Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 07:57 AM EDT

PDB ID	:	2E76
Title	:	Crystal Structure of the Cytochrome b6f Complex with tridecyl-stigmatellin (TDS) from M.laminosus
Authors	:	Cramer, W.A.; Yamashita, E.; Zhang, H.
Deposited on	:	2007-01-05
Resolution	:	3.41 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

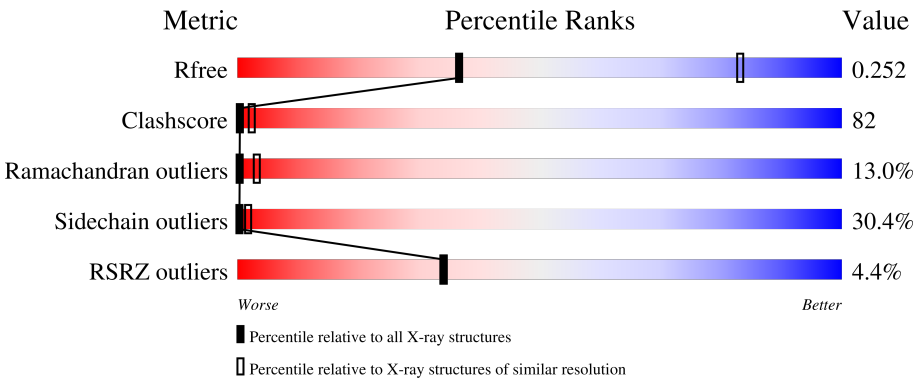
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.41 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}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	23% 42% 24% 11%
2	B	160	3% 18% 40% 31% 11%
3	C	289	6% 18% 47% 28% 7%
4	D	179	10% 19% 42% 22% 11% 6%
5	E	32	6% 12% 50% 25% 12%

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Mol	Chain	Length	Quality of chain
6	F	35	11% 31% 26% 23% 9%
7	G	37	8% 30% 38% 24%
8	H	29	14% 38% 34% 14%

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	302	-	-	X	-
10	HEM	A	303	-	-	X	-
10	HEM	C	301	-	-	X	-
11	OPC	B	1001	-	X	-	-
12	UMQ	A	1101	X	-	-	-
12	UMQ	A	1102	X	-	-	-
12	UMQ	A	1103	X	-	-	-
12	UMQ	A	1104	X	-	-	-
13	CLA	B	201	X	-	-	-
14	TDS	B	1201	-	X	X	-
14	TDS	B	1202	-	X	-	-
16	SQD	D	201	X	X	-	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 8112 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	168	1288	823	221	237	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	283	188	44	50	1	0	0	0

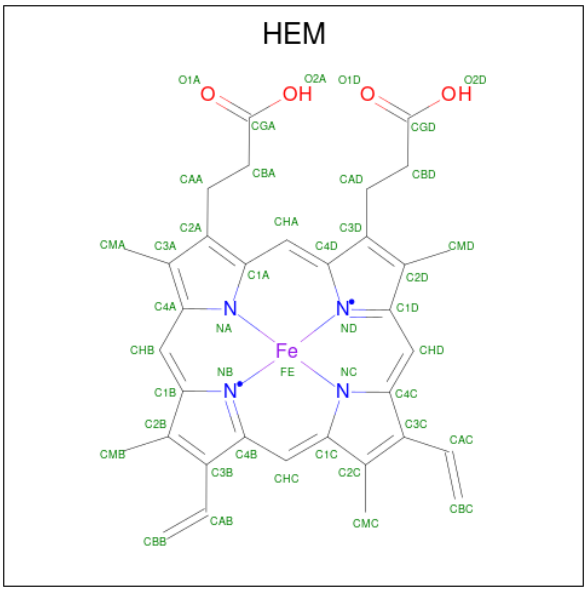
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

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

- Molecule 9 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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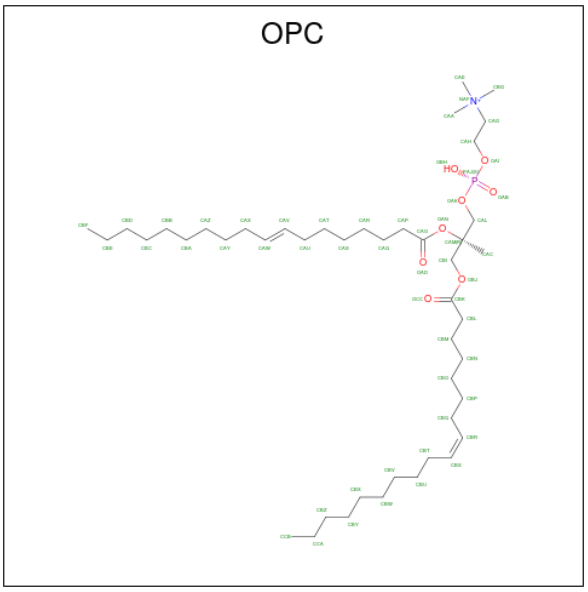
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
10	C	1	43	34	1	4	4	0	0

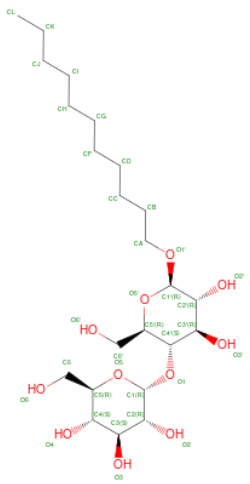
- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: $C_{45}H_{87}NO_8P$).



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

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).

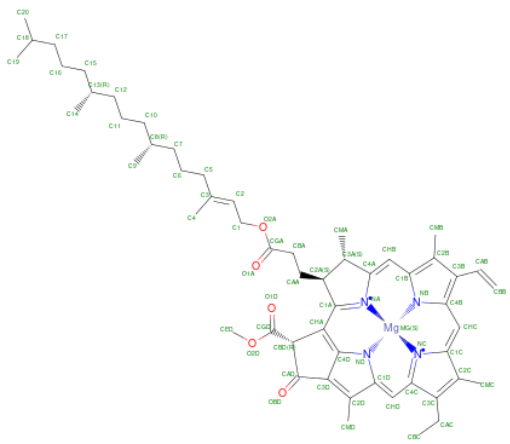
UMQ



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

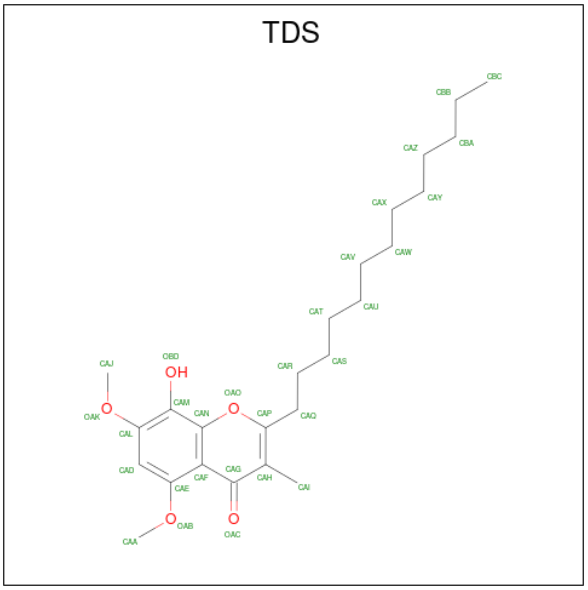
- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).

CLA



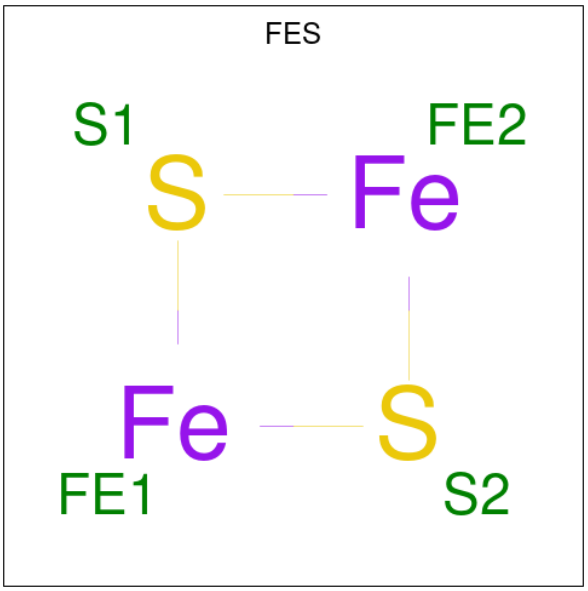
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0

- Molecule 14 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROMEN-4-ONE (three-letter code: TDS) (formula: $C_{25}H_{38}O_5$).



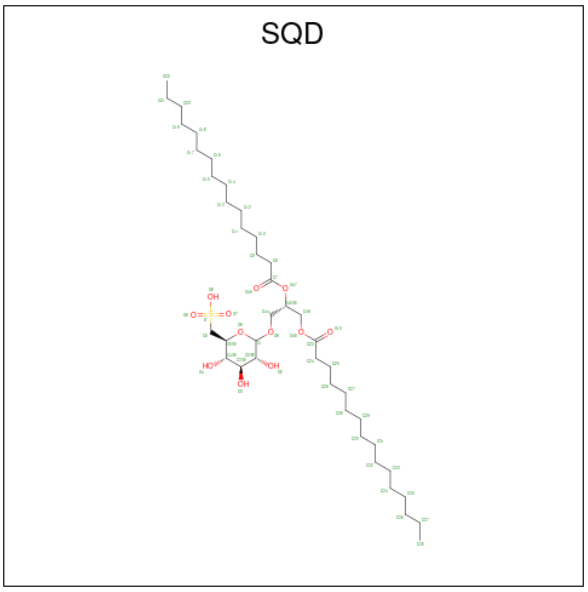
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O				
14	B	1	30	25	5			0	0
14	B	1	Total	C	O			0	0
			30	25	5				

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



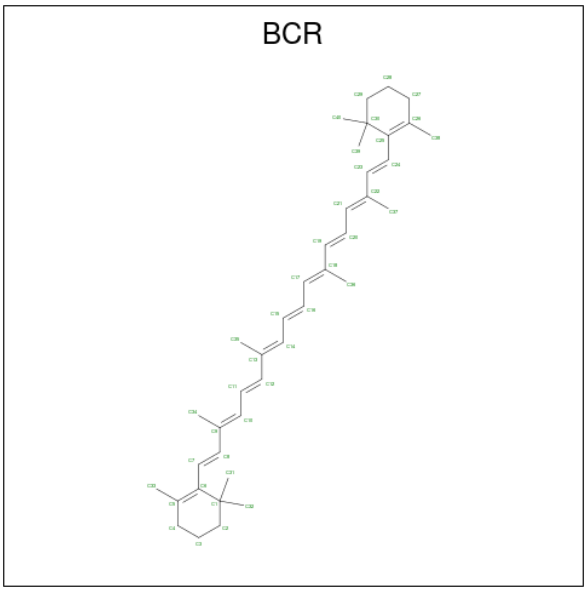
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
15	D	1	4	2	2	0	0

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 18 is water.

