	CAD-CBD-CGD-O2D
10	A	301	HEM	CAA-CBA-CGA-O2A
11	A	303	HEC	CAA-CBA-CGA-O1A
11	A	303	HEC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	501	QNO	N1-C2-C21-C22
17	D	201	SQD	C24-C25-C26-C27
10	C	301	HEM	CAD-CBD-CGD-O2D
10	A	302	HEM	CAD-CBD-CGD-O1D
13	A	1102	UMQ	CC-CD-CF-CG
12	B	1001	OPC	CBL-CBK-OBJ-CBI
13	C	1101	UMQ	CG-CH-CI-CJ
12	A	1002	OPC	OAK-CAL-CAM-CBI
12	A	1002	OPC	CAT-CAU-CAV-CAW
11	A	303	HEC	CAD-CBD-CGD-O1D
12	A	1002	OPC	OCC-CBK-OBJ-CBI
13	A	1103	UMQ	O1'-CA-CB-CC
17	D	201	SQD	C5-C6-S-O9
12	A	1002	OPC	CBU-CBV-CBW-CBX
13	A	1102	UMQ	CH-CI-CJ-CK
12	A	1002	OPC	CBL-CBK-OBJ-CBI
11	A	303	HEC	CAD-CBD-CGD-O2D

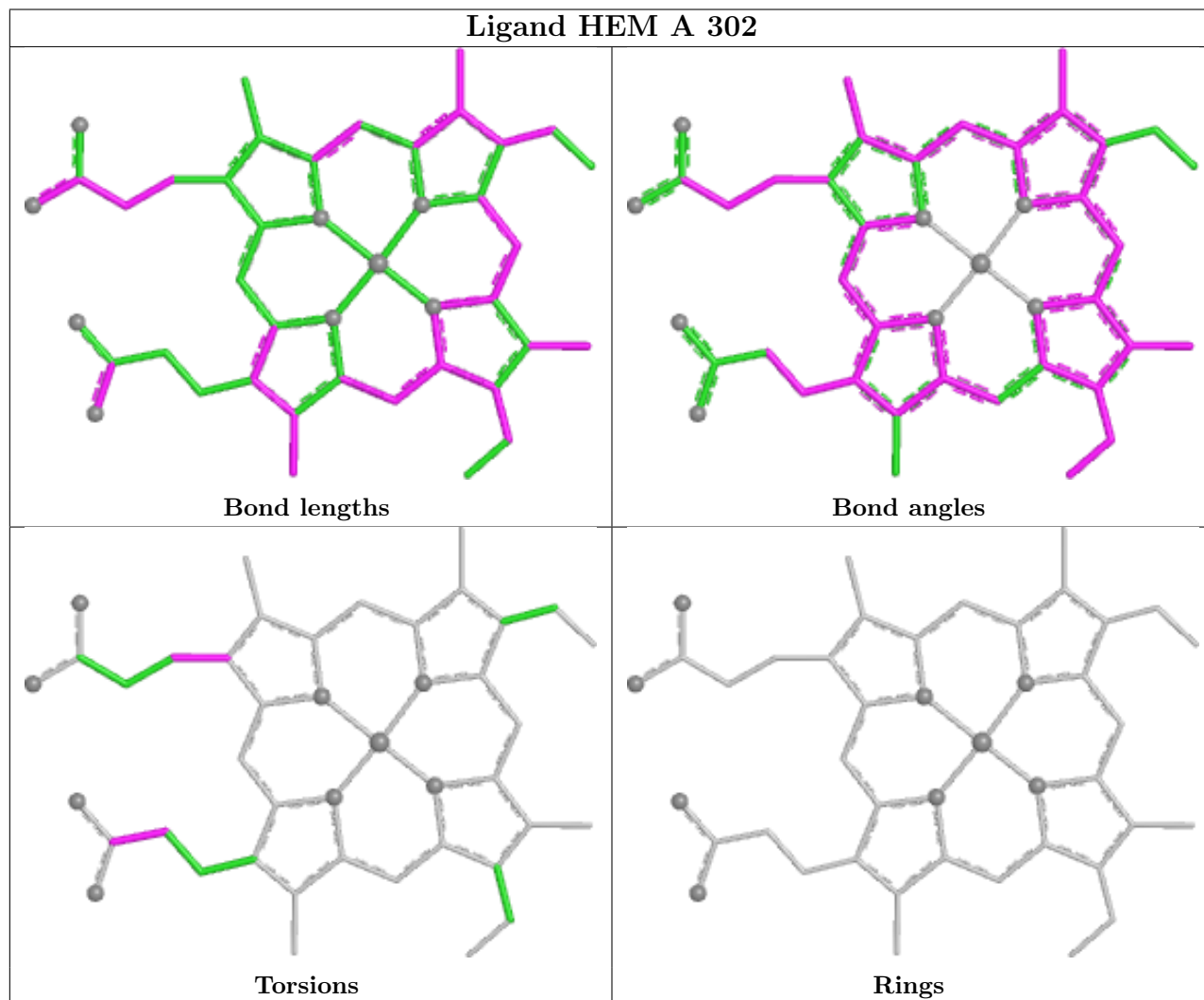
There are no ring outliers.

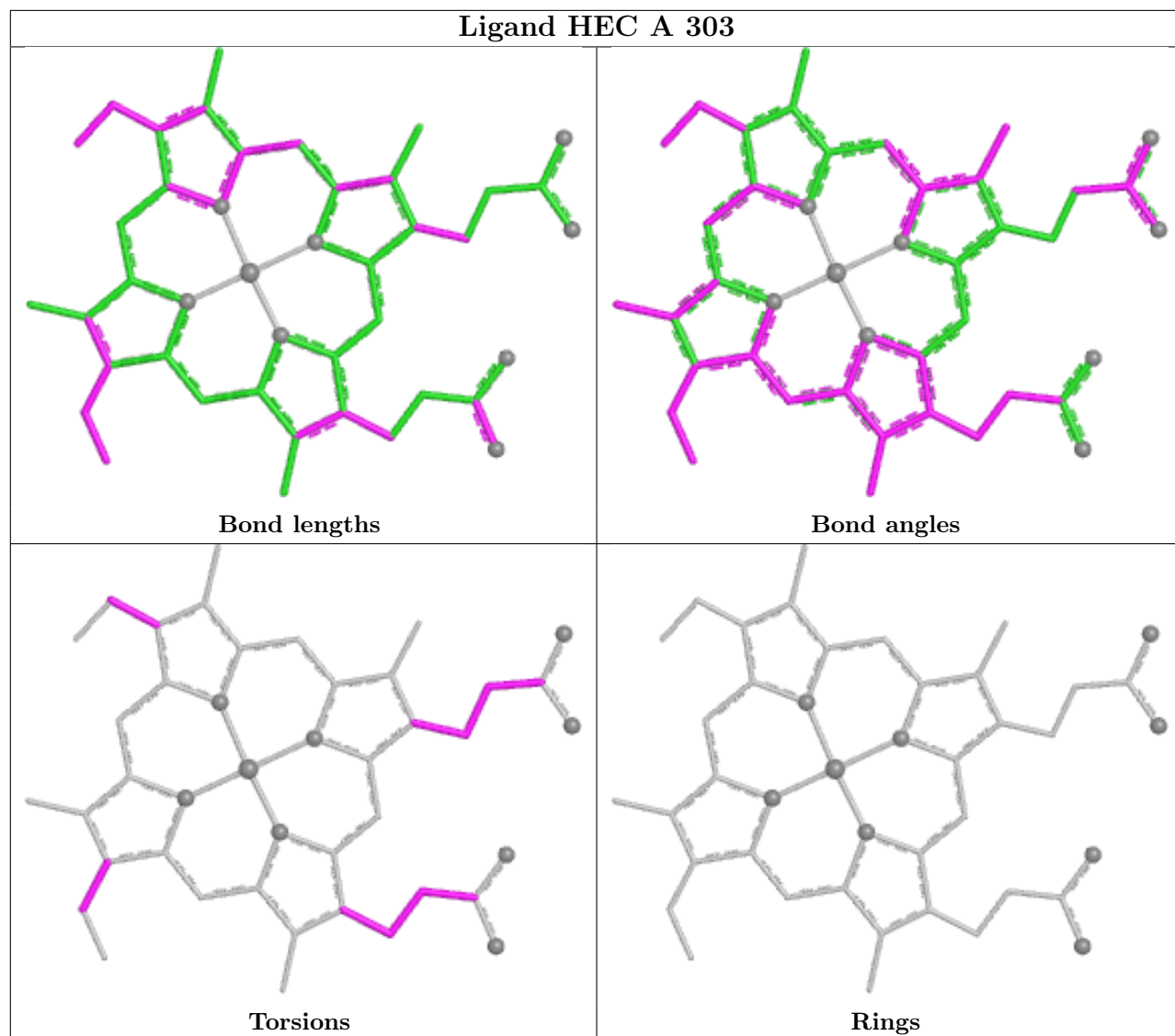
15 monomers are involved in 186 short contacts:

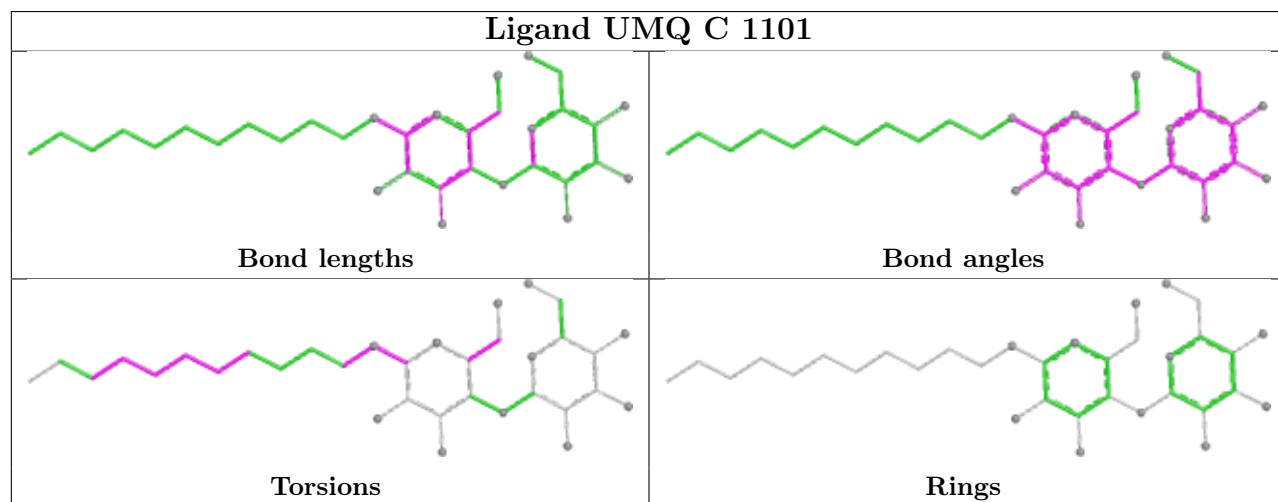
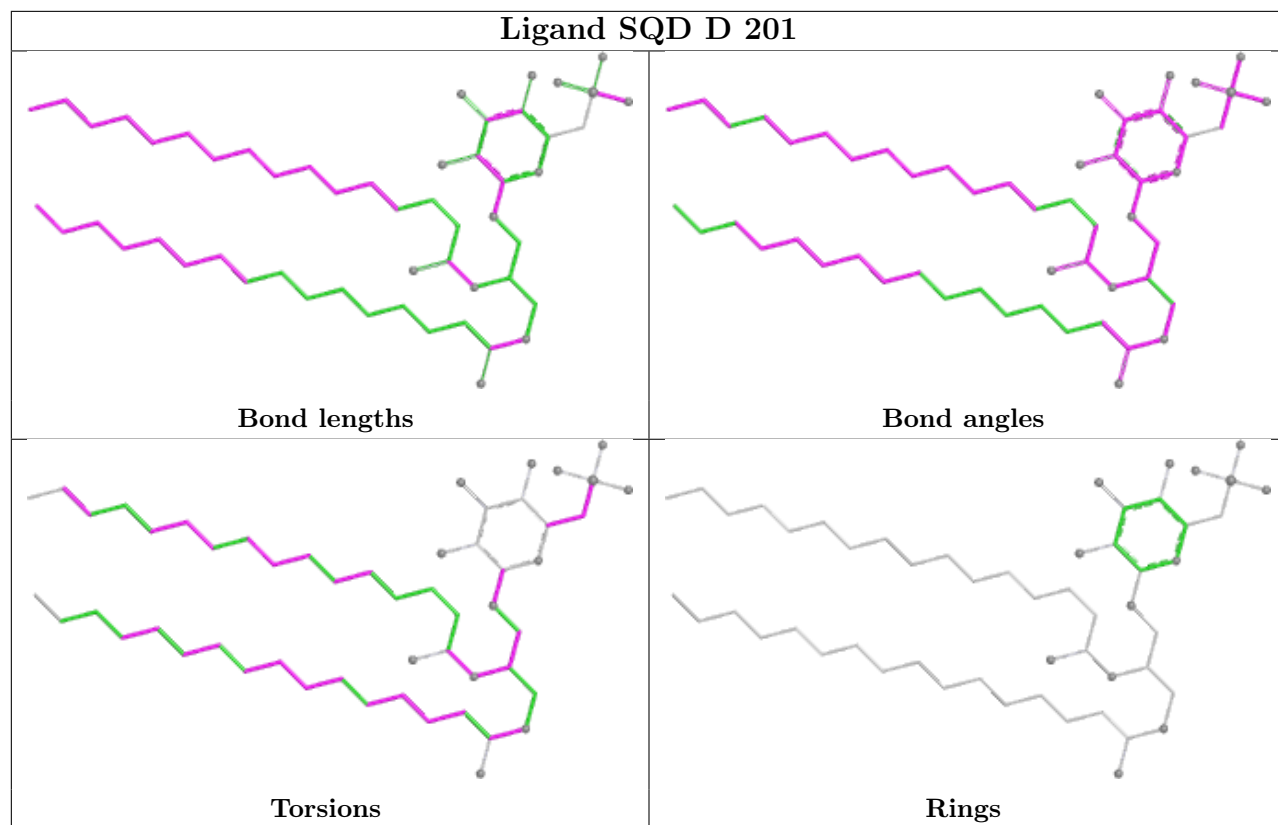
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	302	HEM	25	0
11	A	303	HEC	10	0
16	D	200	FES	3	0
17	D	201	SQD	11	0
13	C	1101	UMQ	10	0
14	A	501	QNO	7	0
13	A	1104	UMQ	2	0
13	A	1102	UMQ	9	0
12	B	1001	OPC	11	0
13	A	1103	UMQ	2	0
12	A	1002	OPC	26	0
10	A	301	HEM	22	0
15	B	201	CLA	14	0
10	C	301	HEM	23	0
18	G	101	BCR	13	0