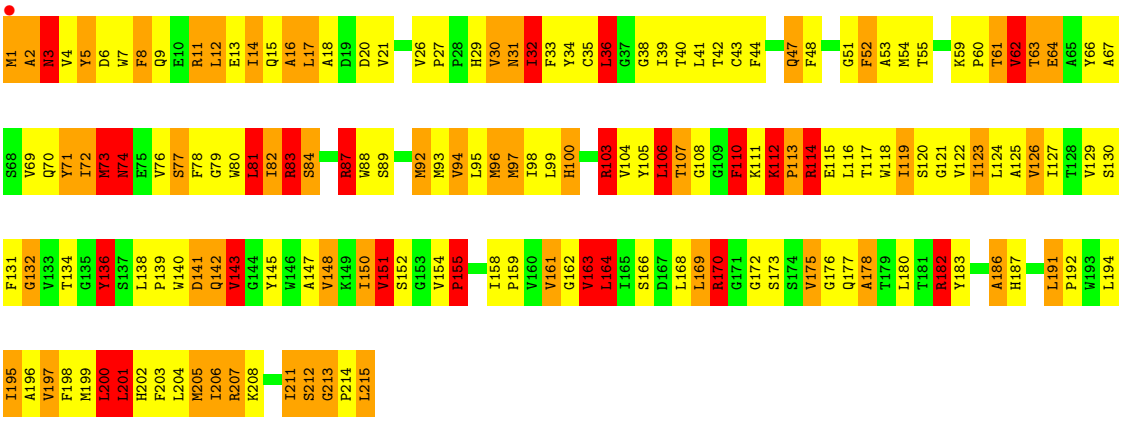
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	2	2	2	0	0
			Total	O		
18	B	2	2	2	0	0
			Total	O		
18	C	1	1	1	0	0

3 Residue-property plots (i)

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.

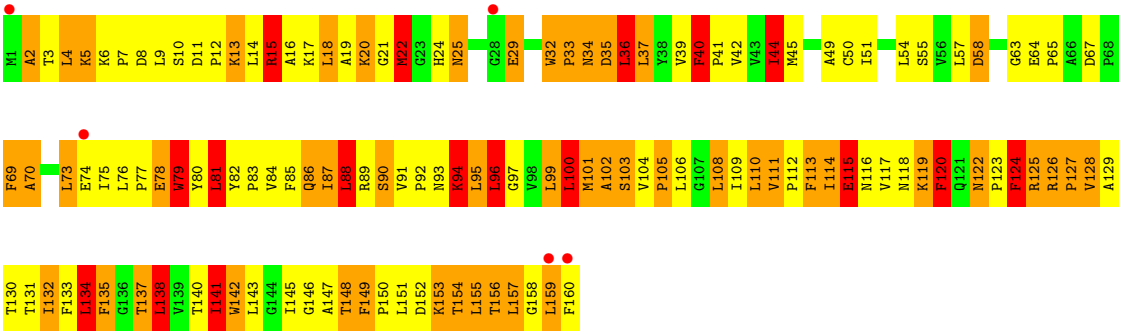
• Molecule 1: Cytochrome b6

Chain A:



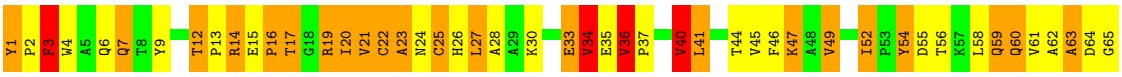
• Molecule 2: Cytochrome b6-f complex subunit 4

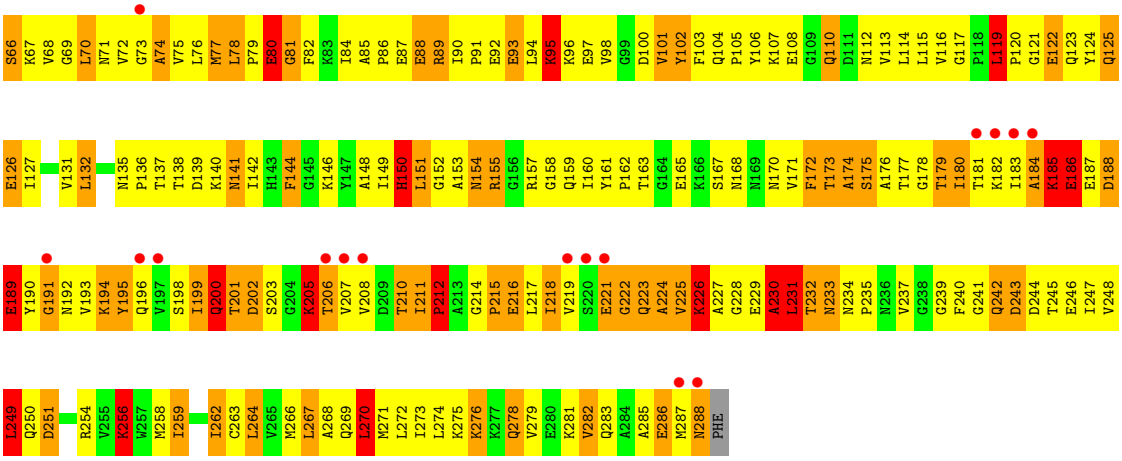
Chain B:



• Molecule 3: Apocytochrome f

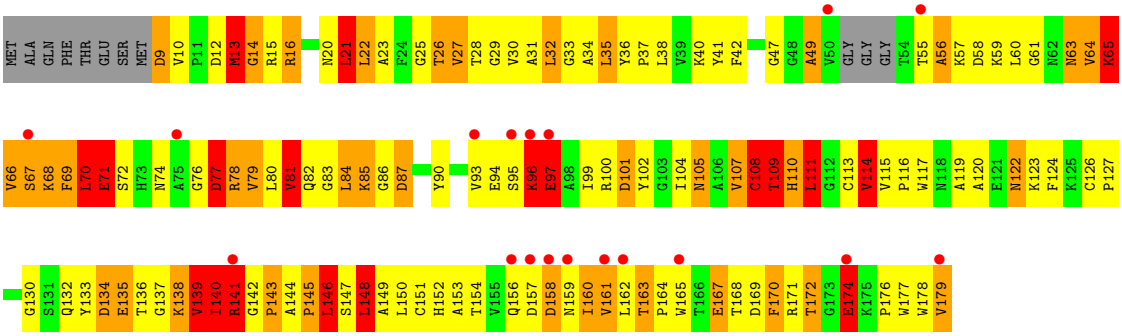
Chain C:





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

Chain D:

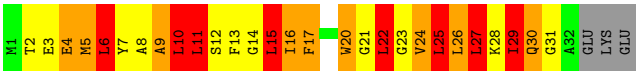


- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:

- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:

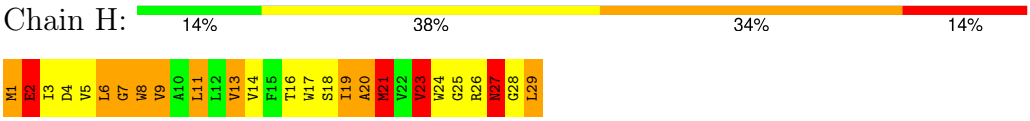


- Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:

- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:


14%
38%
34%
14%
M1
E2
I3
D4
V5
L6
G7
W8
V9
A10
L11
L12
V13
V14
F15
T16
W17
S18
I19
A20
M21
V22
V23
W24
G25
R26
N27
G28
L29

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	157.23Å 157.23Å 363.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.27 – 3.41 39.21 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.27-3.41) 99.7 (39.21-3.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.84 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.256 0.182 , 0.252	Depositor DCC
R_{free} test set	1852 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	92.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 102.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FES, UMQ, CLA, HEM, OPC, TDS, BCR, CD, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.81	32/1763 (1.8%)	1.85	50/2405 (2.1%)
2	B	1.89	26/1288 (2.0%)	1.96	34/1765 (1.9%)
3	C	1.47	21/2264 (0.9%)	1.51	30/3082 (1.0%)
4	D	1.29	6/1320 (0.5%)	1.49	27/1798 (1.5%)
5	E	1.82	5/253 (2.0%)	1.88	8/340 (2.4%)
6	F	2.11	7/246 (2.8%)	2.03	9/331 (2.7%)
7	G	2.14	7/289 (2.4%)	2.25	13/391 (3.3%)
8	H	2.01	5/236 (2.1%)	1.86	8/323 (2.5%)
All	All	1.68	109/7659 (1.4%)	1.74	179/10435 (1.7%)

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	4
2	B	0	3
3	C	0	7
4	D	0	5
5	E	0	1
6	F	0	3
7	G	0	2
8	H	0	2
All	All	0	27

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	3	GLU	CG-CD	16.26	1.76	1.51
3	C	246	GLU	CD-OE2	12.18	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246	GLU	CG-CD	11.96	1.69	1.51
6	F	3	GLU	CB-CG	11.17	1.73	1.52
2	B	115	GLU	CG-CD	11.11	1.68	1.51
2	B	40	PHE	CE2-CZ	10.90	1.58	1.37
1	A	13	GLU	CB-CG	10.22	1.71	1.52
3	C	256	LYS	CE-NZ	10.05	1.74	1.49
1	A	67	ALA	CA-CB	-9.94	1.31	1.52
7	G	3	GLU	CB-CG	9.72	1.70	1.52
6	F	3	GLU	CG-CD	9.48	1.66	1.51
1	A	13	GLU	CG-CD	9.02	1.65	1.51
3	C	246	GLU	CB-CG	9.00	1.69	1.52
8	H	8	TRP	CB-CG	-8.97	1.34	1.50
2	B	15	ARG	CZ-NH1	8.91	1.44	1.33
2	B	142	TRP	CG-CD1	8.55	1.48	1.36
1	A	63	THR	CA-CB	-8.24	1.31	1.53
2	B	115	GLU	CD-OE1	8.15	1.34	1.25
3	C	256	LYS	CG-CD	8.12	1.80	1.52
3	C	33	GLU	CB-CG	7.73	1.66	1.52
1	A	186	ALA	CA-CB	-7.71	1.36	1.52
8	H	26	ARG	CZ-NH1	7.59	1.43	1.33
3	C	33	GLU	CG-CD	7.47	1.63	1.51
2	B	78	GLU	CG-CD	7.16	1.62	1.51
2	B	117	VAL	CB-CG1	7.13	1.67	1.52
1	A	87	ARG	CG-CD	7.07	1.69	1.51
5	E	10	VAL	CB-CG1	6.99	1.67	1.52
2	B	40	PHE	CB-CG	-6.97	1.39	1.51
2	B	79	TRP	CZ3-CH2	6.91	1.51	1.40
6	F	25	LEU	CG-CD1	6.90	1.77	1.51
2	B	15	ARG	CG-CD	6.86	1.69	1.51
5	E	27	LYS	CE-NZ	6.73	1.65	1.49
1	A	71	TYR	CD1-CE1	-6.73	1.29	1.39
3	C	25	CYS	CB-SG	-6.71	1.70	1.82
3	C	40	VAL	CA-CB	-6.66	1.40	1.54
2	B	141	ILE	CA-CB	-6.66	1.39	1.54
3	C	148	ALA	CA-CB	-6.66	1.38	1.52
8	H	13	VAL	CB-CG1	6.61	1.66	1.52
2	B	79	TRP	CB-CG	-6.50	1.38	1.50
2	B	40	PHE	CG-CD1	6.43	1.48	1.38
2	B	49	ALA	CA-CB	-6.38	1.39	1.52
4	D	107	VAL	CA-CB	-6.26	1.41	1.54
2	B	135	PHE	CE1-CZ	6.25	1.49	1.37
3	C	256	LYS	CB-CG	6.22	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	14	VAL	CB-CG2	-6.22	1.39	1.52
7	G	24	ALA	CA-CB	6.21	1.65	1.52
6	F	4	GLU	CG-CD	6.21	1.61	1.51
2	B	50	CYS	CB-SG	-6.20	1.71	1.82
1	A	62	VAL	CA-CB	-6.17	1.41	1.54
2	B	138	LEU	CG-CD1	6.13	1.74	1.51
2	B	29	GLU	CG-CD	6.07	1.61	1.51
1	A	140	TRP	CZ3-CH2	6.01	1.49	1.40
7	G	1	MET	N-CA	5.95	1.58	1.46
3	C	256	LYS	CD-CE	5.95	1.66	1.51
4	D	77	ASP	CB-CG	5.93	1.64	1.51
6	F	2	THR	CA-CB	5.86	1.68	1.53
1	A	110	PHE	CE2-CZ	5.85	1.48	1.37
1	A	8	PHE	CB-CG	-5.82	1.41	1.51
3	C	89	ARG	CB-CG	-5.82	1.36	1.52
4	D	114	VAL	CB-CG1	5.81	1.65	1.52
1	A	197	VAL	CB-CG2	-5.81	1.40	1.52
2	B	148	THR	CB-CG2	5.80	1.71	1.52
8	H	9	VAL	CB-CG2	-5.80	1.40	1.52
3	C	81	GLY	N-CA	5.79	1.54	1.46
3	C	16	PRO	C-O	5.78	1.34	1.23
1	A	52	PHE	CB-CG	-5.78	1.41	1.51
3	C	126	GLU	CG-CD	5.73	1.60	1.51
1	A	143	VAL	CB-CG2	-5.72	1.40	1.52
3	C	144	PHE	CB-CG	-5.70	1.41	1.51
1	A	66	TYR	CD2-CE2	-5.69	1.30	1.39
2	B	117	VAL	CA-CB	5.69	1.66	1.54
1	A	112	LYS	CB-CG	5.65	1.67	1.52
2	B	79	TRP	CD2-CE2	5.65	1.48	1.41
5	E	4	GLY	C-O	5.64	1.32	1.23
1	A	48	PHE	CB-CG	-5.61	1.41	1.51
1	A	113	PRO	N-CA	5.59	1.56	1.47
1	A	134	THR	CB-CG2	-5.57	1.33	1.52
4	D	79	VAL	CB-CG1	5.52	1.64	1.52
2	B	135	PHE	CD1-CE1	5.49	1.50	1.39
1	A	113	PRO	CB-CG	5.48	1.77	1.50
7	G	1	MET	CB-CG	5.42	1.68	1.51
1	A	69	VAL	CB-CG2	-5.40	1.41	1.52
1	A	66	TYR	CE1-CZ	-5.39	1.31	1.38
2	B	135	PHE	CD2-CE2	5.36	1.50	1.39
4	D	141	ARG	N-CA	5.33	1.57	1.46
5	E	27	LYS	CB-CG	5.33	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	TYR	CE1-CZ	5.32	1.45	1.38
1	A	129	VAL	CB-CG2	-5.31	1.41	1.52
4	D	42	PHE	CE2-CZ	5.30	1.47	1.37
1	A	140	TRP	CA-CB	-5.29	1.42	1.53
1	A	169	LEU	CG-CD2	5.29	1.71	1.51
2	B	78	GLU	CB-CG	5.28	1.62	1.52
1	A	178	ALA	CA-CB	-5.24	1.41	1.52
3	C	185	LYS	CB-CG	5.21	1.66	1.52
5	E	11	PHE	CD2-CE2	5.20	1.49	1.39
1	A	94	VAL	CB-CG2	-5.18	1.42	1.52
3	C	1	TYR	CG-CD1	5.18	1.45	1.39
6	F	29	ILE	CA-CB	5.17	1.66	1.54
6	F	20	TRP	C-O	5.14	1.33	1.23
1	A	126	VAL	CB-CG2	-5.13	1.42	1.52
1	A	66	TYR	CE2-CZ	-5.12	1.31	1.38
2	B	64	GLU	CG-CD	5.11	1.59	1.51
2	B	115	GLU	CB-CG	5.10	1.61	1.52
7	G	1	MET	CG-SD	5.09	1.94	1.81
1	A	213	GLY	C-O	5.08	1.31	1.23
1	A	112	LYS	CG-CD	5.07	1.69	1.52
8	H	1	MET	CB-CG	5.06	1.67	1.51
3	C	40	VAL	CB-CG1	-5.01	1.42	1.52
3	C	49	VAL	CA-CB	-5.01	1.44	1.54