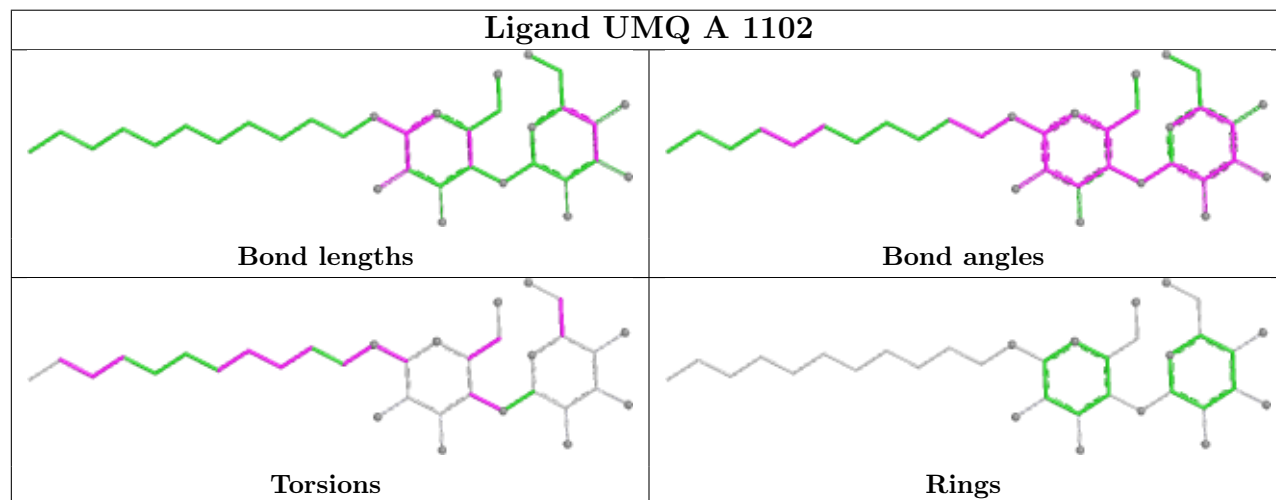
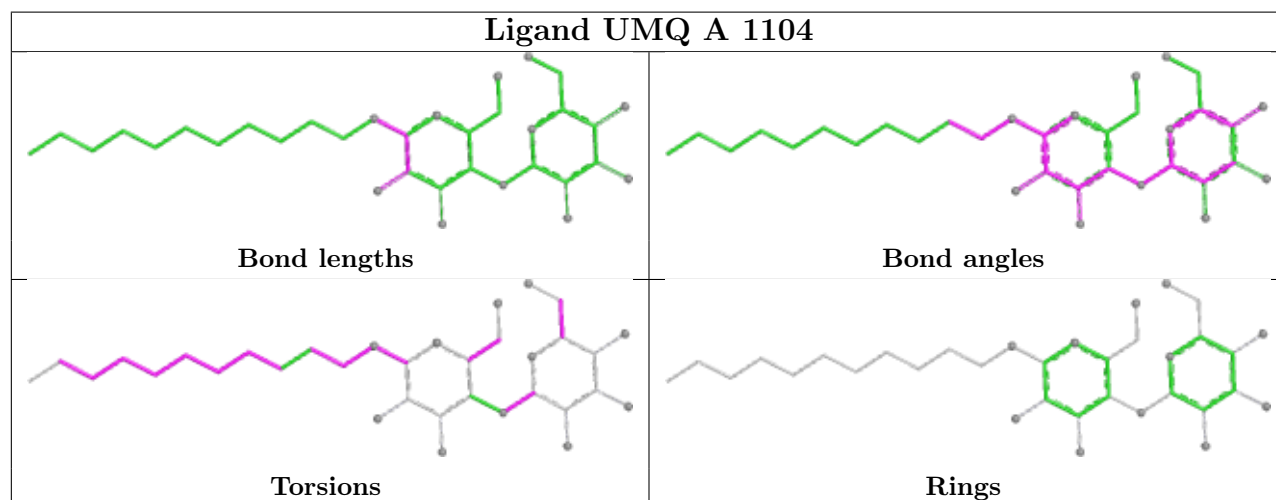
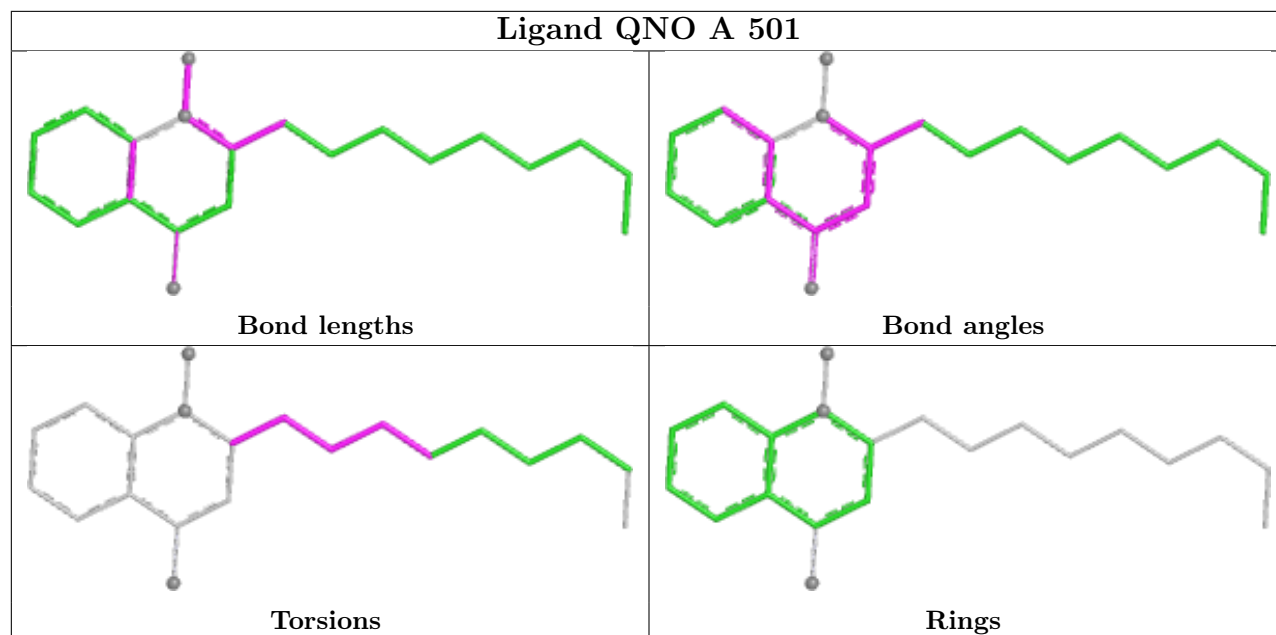
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

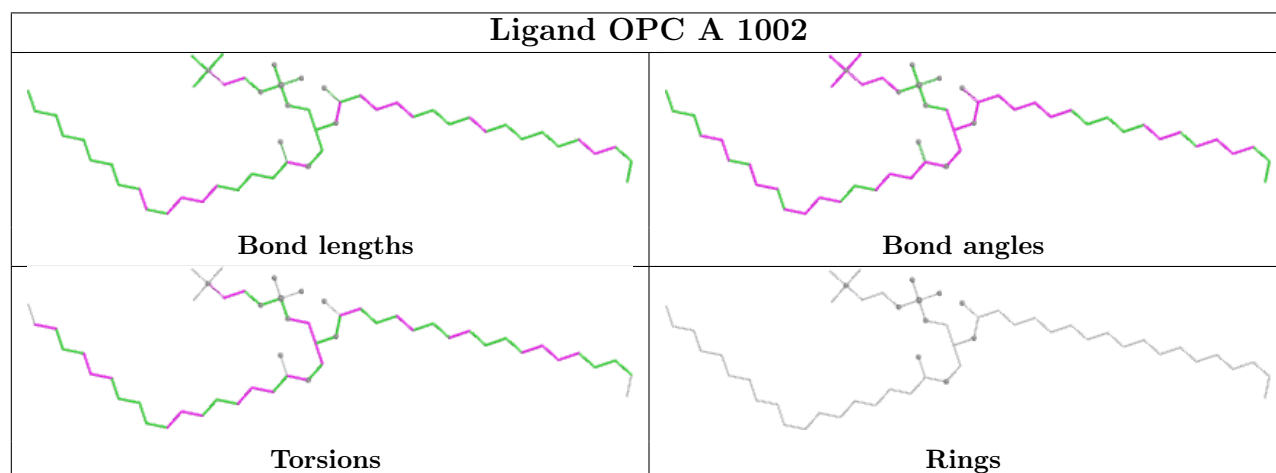
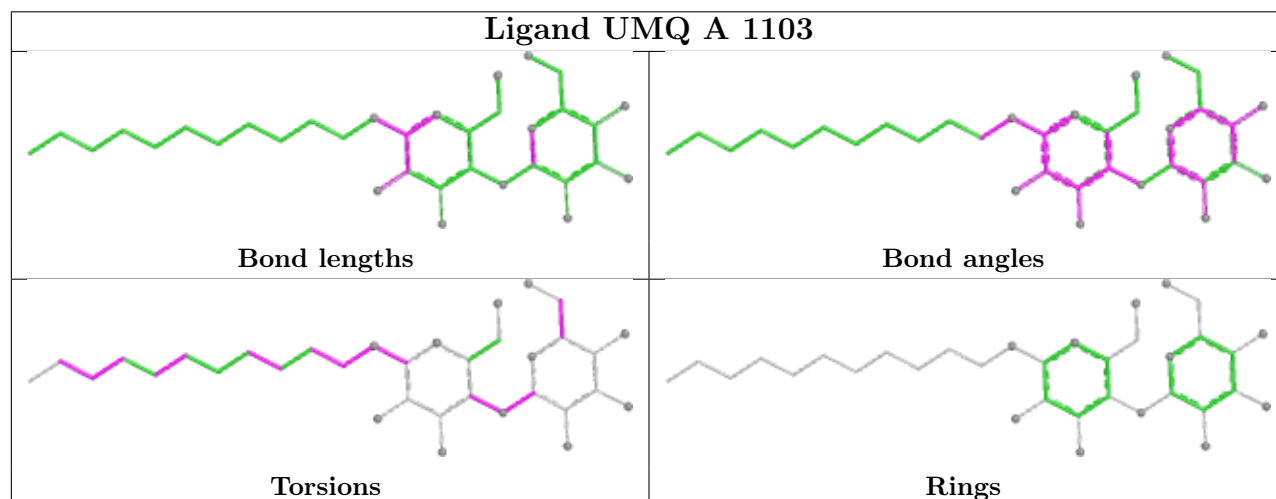
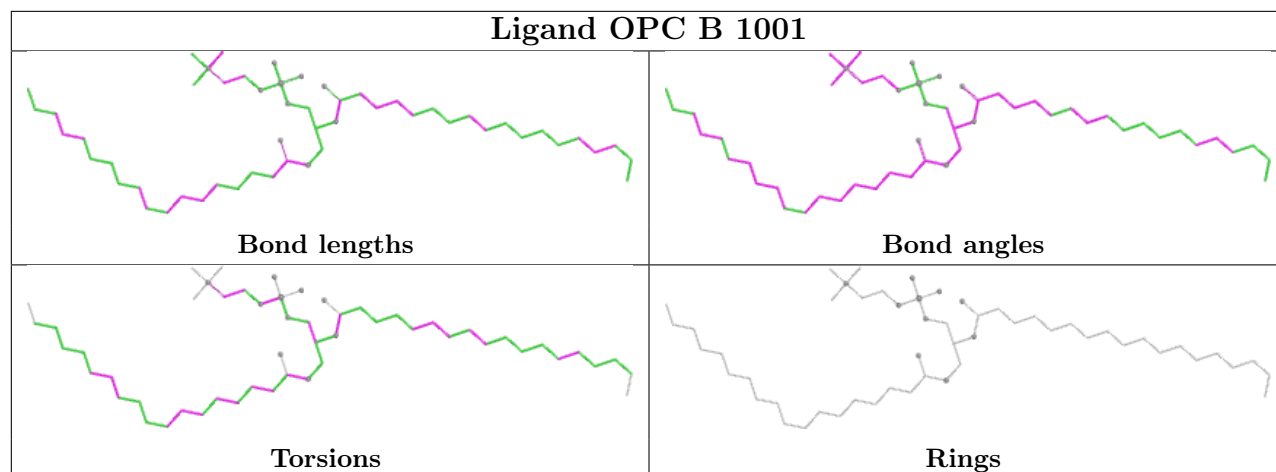
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