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	15	ARG	NE-CZ-NH2	-14.05	113.27	120.30
7	G	7	ASP	CB-CG-OD1	12.97	129.97	118.30
7	G	9	LEU	CA-CB-CG	-12.37	86.84	115.30
2	B	15	ARG	NE-CZ-NH1	11.62	126.11	120.30
5	E	23	ILE	CB-CA-C	-10.85	89.90	111.60
1	A	169	LEU	CB-CG-CD1	-10.71	92.78	111.00
1	A	83	ARG	NE-CZ-NH2	-10.42	115.09	120.30
7	G	1	MET	CG-SD-CE	10.36	116.77	100.20
7	G	7	ASP	CB-CG-OD2	-10.36	108.98	118.30
2	B	110	LEU	CA-CB-CG	-10.31	91.60	115.30
1	A	63	THR	CA-CB-CG2	-10.16	98.18	112.40
2	B	126	ARG	NE-CZ-NH2	-10.11	115.25	120.30
3	C	132	LEU	CB-CG-CD2	-10.01	93.98	111.00
7	G	3	GLU	OE1-CD-OE2	-9.93	111.39	123.30
2	B	81	LEU	CB-CG-CD2	-9.38	95.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	25	LEU	CB-CG-CD2	-9.15	95.45	111.00
1	A	81	LEU	CB-CG-CD2	-9.14	95.47	111.00
2	B	138	LEU	CB-CG-CD2	-8.98	95.73	111.00
3	C	89	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	A	74	ASN	N-CA-C	8.88	134.96	111.00
2	B	70	ALA	C-N-CA	-8.53	100.36	121.70
7	G	5	LEU	CA-CB-CG	-8.49	95.77	115.30
8	H	11	LEU	CB-CG-CD1	-8.35	96.81	111.00
5	E	14	LEU	CB-CG-CD2	-8.34	96.82	111.00
1	A	62	VAL	CG1-CB-CG2	8.23	124.07	110.90
2	B	99	LEU	CA-CB-CG	-8.12	96.63	115.30
1	A	191	LEU	CA-CB-CG	-8.04	96.81	115.30
4	D	113	CYS	CA-CB-SG	-7.97	99.66	114.00
2	B	126	ARG	NE-CZ-NH1	7.81	124.21	120.30
3	C	119	LEU	CB-CG-CD2	-7.79	97.76	111.00
1	A	182	ARG	NE-CZ-NH1	-7.77	116.42	120.30
1	A	62	VAL	CB-CA-C	-7.76	96.65	111.40
2	B	40	PHE	CB-CG-CD1	-7.55	115.52	120.80
1	A	164	LEU	CA-CB-CG	7.54	132.65	115.30
2	B	58	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	3	ASN	N-CA-C	7.33	130.81	111.00
4	D	70	LEU	CA-CB-CG	7.29	132.07	115.30
1	A	180	LEU	CB-CG-CD1	-7.27	98.64	111.00
3	C	243	ASP	CB-CG-OD1	7.24	124.81	118.30
3	C	231	LEU	CA-CB-CG	7.22	131.92	115.30
8	H	1	MET	CB-CG-SD	7.22	134.06	112.40
4	D	35	LEU	CA-CB-CG	-7.20	98.73	115.30
2	B	22	MET	N-CA-C	7.11	130.19	111.00
8	H	21	MET	CB-CG-SD	-7.07	91.20	112.40
7	G	11	LEU	CA-CB-CG	-7.06	99.06	115.30
7	G	9	LEU	CB-CG-CD2	-7.06	99.00	111.00
6	F	11	LEU	CB-CG-CD2	-7.06	99.00	111.00
1	A	114	ARG	N-CA-C	7.03	129.98	111.00
1	A	92	MET	CA-CB-CG	-6.93	101.52	113.30
8	H	26	ARG	NE-CZ-NH2	-6.93	116.84	120.30
3	C	90	ILE	C-N-CD	6.89	142.87	128.40
4	D	21	LEU	CA-CB-CG	-6.83	99.59	115.30
1	A	204	LEU	CB-CG-CD1	-6.80	99.44	111.00
4	D	32	LEU	CB-CG-CD2	6.71	122.40	111.00
4	D	13	MET	CB-CG-SD	-6.63	92.52	112.40
5	E	23	ILE	N-CA-CB	6.58	125.93	110.80
4	D	107	VAL	CB-CA-C	-6.57	98.91	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	VAL	CA-CB-CG1	-6.55	101.07	110.90
7	G	18	LEU	CA-CB-CG	-6.54	100.25	115.30
1	A	126	VAL	CA-CB-CG2	-6.54	101.09	110.90
1	A	200	LEU	CB-CG-CD2	-6.54	99.89	111.00
1	A	59	LYS	C-N-CD	6.47	142.00	128.40
2	B	125	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	A	175	VAL	CB-CA-C	-6.44	99.16	111.40
5	E	14	LEU	CB-CG-CD1	-6.39	100.13	111.00
7	G	11	LEU	CB-CG-CD1	6.37	121.84	111.00
7	G	2	VAL	CB-CA-C	-6.36	99.31	111.40
3	C	95	LYS	CD-CE-NZ	6.32	126.23	111.70
2	B	143	LEU	CB-CG-CD1	-6.25	100.38	111.00
4	D	148	LEU	CB-CG-CD1	-6.24	100.40	111.00
2	B	108	LEU	CB-CG-CD2	-6.23	100.40	111.00
4	D	111	LEU	CB-CG-CD1	-6.20	100.45	111.00
3	C	244	ASP	CB-CG-OD2	-6.18	112.74	118.30
2	B	134	LEU	CA-CB-CG	-6.17	101.11	115.30
3	C	244	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	201	LEU	CA-CB-CG	-6.14	101.18	115.30
2	B	111	VAL	C-N-CD	6.12	141.26	128.40
1	A	83	ARG	CG-CD-NE	-6.10	99.00	111.80
6	F	22	LEU	CB-CG-CD2	6.08	121.34	111.00
6	F	5	MET	CA-CB-CG	-6.02	103.06	113.30
2	B	134	LEU	CB-CG-CD2	6.01	121.22	111.00
3	C	27	LEU	CA-CB-CG	-6.01	101.47	115.30
3	C	226	LYS	N-CA-C	6.00	127.21	111.00
4	D	97	GLU	N-CA-C	5.99	127.18	111.00
3	C	3	PHE	CB-CA-C	5.96	122.32	110.40
2	B	18	LEU	CA-CB-CG	-5.94	101.64	115.30
5	E	10	VAL	CB-CA-C	-5.92	100.14	111.40
7	G	24	ALA	N-CA-CB	5.92	118.39	110.10
2	B	36	LEU	CA-CB-CG	-5.90	101.74	115.30
8	H	1	MET	CG-SD-CE	5.88	109.61	100.20
5	E	29	ILE	N-CA-C	-5.87	95.15	111.00
5	E	10	VAL	CG1-CB-CG2	5.87	120.29	110.90
3	C	36	VAL	N-CA-C	-5.86	95.17	111.00
4	D	81	VAL	CB-CA-C	-5.86	100.27	111.40
2	B	15	ARG	CB-CG-CD	5.84	126.78	111.60
2	B	22	MET	CG-SD-CE	5.82	109.51	100.20
4	D	139	VAL	CB-CA-C	-5.81	100.36	111.40
3	C	41	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	A	136	TYR	CB-CA-C	-5.77	98.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	22	MET	C-N-CA	-5.77	110.19	122.30
1	A	110	PHE	CB-CA-C	-5.73	98.95	110.40
2	B	120	PHE	N-CA-CB	5.70	120.85	110.60
1	A	132	GLY	N-CA-C	5.68	127.31	113.10
2	B	100	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	A	1	MET	CG-SD-CE	5.68	109.29	100.20
3	C	119	LEU	CA-CB-CG	-5.68	102.24	115.30
3	C	80	GLU	N-CA-C	5.64	126.23	111.00
3	C	78	LEU	CA-CB-CG	-5.63	102.35	115.30
1	A	186	ALA	CB-CA-C	-5.60	101.69	110.10
6	F	15	LEU	CA-CB-CG	-5.59	102.43	115.30
2	B	94	LYS	CD-CE-NZ	-5.59	98.84	111.70
1	A	64	GLU	CG-CD-OE1	-5.58	107.13	118.30
8	H	29	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	67	ALA	N-CA-CB	-5.57	102.30	110.10
4	D	108	CYS	N-CA-CB	5.53	120.55	110.60
6	F	22	LEU	CB-CA-C	5.53	120.70	110.20
1	A	73	MET	CG-SD-CE	5.52	109.03	100.20
2	B	88	LEU	CA-CB-CG	-5.51	102.62	115.30
3	C	249	LEU	CB-CG-CD1	-5.51	101.64	111.00
2	B	65	PRO	N-CD-CG	-5.49	94.97	103.20
6	F	10	LEU	CA-CB-CG	-5.49	102.69	115.30
4	D	71	GLU	N-CA-C	5.48	125.79	111.00
1	A	151	VAL	C-N-CA	-5.47	108.03	121.70
3	C	127	ILE	CB-CA-C	-5.46	100.68	111.60
4	D	87	ASP	C-N-CD	5.45	139.84	128.40
1	A	170	ARG	NE-CZ-NH1	5.45	123.02	120.30
3	C	151	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	A	119	ILE	CB-CA-C	-5.41	100.78	111.60
4	D	109	THR	N-CA-C	-5.39	96.44	111.00
1	A	172	GLY	N-CA-C	-5.38	99.64	113.10
3	C	150	HIS	CB-CA-C	-5.38	99.64	110.40
3	C	102	TYR	C-N-CA	-5.38	108.26	121.70
3	C	200	GLN	N-CA-C	5.37	125.50	111.00
2	B	44	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	A	100	HIS	CB-CA-C	5.36	121.11	110.40
1	A	163	VAL	CG1-CB-CG2	-5.36	102.33	110.90
3	C	202	ASP	N-CA-C	5.34	125.41	111.00
1	A	215	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	113	PRO	CA-N-CD	5.31	119.14	111.70
1	A	141	ASP	N-CA-CB	-5.31	101.04	110.60
1	A	13	GLU	OE1-CD-OE2	-5.31	116.93	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	LEU	C-N-CD	5.31	139.55	128.40
3	C	205	LYS	N-CA-C	5.31	125.33	111.00
3	C	34	VAL	CB-CA-C	-5.29	101.35	111.40
1	A	205	MET	CA-CB-CG	-5.29	104.32	113.30
8	H	23	VAL	CA-CB-CG1	-5.29	102.97	110.90
1	A	55	THR	CA-CB-CG2	-5.28	105.01	112.40
4	D	32	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	A	103	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	212	SER	N-CA-C	-5.25	96.81	111.00
7	G	7	ASP	CB-CA-C	5.25	120.91	110.40
2	B	63	GLY	N-CA-C	-5.25	99.99	113.10
2	B	141	ILE	CG1-CB-CG2	5.24	122.93	111.40
3	C	270	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	63	THR	CB-CA-C	-5.23	97.48	111.60
2	B	149	PHE	CB-CA-C	-5.21	99.98	110.40
1	A	64	GLU	CA-CB-CG	-5.18	101.99	113.40
2	B	96	LEU	CB-CG-CD2	5.18	119.81	111.00
4	D	141	ARG	NE-CZ-NH1	5.17	122.88	120.30
4	D	163	THR	C-N-CD	5.14	139.20	128.40
4	D	21	LEU	CB-CG-CD1	-5.13	102.29	111.00
4	D	130	GLY	N-CA-C	5.12	125.91	113.10
4	D	26	THR	N-CA-CB	5.12	120.03	110.30
6	F	27	LEU	CB-CG-CD2	5.11	119.69	111.00
4	D	35	LEU	CB-CG-CD2	-5.08	102.36	111.00
8	H	29	LEU	CB-CG-CD2	5.08	119.64	111.00
4	D	140	ILE	CB-CA-C	5.08	121.76	111.60
4	D	27	VAL	CA-CB-CG2	-5.07	103.29	110.90
1	A	92	MET	CG-SD-CE	-5.06	92.10	100.20
4	D	70	LEU	CB-CG-CD1	5.06	119.60	111.00
3	C	52	ILE	CB-CA-C	-5.06	101.48	111.60
5	E	31	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	A	94	VAL	CG1-CB-CG2	-5.05	102.82	110.90
6	F	6	LEU	CA-CB-CG	-5.05	103.69	115.30
1	A	106	LEU	CB-CG-CD2	5.04	119.58	111.00
4	D	146	LEU	CB-CG-CD1	-5.03	102.44	111.00
3	C	17	THR	CA-CB-CG2	-5.02	105.38	112.40
3	C	167	SER	N-CA-C	-5.01	97.48	111.00
2	B	128	VAL	CA-CB-CG2	-5.00	103.39	110.90

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LYS	Peptide
1	A	161	VAL	Peptide
1	A	2	ALA	Peptide
1	A	73	MET	Peptide
2	B	124	PHE	Peptide
2	B	2	ALA	Peptide
2	B	32	TRP	Peptide
3	C	191	GLY	Peptide
3	C	200	GLN	Peptide
3	C	216	GLU	Peptide
3	C	222	GLY	Peptide
3	C	225	VAL	Peptide
3	C	230	ALA	Peptide
3	C	81	GLY	Peptide
4	D	108	CYS	Peptide
4	D	158	ASP	Peptide
4	D	65	LYS	Peptide
4	D	96	LYS	Peptide
4	D	97	GLU	Peptide
5	E	28	SER	Peptide
6	F	26	LEU	Peptide
6	F	27	LEU	Peptide
6	F	9	ALA	Peptide
7	G	27	GLN	Peptide
7	G	31	ARG	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	303	0
2	B	1249	0	1308	254	0
3	C	2216	0	2233	404	1
4	D	1288	0	1273	229	0
5	E	248	0	284	39	0
6	F	242	0	260	61	0
7	G	283	0	289	75	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	230	0	239	51	0
9	A	1	0	0	0	0
10	A	129	0	90	64	0
10	C	43	0	30	29	0
11	A	54	0	79	18	0
11	B	54	0	83	2	0
12	A	136	0	165	6	0
13	B	65	0	72	5	0
14	B	60	0	70	41	0
15	D	4	0	0	1	0
16	D	54	0	53	9	0
17	G	40	0	52	9	0
18	A	2	0	0	0	0
18	B	2	0	0	0	0
18	C	1	0	0	0	0
All	All	8112	0	8316	1350	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 82.

All (1350) 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)
6:F:25:LEU:CD1	6:F:25:LEU:CG	1.77	1.62
3:C:256:LYS:CG	3:C:256:LYS:CD	1.80	1.59
2:B:138:LEU:CG	2:B:138:LEU:CD1	1.74	1.59
7:G:3:GLU:CD	7:G:3:GLU:CG	1.76	1.52
3:C:256:LYS:CE	3:C:256:LYS:NZ	1.74	1.50
1:A:92:MET:CE	11:A:1002:OPC:HCB2	1.37	1.48
1:A:113:PRO:CG	1:A:113:PRO:CB	1.77	1.46
7:G:29:TYR:O	7:G:29:TYR:CD2	1.69	1.44
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	1.35	1.37
3:C:22:CYS:HB2	10:C:301:HEM:CAB	1.55	1.35
6:F:29:ILE:O	6:F:29:ILE:CD1	1.75	1.35
6:F:29:ILE:O	6:F:29:ILE:HD12	1.20	1.33
4:D:85:LYS:HB2	4:D:85:LYS:NZ	1.17	1.31
2:B:93:ASN:OD1	2:B:96:LEU:HB2	1.25	1.28
6:F:7:TYR:O	6:F:11:LEU:CD1	1.83	1.27
4:D:122:ASN:HB3	4:D:135:GLU:OE2	1.33	1.26
3:C:65:GLY:O	3:C:66:SER:O	1.52	1.26
2:B:9:LEU:O	2:B:15:ARG:HD2	1.31	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:GLN:HG3	3:C:205:LYS:O	1.37	1.24
4:D:111:LEU:N	4:D:111:LEU:CD1	2.04	1.19
3:C:15:GLU:HB3	3:C:16:PRO:HD2	1.23	1.19
12:A:1104:UMQ:H31	12:A:1104:UMQ:H6'2	1.20	1.15
2:B:142:TRP:CH2	2:B:155:LEU:O	1.99	1.15
4:D:85:LYS:NZ	4:D:85:LYS:CB	2.11	1.14
3:C:157:ARG:HB2	10:C:301:HEM:HAD2	1.25	1.14
4:D:111:LEU:N	4:D:111:LEU:HD13	1.51	1.14
1:A:92:MET:HE2	11:A:1002:OPC:HCB2	1.29	1.14
10:A:301:HEM:CBB	10:A:301:HEM:HMB2	1.77	1.13
1:A:54:MET:CE	10:A:301:HEM:HBD1	1.78	1.13
4:D:139:VAL:HG22	4:D:147:SER:CA	1.77	1.13
1:A:92:MET:CE	11:A:1002:OPC:CCB	2.27	1.12
2:B:34:ASN:ND2	3:C:283:GLN:HE22	1.47	1.12
3:C:93:GLU:N	3:C:93:GLU:OE1	1.83	1.11
3:C:188:ASP:O	3:C:190:TYR:N	1.81	1.11
6:F:11:LEU:HB3	6:F:15:LEU:HD12	1.32	1.11
4:D:109:THR:CG2	4:D:144:ALA:HB1	1.80	1.11
4:D:146:LEU:HD12	4:D:177:TRP:CD2	1.84	1.11
2:B:95:LEU:O	2:B:95:LEU:HD23	1.49	1.11
3:C:19:ARG:O	3:C:20:ILE:HB	1.46	1.11
3:C:211:ILE:O	3:C:211:ILE:HG13	1.38	1.10
2:B:152:ASP:HA	2:B:154:THR:HG22	1.12	1.10
6:F:7:TYR:O	6:F:11:LEU:HD12	0.92	1.10
1:A:39:ILE:HD11	17:G:101:BCR:H312	1.17	1.09
4:D:109:THR:HG22	4:D:144:ALA:CB	1.82	1.09
2:B:96:LEU:HD13	2:B:100:LEU:CD1	1.81	1.09
11:A:1002:OPC:HBV1	7:G:9:LEU:HD21	1.34	1.09
13:B:201:CLA:HBB1	13:B:201:CLA:HMB1	1.33	1.09
14:B:1202:TDS:HAA3	14:B:1202:TDS:OAC	1.51	1.08
1:A:163:VAL:HG12	1:A:164:LEU:N	1.58	1.08
3:C:171:VAL:HG12	3:C:235:PRO:HD2	1.11	1.08
3:C:171:VAL:HG12	3:C:235:PRO:CD	1.84	1.08
2:B:91:VAL:HG12	2:B:91:VAL:O	1.29	1.07
7:G:2:VAL:CG1	7:G:4:PRO:HD3	1.84	1.07
3:C:22:CYS:CB	10:C:301:HEM:HAB	1.83	1.07
7:G:26:TYR:O	7:G:28:GLN:N	1.86	1.07
1:A:97:MET:HE1	1:A:125:ALA:HA	1.10	1.06
1:A:97:MET:CE	1:A:125:ALA:HA	1.83	1.06
2:B:124:PHE:HE1	7:G:26:TYR:HB2	1.20	1.06
3:C:171:VAL:CG1	3:C:235:PRO:HD2	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:GLY:HA3	4:D:171:ARG:NH1	1.71	1.06
1:A:92:MET:HB3	11:A:1002:OPC:HCB1	1.38	1.05
3:C:70:LEU:N	3:C:70:LEU:HD23	1.69	1.05
3:C:144:PHE:CZ	3:C:251:ASP:HB2	1.91	1.05
1:A:7:TRP:CE2	1:A:11:ARG:NH2	2.24	1.04
4:D:139:VAL:H	4:D:147:SER:HB3	1.16	1.04
2:B:132:ILE:HD12	2:B:132:ILE:H	1.22	1.03
1:A:36:LEU:HB3	1:A:100:HIS:HB2	1.38	1.03
4:D:85:LYS:CB	4:D:85:LYS:HZ2	1.70	1.03
10:A:302:HEM:HBC2	10:A:302:HEM:HMC2	1.40	1.03
1:A:106:LEU:HD21	2:B:133:PHE:CE1	1.93	1.02
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.24	1.02
4:D:122:ASN:CB	4:D:135:GLU:OE2	2.07	1.02
7:G:29:TYR:O	7:G:29:TYR:CG	2.10	1.02
6:F:11:LEU:HB3	6:F:15:LEU:CD1	1.89	1.02
10:A:301:HEM:CMB	10:A:301:HEM:CBB	2.30	1.01
3:C:70:LEU:HD23	3:C:70:LEU:H	1.18	1.01
3:C:84:ILE:HD11	3:C:114:LEU:HD13	1.42	1.01
6:F:13:PHE:CE2	6:F:17:PHE:HE1	1.79	1.01
1:A:47:GLN:HE21	1:A:47:GLN:CA	1.74	1.01
2:B:96:LEU:HD13	2:B:100:LEU:HD11	1.39	1.00
4:D:139:VAL:CG2	4:D:147:SER:HB3	1.90	1.00
1:A:92:MET:HE3	11:A:1002:OPC:CCB	1.89	1.00
1:A:113:PRO:HG3	2:B:21:GLY:HA3	1.39	1.00
3:C:70:LEU:N	3:C:70:LEU:CD2	2.25	0.99
4:D:133:TYR:CE2	4:D:148:LEU:HD23	1.96	0.99
1:A:54:MET:HE3	10:A:301:HEM:HBD1	1.00	0.99
1:A:61:THR:HA	1:A:177:GLN:HE22	1.25	0.99
3:C:171:VAL:CG1	3:C:234:ASN:HD22	1.75	0.98
1:A:41:LEU:HD23	10:A:303:HEM:CBC	1.93	0.98
1:A:32:ILE:HG22	1:A:33:PHE:CD2	1.99	0.97
1:A:92:MET:HE3	11:A:1002:OPC:HCB2	1.00	0.97
5:E:22:ILE:O	5:E:26:ILE:HB	1.63	0.97
2:B:128:VAL:O	2:B:132:ILE:CD1	2.12	0.97
3:C:28:ALA:HB3	3:C:239:GLY:HA3	1.45	0.97
3:C:15:GLU:CB	3:C:16:PRO:HD2	1.95	0.97
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.26	0.97
1:A:150:ILE:HD13	14:B:1201:TDS:CAA	1.95	0.96
5:E:18:ILE:O	5:E:22:ILE:HG22	1.63	0.96
3:C:176:ALA:HB1	3:C:205:LYS:NZ	1.80	0.96
1:A:26:VAL:HG21	1:A:30:VAL:HG11	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:H	1:A:110:PHE:HD2	1.09	0.96
2:B:91:VAL:O	2:B:91:VAL:CG1	2.07	0.96
3:C:189:GLU:O	3:C:190:TYR:CD2	2.18	0.96
3:C:273:ILE:HG13	8:H:21:MET:HG3	1.44	0.96
2:B:82:TYR:N	2:B:83:PRO:HD2	1.78	0.96
2:B:142:TRP:HH2	2:B:155:LEU:O	1.45	0.96
3:C:120:PRO:HD2	3:C:124:TYR:HD1	1.30	0.96
4:D:85:LYS:HB2	4:D:85:LYS:HZ3	1.18	0.95
6:F:20:TRP:O	6:F:24:VAL:HG23	1.65	0.95
2:B:128:VAL:O	2:B:132:ILE:HD12	1.65	0.95
1:A:150:ILE:HD13	14:B:1201:TDS:HAA3	1.48	0.95
10:A:301:HEM:O2D	10:A:301:HEM:HBA2	1.66	0.95
3:C:15:GLU:HB3	3:C:16:PRO:CD	1.96	0.95
4:D:84:LEU:HD12	4:D:84:LEU:H	1.31	0.95
2:B:34:ASN:HD21	3:C:283:GLN:NE2	1.65	0.95
3:C:141:ASN:N	3:C:141:ASN:HD22	1.59	0.95
1:A:163:VAL:CG1	1:A:164:LEU:N	2.30	0.95
2:B:40:PHE:CB	2:B:41:PRO:HD3	1.95	0.95
7:G:2:VAL:HG13	7:G:4:PRO:HD3	1.46	0.94
1:A:39:ILE:HD11	17:G:101:BCR:C31	1.97	0.94
10:C:301:HEM:HMC2	10:C:301:HEM:HBC2	1.49	0.94
2:B:25:ASN:HD22	2:B:25:ASN:H	1.15	0.94
3:C:170:ASN:O	3:C:235:PRO:HG3	1.67	0.94
4:D:146:LEU:CD1	4:D:177:TRP:CG	2.50	0.94