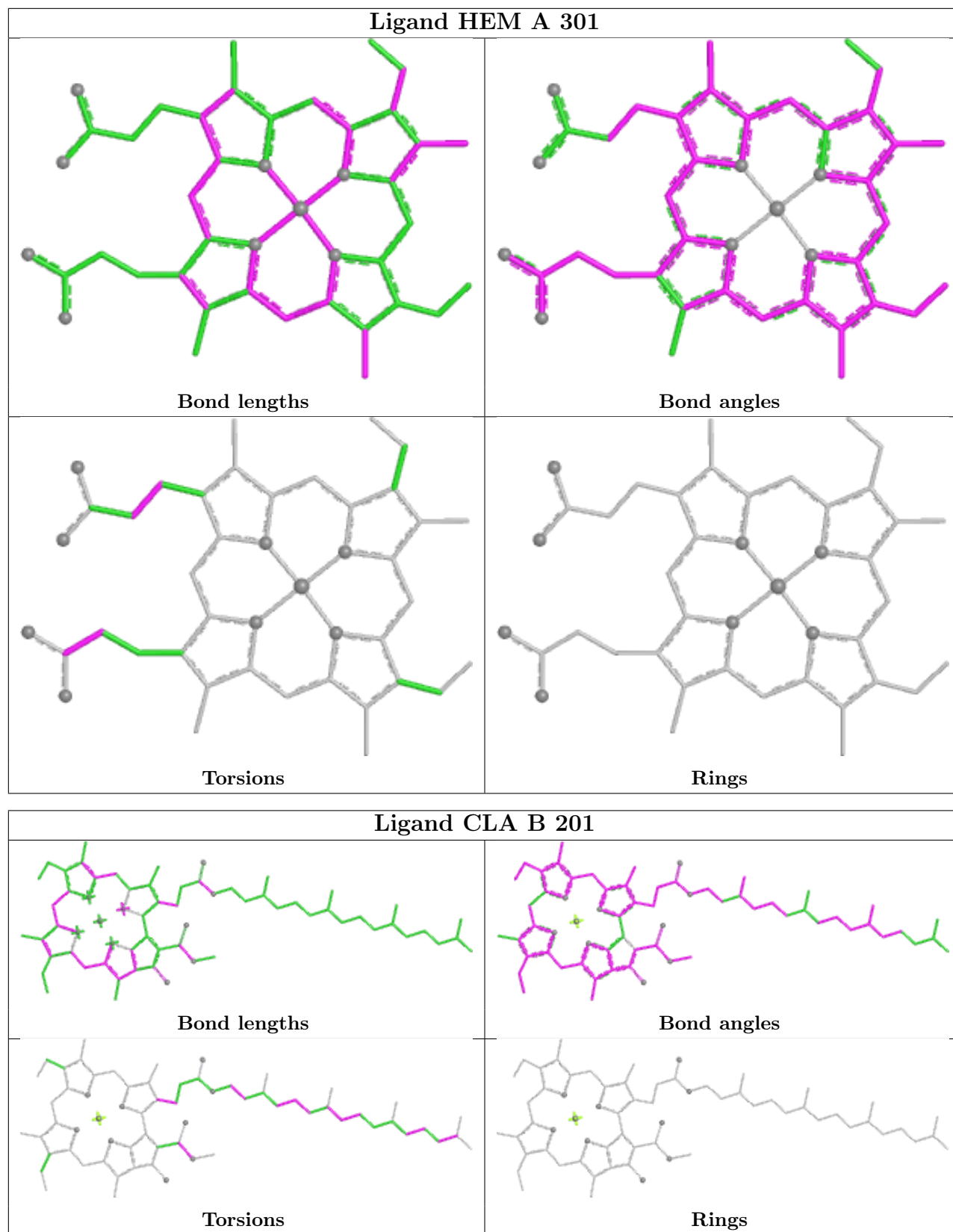


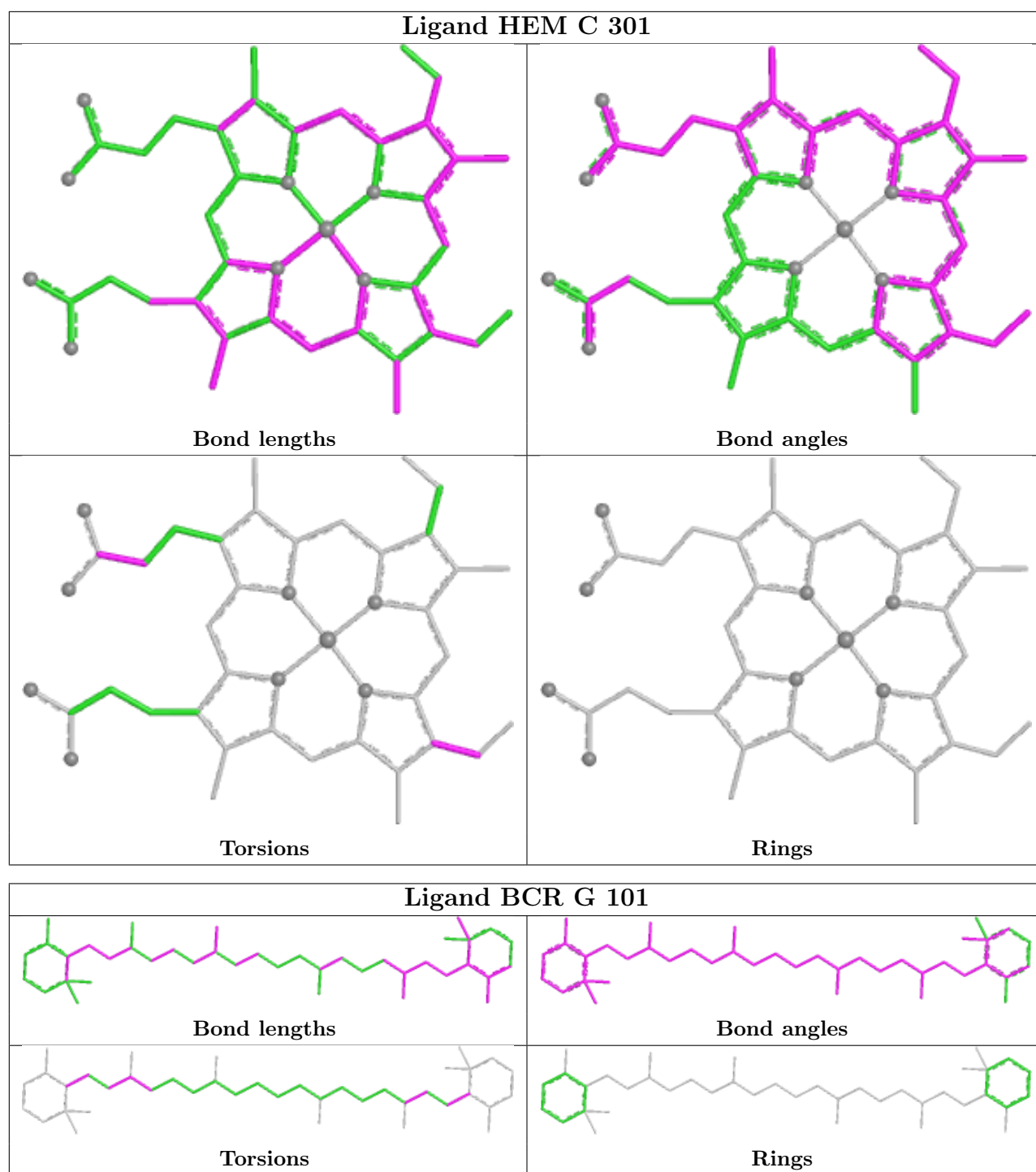












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/215 (100%)	-0.54	1 (0%) 87 66	4, 22, 60, 162	0
2	B	160/160 (100%)	-0.12	5 (3%) 51 28	9, 41, 93, 133	0
3	C	288/289 (99%)	1.06	63 (21%) 2 2	2, 47, 145, 170	1 (0%)
4	D	166/179 (92%)	1.70	48 (28%) 1 1	8, 101, 150, 182	0
5	E	32/32 (100%)	-0.25	1 (3%) 51 28	22, 52, 98, 119	0
6	F	32/35 (91%)	0.10	1 (3%) 51 28	10, 41, 112, 123	0
7	G	37/37 (100%)	-0.06	2 (5%) 31 18	13, 33, 115, 123	0
8	H	29/29 (100%)	-0.40	1 (3%) 48 26	15, 28, 50, 97	0
All	All	959/976 (98%)	0.45	122 (12%) 8 6	2, 42, 139, 182	1 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	145	PRO	13.5
4	D	144	ALA	13.4
4	D	179	VAL	11.9
4	D	177	TRP	9.5
4	D	143	PRO	8.7
3	C	40	VAL	6.7
4	D	146	LEU	6.6
4	D	141	ARG	6.1
7	G	37	GLY	6.1
4	D	142	GLY	6.1
3	C	241	GLY	6.0
4	D	173	GLY	5.8
4	D	157	ASP	5.7
3	C	184	ALA	5.5
4	D	175	LYS	5.4
4	D	156	GLN	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	49	ALA	5.2
3	C	80	GLU	5.2
3	C	287	MET	5.1
4	D	50	VAL	5.0
4	D	147	SER	5.0
3	C	244	ASP	4.9
3	C	196	GLN	4.9
3	C	285	ALA	4.5
4	D	168	THR	4.4
3	C	208	VAL	4.3
3	C	286	GLU	4.2
3	C	288	ASN	4.2
4	D	160	ILE	4.1
4	D	178	TRP	4.1
3	C	189	GLU	4.0
3	C	20	ILE	3.9
3	C	195	TYR	3.9
4	D	174	GLU	3.9
4	D	71	GLU	3.8
4	D	109	THR	3.7
3	C	100	ASP	3.7
3	C	68	VAL	3.5
4	D	75	ALA	3.5
5	E	2	ILE	3.5
4	D	77	ASP	3.5
3	C	193	VAL	3.4
3	C	207	VAL	3.4
3	C	18	GLY	3.4
3	C	165	GLU	3.4
3	C	243	ASP	3.4
4	D	128	CYS	3.3
8	H	1	MET	3.2
3	C	109	GLY	3.2
4	D	10	VAL	3.2
3	C	14	ARG	3.1
3	C	32	ALA	3.1
3	C	240	PHE	3.0
3	C	242	GLN	3.0
4	D	73	HIS	3.0
4	D	85	LYS	2.9
4	D	62	ASN	2.9
4	D	91	ILE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	194	LYS	2.8
3	C	29	ALA	2.8
3	C	281	LYS	2.8
7	G	32	PRO	2.8
3	C	13	PRO	2.7
4	D	61	GLY	2.7
3	C	190	TYR	2.7
3	C	186	GLU	2.7
3	C	140	LYS	2.6
4	D	172	THR	2.6
1	A	160	VAL	2.5
4	D	170	PHE	2.5
3	C	256	LYS	2.5
2	B	16	ALA	2.5