1:A:147:ALA:HB2	14:B:1201:TDS:HAJ3	1.46	0.94
10:A:301:HEM:HBB2	10:A:301:HEM:HMB2	0.95	0.94
2:B:152:ASP:CA	2:B:154:THR:HG22	1.97	0.94
1:A:103:ARG:HD2	1:A:103:ARG:C	1.86	0.93
2:B:93:ASN:OD1	2:B:96:LEU:CB	2.17	0.93
6:F:29:ILE:O	6:F:29:ILE:HD13	1.67	0.93
1:A:70:GLN:O	1:A:74:ASN:HB2	1.69	0.93
4:D:66:VAL:HG23	4:D:158:ASP:O	1.69	0.93
4:D:109:THR:HG22	4:D:144:ALA:HB1	0.94	0.93
2:B:109:ILE:O	2:B:112:PRO:HD2	1.69	0.93
3:C:200:GLN:CG	3:C:205:LYS:O	2.16	0.93
3:C:193:VAL:O	3:C:194:LYS:HG2	1.69	0.92
3:C:178:GLY:O	3:C:224:ALA:HA	1.69	0.92
2:B:79:TRP:CD1	2:B:80:TYR:N	2.38	0.92
10:A:303:HEM:CGA	14:B:1202:TDS:HAA2	2.00	0.92
3:C:170:ASN:O	3:C:235:PRO:CG	2.17	0.92
3:C:180:ILE:HD11	3:C:183:ILE:CD1	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ASN:HD22	3:C:141:ASN:H	1.12	0.91
1:A:103:ARG:NH1	1:A:104:VAL:HG23	1.86	0.91
3:C:144:PHE:CE2	3:C:251:ASP:HB2	2.05	0.91
1:A:39:ILE:CD1	17:G:101:BCR:H312	2.01	0.90
2:B:96:LEU:CD1	2:B:100:LEU:HD11	2.01	0.90
1:A:47:GLN:HE21	1:A:47:GLN:HA	1.31	0.90
4:D:94:GLU:OE2	4:D:100:ARG:HG2	1.70	0.90
3:C:200:GLN:O	3:C:205:LYS:HG2	1.70	0.90
7:G:11:LEU:N	7:G:11:LEU:HD23	1.85	0.90
2:B:115:GLU:OE2	2:B:126:ARG:NH1	2.04	0.90
4:D:146:LEU:HD12	4:D:177:TRP:CG	2.06	0.90
1:A:26:VAL:CG2	1:A:30:VAL:HG11	2.02	0.90
10:A:303:HEM:O2A	14:B:1202:TDS:HAA2	1.71	0.90
2:B:57:LEU:HD12	8:H:8:TRP:CE3	2.06	0.90
2:B:138:LEU:CD1	2:B:138:LEU:HG	2.01	0.90
4:D:139:VAL:HG22	4:D:147:SER:CB	2.01	0.90
3:C:211:ILE:O	3:C:212:PRO:O	1.91	0.89
3:C:119:LEU:CD2	3:C:124:TYR:CD1	2.55	0.89
1:A:31:ASN:C	1:A:31:ASN:HD22	1.74	0.89
1:A:92:MET:HE2	11:A:1002:OPC:CCB	1.96	0.89
2:B:88:LEU:HD13	14:B:1201:TDS:CAI	2.03	0.89
2:B:124:PHE:CE1	7:G:26:TYR:HB2	2.07	0.89
1:A:30:VAL:HG22	1:A:34:TYR:CG	2.08	0.89
1:A:47:GLN:HA	1:A:47:GLN:NE2	1.87	0.89
4:D:139:VAL:HG23	4:D:147:SER:HB3	1.54	0.89
3:C:60:GLN:HE22	3:C:157:ARG:HG2	1.36	0.89
1:A:108:GLY:HA2	1:A:110:PHE:CE2	2.07	0.88
7:G:10:VAL:HG12	7:G:11:LEU:HD23	1.55	0.88
3:C:285:ALA:C	3:C:286:GLU:OE1	2.11	0.88
2:B:152:ASP:HA	2:B:154:THR:CG2	2.03	0.88
6:F:6:LEU:O	6:F:10:LEU:HB2	1.74	0.88
7:G:29:TYR:O	7:G:29:TYR:HD2	1.55	0.88
3:C:288:ASN:C	3:C:288:ASN:HD22	1.76	0.88
4:D:139:VAL:HG22	4:D:147:SER:HA	1.54	0.88
3:C:171:VAL:HG11	3:C:234:ASN:HD22	1.36	0.88
1:A:103:ARG:HH12	1:A:104:VAL:HG23	1.38	0.87
3:C:22:CYS:HB2	10:C:301:HEM:HAB	0.89	0.87
3:C:71:ASN:HB2	10:C:301:HEM:O2A	1.74	0.87
2:B:118:ASN:HD22	2:B:120:PHE:H	1.22	0.87
1:A:100:HIS:HE1	10:A:302:HEM:C1A	1.93	0.87
3:C:119:LEU:HD23	3:C:124:TYR:CD1	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:HIS:HB3	15:D:200:FES:S2	2.14	0.87
1:A:54:MET:HE3	10:A:301:HEM:CBD	1.97	0.86
2:B:4:LEU:H	3:C:287:MET:CE	1.87	0.86
2:B:79:TRP:CG	2:B:80:TYR:N	2.43	0.86
3:C:52:ILE:O	3:C:52:ILE:HG22	1.75	0.86
6:F:29:ILE:HD12	6:F:29:ILE:C	1.96	0.86
1:A:163:VAL:HG12	1:A:164:LEU:H	1.40	0.86
4:D:109:THR:HG21	4:D:146:LEU:O	1.74	0.86
1:A:61:THR:HG22	1:A:64:GLU:H	1.41	0.86
3:C:22:CYS:CB	10:C:301:HEM:CAB	2.50	0.86
3:C:211:ILE:O	3:C:211:ILE:CG1	2.22	0.86
3:C:219:VAL:HG12	3:C:219:VAL:O	1.73	0.86
6:F:25:LEU:CD1	6:F:25:LEU:HG	2.05	0.86
3:C:223:GLN:HG3	3:C:224:ALA:H	1.41	0.85
4:D:21:LEU:HD11	16:D:201:SQD:H301	1.58	0.85
4:D:102:TYR:HA	4:D:151:CYS:O	1.76	0.85
1:A:112:LYS:O	1:A:113:PRO:C	2.12	0.85
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.59	0.85
1:A:26:VAL:CG2	1:A:30:VAL:CG1	2.54	0.85
1:A:39:ILE:HG22	1:A:96:MET:HG3	1.56	0.85
6:F:13:PHE:CE2	6:F:17:PHE:CE1	2.64	0.85
3:C:60:GLN:NE2	3:C:157:ARG:HG2	1.90	0.85
3:C:71:ASN:N	10:C:301:HEM:O2A	2.10	0.85
3:C:28:ALA:HB3	3:C:239:GLY:CA	2.07	0.85
2:B:77:PRO:HB3	14:B:1201:TDS:CAM	2.07	0.85
4:D:68:LYS:HA	4:D:71:GLU:HB2	1.59	0.85
3:C:259:ILE:HD12	8:H:6:LEU:HD13	1.57	0.84
2:B:114:ILE:HG22	2:B:115:GLU:N	1.90	0.84
6:F:5:MET:HG2	6:F:6:LEU:N	1.92	0.84
1:A:41:LEU:HD23	10:A:303:HEM:HBC1	1.59	0.84
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.13	0.83
1:A:142:GLN:OE1	1:A:142:GLN:HA	1.78	0.83
10:C:301:HEM:HBC2	10:C:301:HEM:CMC	2.09	0.83
2:B:34:ASN:HD21	3:C:283:GLN:HE22	0.88	0.83
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.59	0.83
1:A:103:ARG:HD2	1:A:103:ARG:O	1.79	0.83
4:D:143:PRO:O	4:D:145:PRO:HD3	1.79	0.82
1:A:92:MET:CB	11:A:1002:OPC:HCB1	2.08	0.82
4:D:69:PHE:HD2	4:D:69:PHE:C	1.83	0.82
5:E:5:ALA:O	5:E:9:ILE:HG13	1.80	0.82
2:B:159:LEU:O	2:B:160:PHE:CD2	2.33	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:CYS:HG	10:C:301:HEM:CAC	1.93	0.82
1:A:215:LEU:HD13	2:B:122:ASN:HA	1.61	0.82
2:B:70:ALA:HB1	3:C:17:THR:HG22	1.61	0.82
4:D:111:LEU:N	4:D:111:LEU:HD12	1.90	0.82
4:D:139:VAL:H	4:D:147:SER:CB	1.92	0.82
4:D:133:TYR:CD2	4:D:148:LEU:HD23	2.15	0.81
6:F:22:LEU:HD13	6:F:22:LEU:C	1.99	0.81
4:D:21:LEU:CD1	16:D:201:SQD:H301	2.10	0.81
1:A:26:VAL:HG21	1:A:30:VAL:CG1	2.10	0.81
3:C:270:LEU:HB2	8:H:21:MET:HE2	1.61	0.81
4:D:102:TYR:OH	4:D:136:THR:HG22	1.80	0.81
4:D:134:ASP:OD1	4:D:134:ASP:C	2.18	0.81
1:A:108:GLY:HA2	1:A:110:PHE:HE2	1.45	0.81
3:C:229:GLU:HA	3:C:229:GLU:OE1	1.78	0.81
3:C:13:PRO:O	3:C:21:VAL:HG22	1.81	0.81
2:B:130:THR:CG2	7:G:22:PHE:HE2	1.93	0.81
2:B:82:TYR:N	2:B:83:PRO:CD	2.44	0.81
3:C:119:LEU:CD2	3:C:124:TYR:CE1	2.64	0.81
1:A:207:ARG:HH12	14:B:1202:TDS:HAI1	1.46	0.81
3:C:226:LYS:HB3	3:C:226:LYS:HZ3	1.45	0.81
1:A:155:PRO:HD3	14:B:1201:TDS:HAX2	1.63	0.80
3:C:171:VAL:CG1	3:C:234:ASN:HA	2.11	0.80
5:E:10:VAL:O	5:E:14:LEU:HB2	1.81	0.80
10:A:302:HEM:HMC2	10:A:302:HEM:CBC	2.11	0.80
4:D:137:GLY:HA3	4:D:171:ARG:HH11	1.46	0.80
2:B:57:LEU:HD12	8:H:8:TRP:CD2	2.17	0.80
3:C:250:GLN:HG3	3:C:251:ASP:N	1.97	0.80
2:B:118:ASN:ND2	2:B:120:PHE:H	1.78	0.80
2:B:90:SER:O	2:B:91:VAL:HG23	1.81	0.80
2:B:57:LEU:CD1	8:H:8:TRP:CD2	2.64	0.80
2:B:95:LEU:HD23	2:B:95:LEU:C	2.02	0.80
4:D:139:VAL:HG22	4:D:147:SER:HB3	1.60	0.80
4:D:139:VAL:HG22	4:D:147:SER:N	1.97	0.80
2:B:91:VAL:O	2:B:93:ASN:N	2.15	0.79
4:D:110:HIS:C	4:D:111:LEU:CD1	2.50	0.79
3:C:107:LYS:HE3	3:C:110:GLN:HE22	1.45	0.79
3:C:177:THR:HG21	3:C:226:LYS:HD2	1.62	0.79
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.17	0.79
6:F:24:VAL:O	6:F:27:LEU:HB2	1.81	0.79
1:A:7:TRP:NE1	1:A:11:ARG:NH2	2.29	0.79
3:C:84:ILE:HD11	3:C:114:LEU:CD1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:ASP:OD1	3:C:139:ASP:C	2.19	0.79
1:A:110:PHE:CD1	2:B:112:PRO:HB3	2.15	0.79
3:C:226:LYS:HB3	3:C:226:LYS:NZ	1.96	0.79
4:D:105:ASN:HB3	4:D:149:ALA:HB3	1.63	0.79
2:B:104:VAL:O	2:B:108:LEU:HB2	1.81	0.79
3:C:206:THR:CG2	3:C:206:THR:O	2.30	0.78
1:A:36:LEU:HD21	1:A:99:LEU:HB3	1.65	0.78
2:B:79:TRP:CD1	2:B:79:TRP:C	2.57	0.78
3:C:107:LYS:HE3	3:C:110:GLN:NE2	1.97	0.78
3:C:141:ASN:N	3:C:141:ASN:ND2	2.31	0.78
4:D:105:ASN:HD21	4:D:107:VAL:HG23	1.46	0.78
3:C:46:PHE:CZ	3:C:131:VAL:HG22	2.19	0.78
10:A:302:HEM:HHA	10:A:302:HEM:HBA1	1.66	0.78
1:A:83:ARG:HD2	10:A:301:HEM:O1D	1.84	0.78
3:C:171:VAL:CG1	3:C:234:ASN:ND2	2.46	0.78
3:C:199:ILE:O	3:C:200:GLN:HB2	1.82	0.78
3:C:120:PRO:HD2	3:C:124:TYR:CD1	2.18	0.77
2:B:4:LEU:H	3:C:287:MET:HE1	1.49	0.77
3:C:107:LYS:CE	3:C:110:GLN:HE22	1.96	0.77
3:C:219:VAL:O	3:C:219:VAL:CG1	2.32	0.77
3:C:286:GLU:OE1	3:C:286:GLU:N	2.17	0.77
4:D:21:LEU:HD12	16:D:201:SQD:H282	1.66	0.77
2:B:40:PHE:HB2	2:B:41:PRO:HD3	1.64	0.77
3:C:176:ALA:HB1	3:C:205:LYS:HZ1	1.49	0.77
3:C:19:ARG:O	3:C:20:ILE:CB	2.20	0.77
3:C:180:ILE:HD11	3:C:183:ILE:HD12	1.67	0.77
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.67	0.77
10:A:301:HEM:HBB2	10:A:301:HEM:HMB3	1.63	0.77
3:C:119:LEU:HD23	3:C:124:TYR:CE1	2.19	0.77
3:C:270:LEU:HA	8:H:21:MET:CE	2.15	0.77
5:E:29:ILE:HG22	5:E:29:ILE:O	1.85	0.77
1:A:207:ARG:NH1	14:B:1202:TDS:HAI1	1.99	0.77
3:C:171:VAL:HG11	3:C:234:ASN:HA	1.64	0.77
4:D:139:VAL:CG2	4:D:147:SER:N	2.48	0.77
1:A:207:ARG:HH11	1:A:207:ARG:CG	1.97	0.77
2:B:16:ALA:O	2:B:19:ALA:HB3	1.85	0.77
3:C:178:GLY:O	3:C:224:ALA:CA	2.32	0.77
3:C:178:GLY:O	3:C:224:ALA:CB	2.33	0.76
11:A:1002:OPC:CBV	7:G:9:LEU:HD21	2.13	0.76
4:D:161:VAL:HG12	4:D:161:VAL:O	1.83	0.76
4:D:12:ASP:O	4:D:14:GLY:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:CD1	14:B:1201:TDS:CAA	2.64	0.76
2:B:10:SER:O	2:B:12:PRO:HD3	1.86	0.76
3:C:14:ARG:CZ	3:C:150:HIS:CD2	2.69	0.76
3:C:200:GLN:NE2	3:C:206:THR:OG1	2.19	0.76
4:D:80:LEU:C	4:D:81:VAL:HG23	2.05	0.76
6:F:13:PHE:HE2	6:F:17:PHE:CE1	2.02	0.76
4:D:12:ASP:O	4:D:13:MET:C	2.23	0.76
4:D:69:PHE:O	4:D:70:LEU:O	2.03	0.76
4:D:108:CYS:HB2	4:D:133:TYR:OH	1.86	0.76
3:C:71:ASN:OD1	3:C:120:PRO:HA	1.86	0.75
4:D:139:VAL:CG2	4:D:147:SER:CB	2.60	0.75
4:D:150:LEU:HD21	4:D:171:ARG:NH1	2.01	0.75
3:C:172:PHE:CD1	3:C:172:PHE:N	2.54	0.75
4:D:111:LEU:HD13	4:D:111:LEU:H	1.45	0.75
2:B:81:LEU:CD1	14:B:1201:TDS:HAR1	2.16	0.75
4:D:15:ARG:HB3	5:E:31:LEU:CD2	2.15	0.75
3:C:171:VAL:HG13	3:C:234:ASN:HD22	1.50	0.75
3:C:225:VAL:HG12	3:C:229:GLU:CG	2.17	0.75
3:C:270:LEU:HB2	8:H:21:MET:CE	2.16	0.75
4:D:64:VAL:HG13	4:D:69:PHE:HD1	1.51	0.75
3:C:180:ILE:HD11	3:C:183:ILE:HD11	1.68	0.75
3:C:171:VAL:HG13	3:C:234:ASN:ND2	2.03	0.74
1:A:147:ALA:HB2	14:B:1201:TDS:CAJ	2.16	0.74
2:B:123:PRO:HA	2:B:126:ARG:HG3	1.69	0.74
7:G:26:TYR:C	7:G:28:GLN:H	1.91	0.74
4:D:146:LEU:HD13	4:D:177:TRP:CG	2.23	0.74
1:A:202:HIS:O	1:A:206:ILE:HG13	1.87	0.74
1:A:150:ILE:CD1	14:B:1201:TDS:HAA3	2.18	0.74
2:B:25:ASN:H	2:B:25:ASN:ND2	1.86	0.74
10:A:303:HEM:O2A	14:B:1202:TDS:CAA	2.35	0.74
3:C:285:ALA:HB2	4:D:10:VAL:HG21	1.68	0.74
4:D:146:LEU:CD1	4:D:177:TRP:CD2	2.66	0.74
8:H:19:ILE:HG22	8:H:20:ALA:N	2.03	0.74
12:A:1101:UMQ:H51	12:A:1101:UMQ:H6'1	1.69	0.73
3:C:119:LEU:HD22	3:C:124:TYR:CD1	2.21	0.73
3:C:4:TRP:CD2	3:C:162:PRO:HG3	2.23	0.73
3:C:221:GLU:OE1	3:C:222:GLY:N	2.22	0.73
1:A:127:ILE:CG2	1:A:195:ILE:HG13	2.18	0.73
1:A:47:GLN:HE21	1:A:47:GLN:N	1.87	0.73
4:D:80:LEU:C	4:D:81:VAL:CG2	2.56	0.73
3:C:94:LEU:O	3:C:94:LEU:HD23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:O	1:A:114:ARG:N	2.21	0.73
2:B:82:TYR:H	2:B:83:PRO:HD2	1.53	0.73
2:B:9:LEU:O	2:B:15:ARG:CD	2.25	0.73
4:D:69:PHE:C	4:D:69:PHE:CD2	2.61	0.73
7:G:2:VAL:HG12	7:G:2:VAL:O	1.87	0.73
3:C:226:LYS:NZ	3:C:226:LYS:CB	2.52	0.72
8:H:1:MET:O	8:H:2:GLU:HB3	1.87	0.72
2:B:124:PHE:HE1	7:G:26:TYR:CB	1.99	0.72
6:F:29:ILE:CD1	6:F:29:ILE:C	2.57	0.72
1:A:33:PHE:CD1	7:G:21:LEU:HD13	2.24	0.72
3:C:23:ALA:HB2	3:C:240:PHE:CE2	2.24	0.72
3:C:189:GLU:O	3:C:190:TYR:HD2	1.70	0.72
1:A:100:HIS:CE1	10:A:302:HEM:C1A	2.76	0.72
3:C:237:VAL:HG22	3:C:237:VAL:O	1.88	0.72
1:A:111:LYS:O	1:A:113:PRO:HD2	1.90	0.72
2:B:14:LEU:HD11	2:B:18:LEU:HD11	1.71	0.72
5:E:10:VAL:HG12	5:E:14:LEU:HD12	1.69	0.72
8:H:23:VAL:HA	8:H:28:GLY:HA3	1.72	0.72
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.04	0.72
3:C:15:GLU:CB	3:C:16:PRO:CD	2.60	0.72
4:D:110:HIS:C	4:D:111:LEU:HD12	2.08	0.72
6:F:27:LEU:O	6:F:30:GLN:HG3	1.89	0.72
10:A:303:HEM:CHB	14:B:1202:TDS:OAK	2.37	0.72
2:B:126:ARG:N	2:B:127:PRO:HD3	2.04	0.72
3:C:54:TYR:HE1	3:C:70:LEU:HD21	1.54	0.72
2:B:132:ILE:HD12	2:B:132:ILE:N	2.00	0.72
2:B:149:PHE:HB3	2:B:150:PRO:CD	2.19	0.72
3:C:19:ARG:O	3:C:242:GLN:OE1	2.08	0.72
5:E:6:VAL:O	5:E:10:VAL:HG23	1.89	0.71
7:G:24:ALA:O	7:G:28:GLN:HB2	1.90	0.71
12:A:1104:UMQ:H31	12:A:1104:UMQ:C6'	2.10	0.71