3	C	28	ALA	2.5
3	C	198	SER	2.5
3	C	145	GLY	2.5
3	C	206	THR	2.5
4	D	155	VAL	2.5
3	C	67	LYS	2.4
3	C	192	ASN	2.4
4	D	16	ARG	2.4
4	D	158	ASP	2.4
3	C	74	ALA	2.4
3	C	148	ALA	2.4
3	C	111	ASP	2.3
3	C	15	GLU	2.3
4	D	135	GLU	2.3
3	C	147	TYR	2.3
3	C	185	LYS	2.3
4	D	120	ALA	2.3
2	B	155	LEU	2.3
4	D	140	ILE	2.3
3	C	59	GLN	2.3
3	C	11	PRO	2.3
3	C	211	ILE	2.3
4	D	65	LYS	2.2
6	F	1	MET	2.2
2	B	154	THR	2.2
3	C	181	THR	2.2
3	C	150	HIS	2.2
4	D	122	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	56	ALA	2.2
4	D	149	ALA	2.2
3	C	218	ILE	2.2
4	D	59	LYS	2.2
4	D	130	GLY	2.2
4	D	60	LEU	2.2
2	B	74	GLU	2.2
4	D	127	PRO	2.2
4	D	113	CYS	2.2
3	C	19	ARG	2.1
3	C	79	PRO	2.1
3	C	226	LYS	2.1
3	C	41	LEU	2.1
4	D	132	GLN	2.1
2	B	64	GLU	2.1
3	C	33	GLU	2.1
3	C	246	GLU	2.1
3	C	182	LYS	2.1
3	C	219	VAL	2.0
3	C	199	ILE	2.0
3	C	209	ASP	2.0
3	C	171	VAL	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, 95<sup>th</sup> 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
13	UMQ	C	1101	34/34	0.79	0.22	4,86,151,160	0

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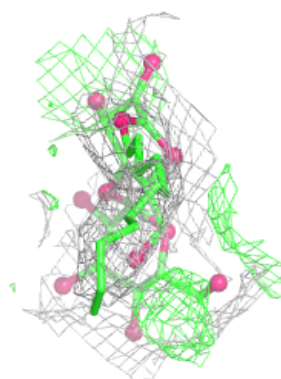
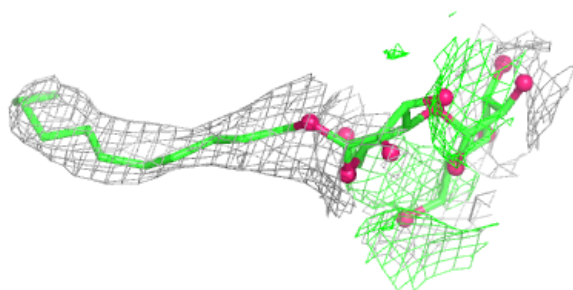
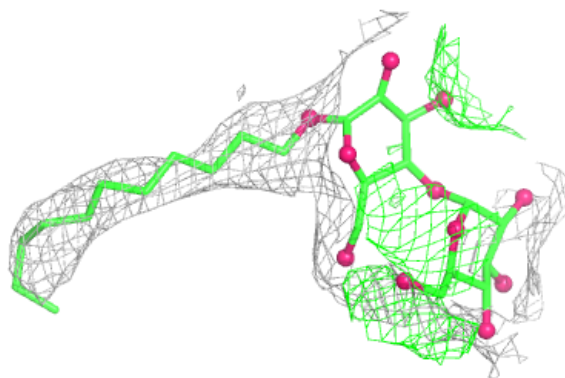
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	UMQ	A	1104	34/34	0.86	0.19	23,131,208,216	0
17	SQD	D	201	54/54	0.86	0.26	39,165,201,204	0
12	OPC	A	1002	54/55	0.87	0.22	2,64,206,220	0
18	BCR	G	101	40/40	0.89	0.20	2,49,145,149	0
13	UMQ	A	1102	34/34	0.91	0.18	31,112,145,149	0
14	QNO	A	501	21/21	0.92	0.18	45,63,95,120	0
12	OPC	B	1001	54/55	0.93	0.18	8,70,138,157	0
13	UMQ	A	1103	34/34	0.94	0.11	40,101,144,155	0
15	CLA	B	201	65/65	0.97	0.10	12,42,72,111	0
16	FES	D	200	4/4	0.97	0.09	89,90,95,104	0
11	HEC	A	303	43/43	0.98	0.07	2,35,56,61	0
9	CD	B	161	1/1	0.98	0.10	161,161,161,161	0
10	HEM	A	302	43/43	0.98	0.07	2,8,43,49	0
10	HEM	C	301	43/43	0.98	0.07	2,33,74,95	0
10	HEM	A	301	43/43	0.99	0.07	2,13,37,60	0
9	CD	A	216	1/1	1.00	0.03	47,47,47,47	0

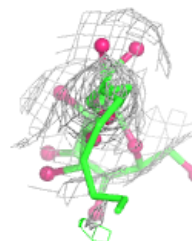
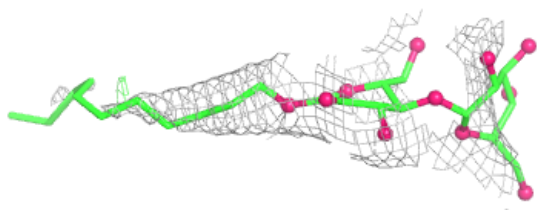
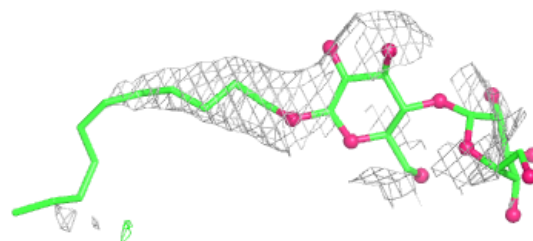
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

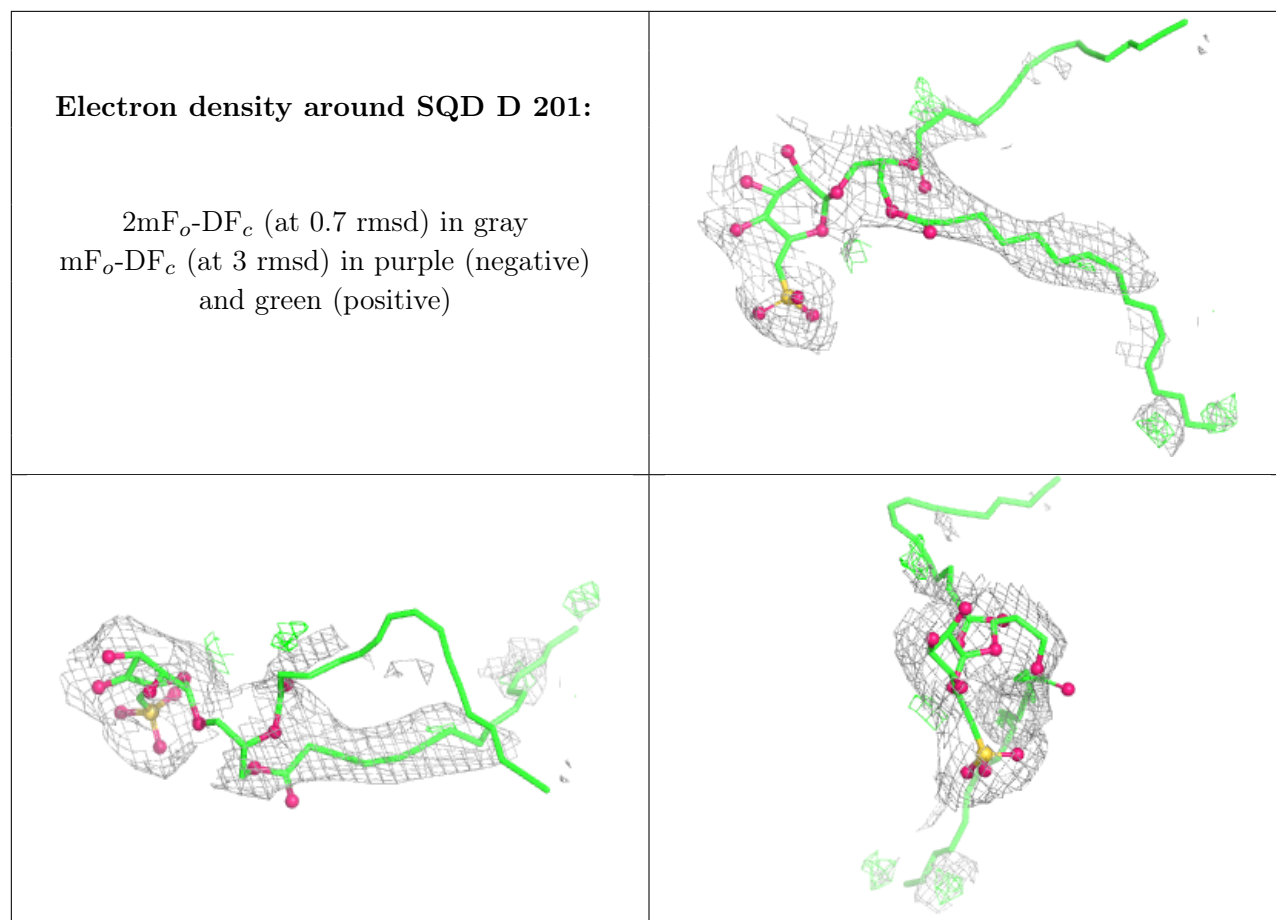
**Electron density around UMQ C 1101:**

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

**Electron density around UMQ A 1104:**

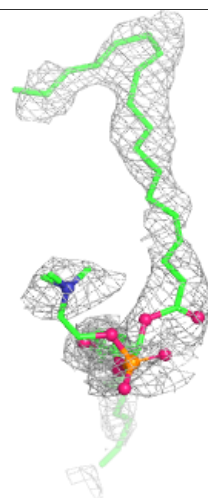
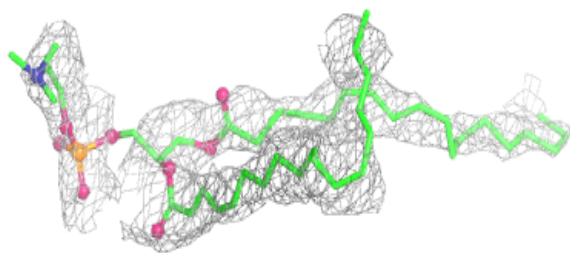
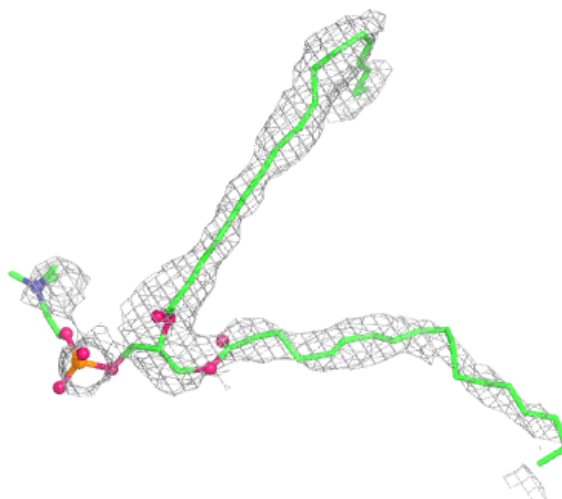
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





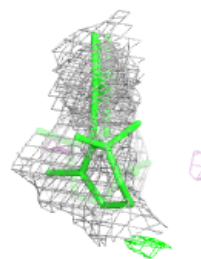
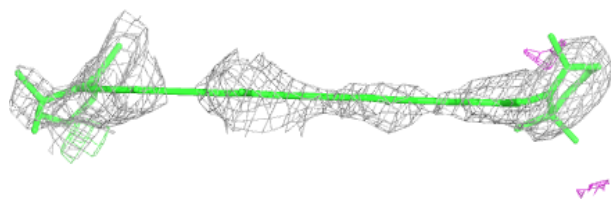
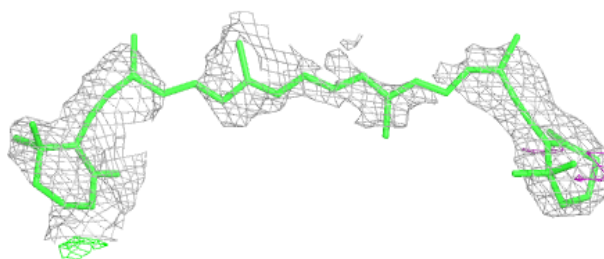
**Electron density around OPC A 1002:**

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

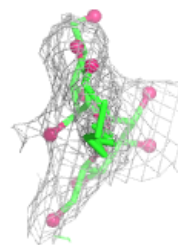
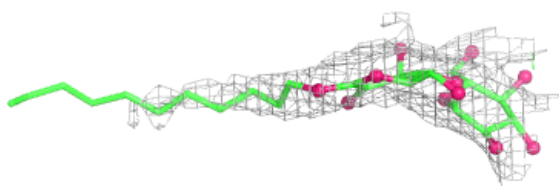
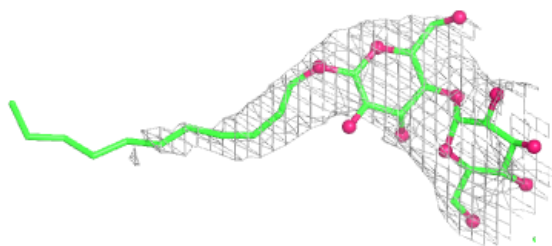


**Electron density around BCR G 101:**

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

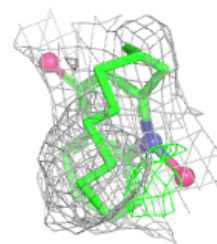
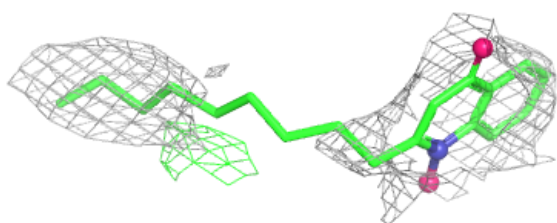
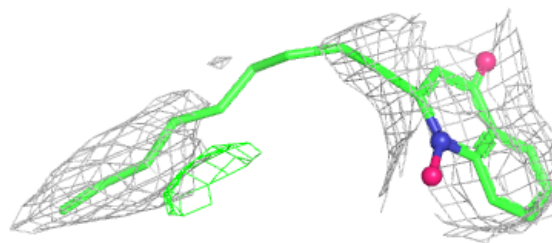
**Electron density around UMQ A 1102:**

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

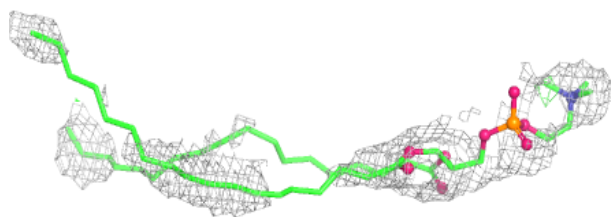
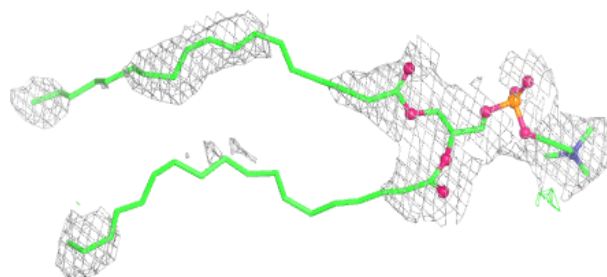


**Electron density around QNO A 501:**

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

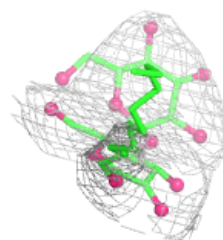
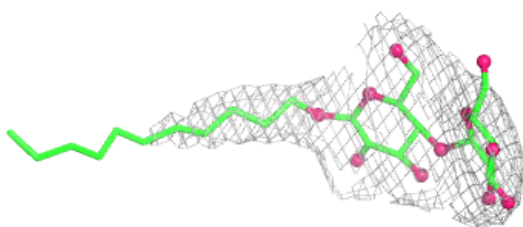
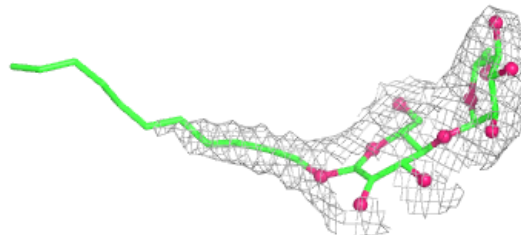
**Electron density around OPC B 1001:**

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

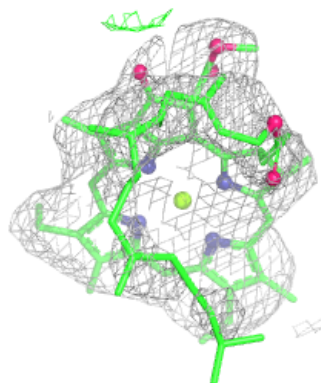
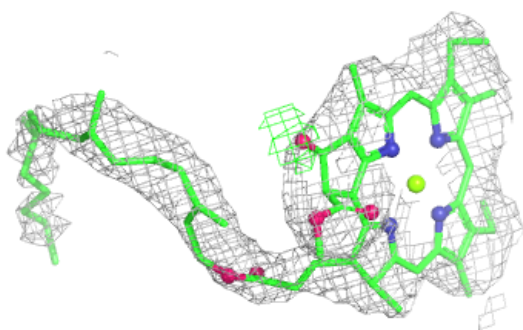
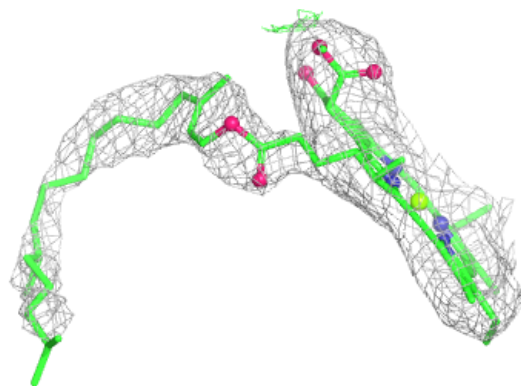


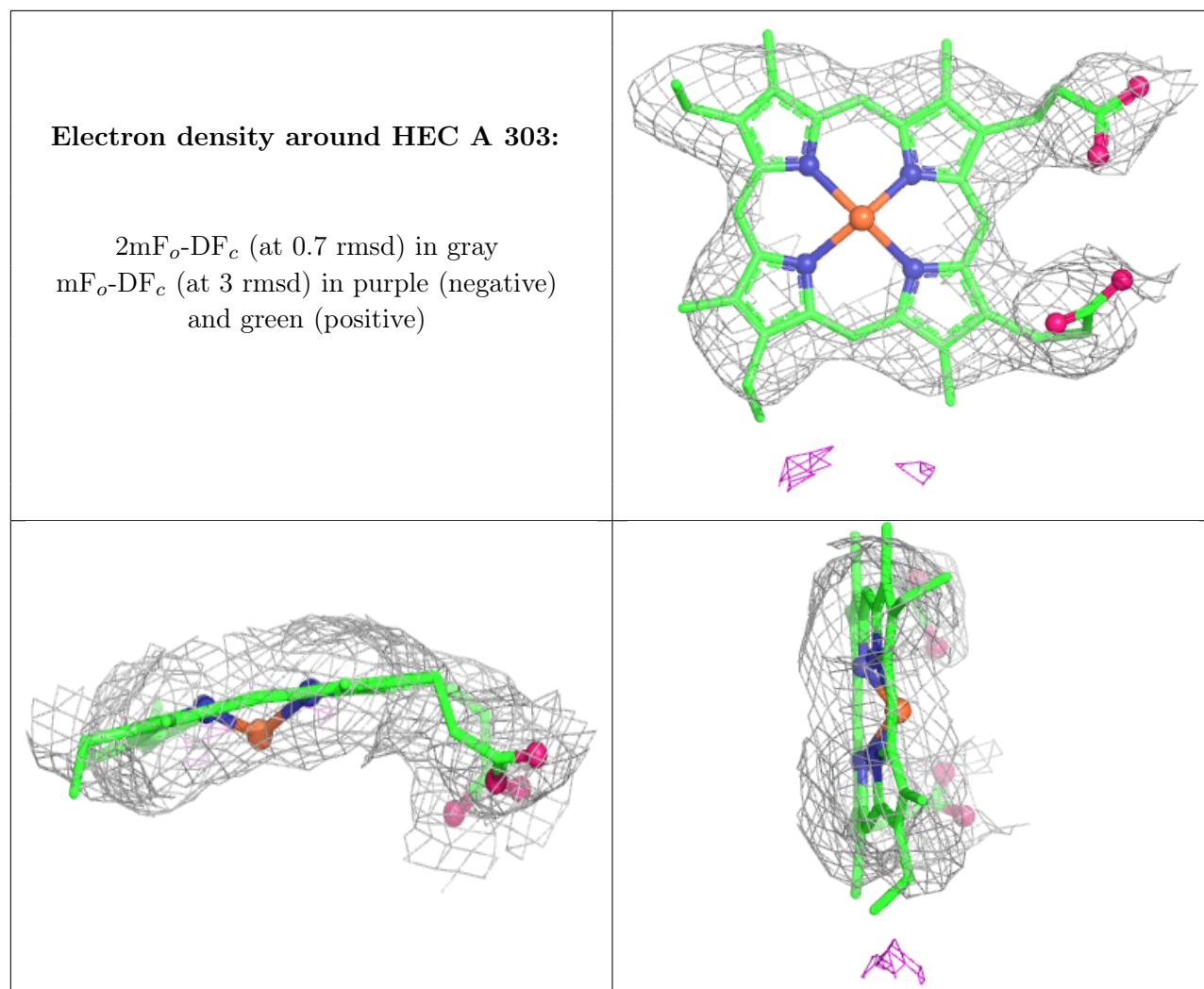
**Electron density around UMQ A 1103:**

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

**Electron density around CLA B 201:**

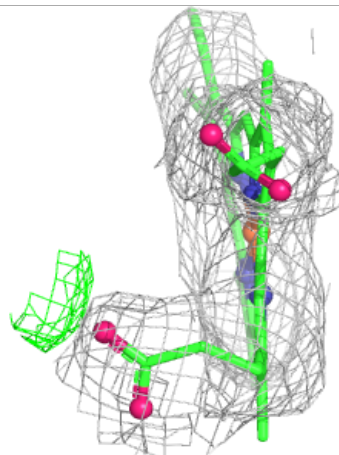
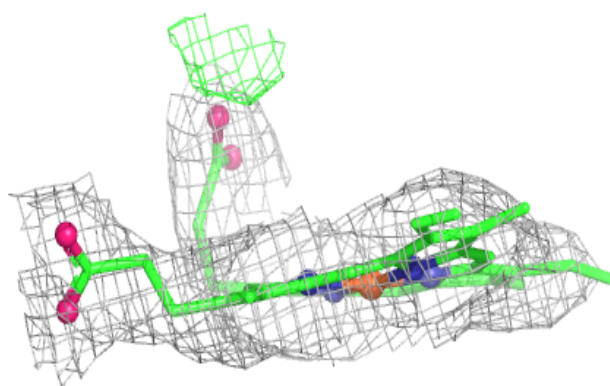
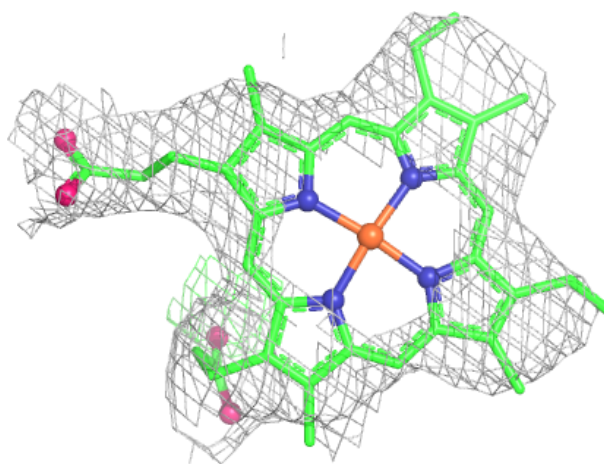
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





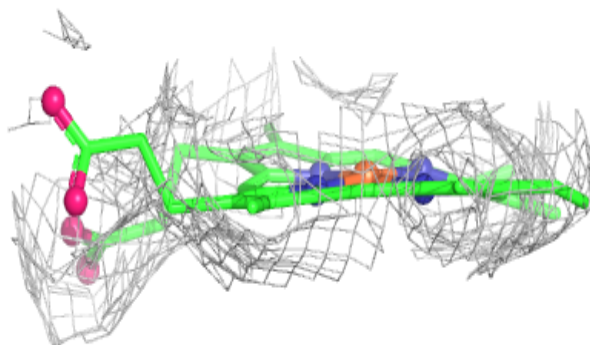
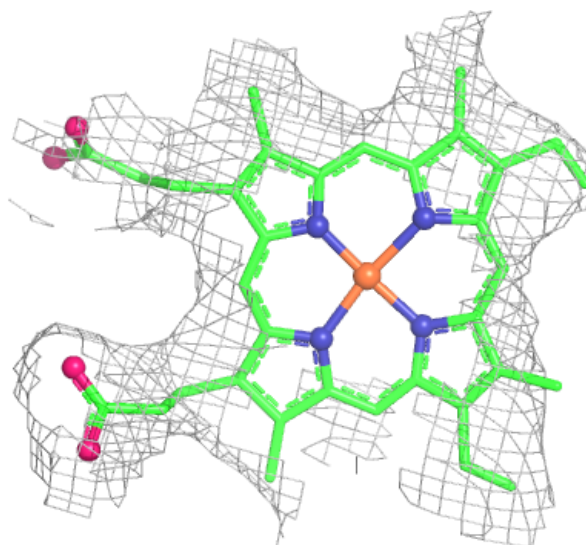
**Electron density around HEM A 302:**

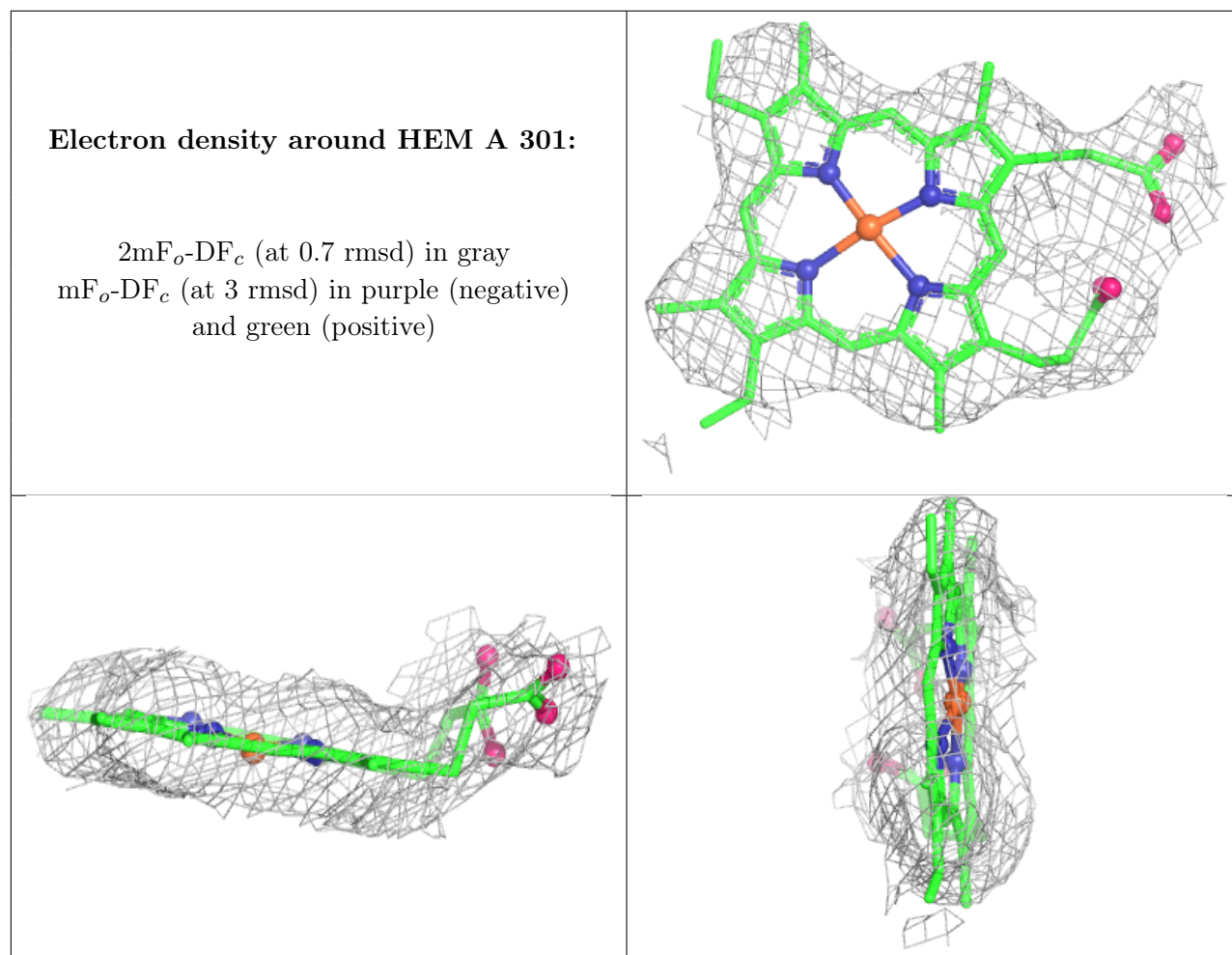
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 301:**

$2mF_o-DF_c$  (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.