1:A:36:LEU:HB3	1:A:100:HIS:CB	2.20	0.71
1:A:36:LEU:CD2	1:A:99:LEU:HB3	2.20	0.71
10:A:303:HEM:CBA	14:B:1202:TDS:HAA2	2.21	0.71
2:B:118:ASN:ND2	2:B:120:PHE:CD1	2.59	0.71
3:C:223:GLN:HG3	3:C:224:ALA:N	2.05	0.71
1:A:20:ASP:O	1:A:20:ASP:OD2	2.08	0.71
1:A:83:ARG:NH1	10:A:301:HEM:O2A	2.23	0.71
4:D:170:PHE:CE2	4:D:171:ARG:HG3	2.26	0.71
3:C:174:ALA:HB2	3:C:231:LEU:HD23	1.73	0.71
5:E:9:ILE:O	5:E:13:ALA:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:HE2	2:B:115:GLU:O	1.91	0.71
2:B:77:PRO:HA	14:B:1201:TDS:HAJ2	1.73	0.71
3:C:259:ILE:CD1	8:H:6:LEU:HD13	2.21	0.70
1:A:31:ASN:C	1:A:31:ASN:ND2	2.45	0.70
3:C:9:TYR:CG	3:C:21:VAL:HG11	2.26	0.70
6:F:16:ILE:HG22	6:F:17:PHE:N	2.05	0.70
1:A:32:ILE:CG2	1:A:33:PHE:N	2.54	0.70
3:C:275:LYS:HE2	4:D:20:ASN:OD1	1.90	0.70
3:C:264:LEU:O	3:C:264:LEU:HD22	1.91	0.70
1:A:95:LEU:HD22	1:A:96:MET:HE2	1.72	0.70
1:A:110:PHE:N	1:A:110:PHE:CD2	2.56	0.70
12:A:1104:UMQ:O3'	12:A:1104:UMQ:H11	1.92	0.70
3:C:22:CYS:O	3:C:24:ASN:N	2.24	0.70
2:B:123:PRO:HD3	7:G:25:ALA:HB1	1.73	0.70
4:D:55:THR:HG23	4:D:159:ASN:HB3	1.74	0.70
6:F:11:LEU:O	6:F:15:LEU:HB2	1.91	0.70
3:C:270:LEU:HA	8:H:21:MET:HE3	1.73	0.69
2:B:40:PHE:CB	2:B:41:PRO:CD	2.70	0.69
1:A:127:ILE:HG22	1:A:195:ILE:HG13	1.74	0.69
4:D:66:VAL:HG23	4:D:158:ASP:C	2.13	0.69
4:D:146:LEU:HD13	4:D:177:TRP:CB	2.23	0.69
1:A:39:ILE:CG2	1:A:96:MET:HG3	2.22	0.69
2:B:152:ASP:C	2:B:154:THR:H	1.94	0.69
1:A:61:THR:HA	1:A:177:GLN:NE2	2.03	0.69
3:C:60:GLN:OE1	3:C:70:LEU:HB3	1.91	0.69
4:D:9:ASP:HA	5:E:30:LYS:NZ	2.07	0.69
2:B:40:PHE:HZ	14:B:1202:TDS:HBD	1.40	0.69
4:D:55:THR:HG21	4:D:63:ASN:OD1	1.92	0.69
5:E:26:ILE:CG2	5:E:32:ILE:HG13	2.22	0.69
2:B:57:LEU:HD11	8:H:8:TRP:HA	1.75	0.69
3:C:270:LEU:HD13	3:C:271:MET:N	2.08	0.69
4:D:178:TRP:CD1	4:D:179:VAL:HB	2.27	0.69
1:A:72:ILE:O	1:A:79:GLY:HA3	1.93	0.69
3:C:259:ILE:HD12	8:H:6:LEU:CD1	2.22	0.69
3:C:172:PHE:HD1	3:C:172:PHE:H	1.41	0.68
3:C:229:GLU:CD	3:C:230:ALA:H	1.96	0.68
3:C:25:CYS:SG	10:C:301:HEM:CBC	2.81	0.68
3:C:180:ILE:CD1	3:C:183:ILE:HD11	2.23	0.68
4:D:117:TRP:CH2	4:D:122:ASN:C	2.67	0.68
3:C:176:ALA:HB1	3:C:205:LYS:HZ2	1.57	0.68
3:C:221:GLU:OE1	3:C:221:GLU:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:LEU:O	5:E:18:ILE:HG12	1.92	0.68
2:B:42:VAL:HG13	3:C:269:GLN:HB3	1.75	0.68
6:F:11:LEU:CB	6:F:15:LEU:HD12	2.19	0.68
10:A:303:HEM:HBB2	10:A:303:HEM:CMB	2.24	0.68
2:B:95:LEU:HD21	2:B:99:LEU:HD11	1.74	0.68
2:B:122:ASN:HD21	7:G:29:TYR:HB2	1.59	0.68
1:A:26:VAL:HG22	1:A:30:VAL:HG12	1.75	0.68
1:A:127:ILE:HG21	1:A:195:ILE:CG1	2.22	0.68
3:C:25:CYS:SG	10:C:301:HEM:C3C	2.86	0.68
3:C:34:VAL:HG21	3:C:151:LEU:CB	2.24	0.68
14:B:1202:TDS:OAC	14:B:1202:TDS:CAA	2.38	0.67
4:D:104:ILE:HG22	4:D:148:LEU:HD12	1.77	0.67
1:A:88:TRP:CZ3	2:B:54:LEU:HD13	2.29	0.67
3:C:23:ALA:HB2	3:C:240:PHE:CD2	2.29	0.67
3:C:14:ARG:NH2	3:C:150:HIS:CD2	2.63	0.67
4:D:85:LYS:HB2	4:D:85:LYS:HZ2	0.84	0.67
4:D:117:TRP:CZ2	4:D:122:ASN:HA	2.28	0.67
4:D:100:ARG:NH1	4:D:102:TYR:OH	2.28	0.67
1:A:41:LEU:HD23	10:A:303:HEM:HBC2	1.77	0.67
2:B:128:VAL:O	2:B:132:ILE:HD11	1.93	0.67
3:C:101:VAL:HG11	3:C:103:PHE:CE2	2.29	0.67
3:C:288:ASN:C	3:C:288:ASN:ND2	2.48	0.66
2:B:21:GLY:O	2:B:22:MET:HB3	1.93	0.66
3:C:94:LEU:HD23	3:C:94:LEU:C	2.15	0.66
7:G:20:GLY:N	17:G:101:BCR:H363	2.10	0.66
1:A:82:ILE:HG12	4:D:41:TYR:CD1	2.31	0.66
3:C:41:LEU:HB2	8:H:1:MET:SD	2.36	0.66
3:C:215:PRO:HB3	3:C:232:THR:HG22	1.76	0.66
3:C:1:TYR:HA	10:C:301:HEM:C4A	2.30	0.66
3:C:229:GLU:O	3:C:231:LEU:N	2.29	0.66
3:C:262:ILE:HG22	3:C:263:CYS:N	2.11	0.66
4:D:65:LYS:CB	4:D:68:LYS:HZ3	2.09	0.66
4:D:90:TYR:OH	4:D:116:PRO:HA	1.96	0.66
3:C:36:VAL:HG11	3:C:149:ILE:CD1	2.25	0.65
3:C:65:GLY:C	3:C:66:SER:O	2.32	0.65
2:B:17:LYS:O	2:B:20:LYS:N	2.17	0.65
3:C:136:PRO:HB3	3:C:142:ILE:O	1.97	0.65
4:D:117:TRP:CH2	4:D:123:LYS:N	2.65	0.65
6:F:28:LYS:O	6:F:30:GLN:N	2.29	0.65
7:G:26:TYR:C	7:G:28:GLN:N	2.48	0.65
17:G:101:BCR:C8	17:G:101:BCR:H321	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:GLN:O	3:C:278:GLN:HG2	1.97	0.65
6:F:13:PHE:C	6:F:13:PHE:CD2	2.70	0.65
3:C:195:TYR:CD1	3:C:195:TYR:N	2.59	0.65
14:B:1202:TDS:CAS	14:B:1202:TDS:OAO	2.44	0.65
3:C:200:GLN:HG3	3:C:205:LYS:HB3	1.77	0.65
1:A:80:TRP:O	1:A:84:SER:HB2	1.97	0.65
10:A:303:HEM:CBB	10:A:303:HEM:HMB1	2.27	0.65
2:B:147:ALA:C	2:B:149:PHE:N	2.48	0.65
4:D:63:ASN:O	4:D:64:VAL:C	2.34	0.65
3:C:14:ARG:CZ	3:C:150:HIS:HD2	2.10	0.65
3:C:285:ALA:CB	4:D:10:VAL:HG21	2.26	0.65
4:D:65:LYS:HB3	4:D:68:LYS:NZ	2.12	0.64
4:D:161:VAL:O	4:D:161:VAL:CG1	2.44	0.64
7:G:26:TYR:O	7:G:27:GLN:C	2.32	0.64
4:D:139:VAL:N	4:D:147:SER:HB3	2.01	0.64
2:B:104:VAL:N	2:B:105:PRO:HD2	2.12	0.64
3:C:71:ASN:CB	10:C:301:HEM:O2A	2.45	0.64
3:C:206:THR:O	3:C:206:THR:HG22	1.97	0.64
3:C:270:LEU:HD13	3:C:270:LEU:C	2.17	0.64
4:D:150:LEU:HD21	4:D:171:ARG:CZ	2.28	0.64
1:A:150:ILE:CD1	14:B:1201:TDS:HAA2	2.27	0.64
2:B:106:LEU:O	2:B:109:ILE:HB	1.96	0.64
4:D:69:PHE:HD2	4:D:69:PHE:O	1.78	0.64
1:A:207:ARG:NH1	14:B:1202:TDS:CAI	2.60	0.64
10:A:303:HEM:CMB	10:A:303:HEM:CBB	2.76	0.64
1:A:136:TYR:HE2	14:B:1201:TDS:CAJ	2.11	0.64
3:C:60:GLN:OE1	3:C:70:LEU:CB	2.46	0.64
4:D:25:GLY:HA3	16:D:201:SQD:H341	1.78	0.64
1:A:26:VAL:CG2	1:A:30:VAL:HG12	2.26	0.63
3:C:232:THR:O	3:C:233:ASN:HB3	1.97	0.63
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.28	0.63
6:F:14:GLY:O	6:F:17:PHE:HB2	1.97	0.63
2:B:22:MET:HA	2:B:24:HIS:HD2	1.63	0.63
4:D:146:LEU:CD1	4:D:177:TRP:CB	2.76	0.63
3:C:188:ASP:C	3:C:190:TYR:H	1.99	0.63
1:A:54:MET:CE	10:A:301:HEM:CBD	2.66	0.63
3:C:2:PRO:HD3	10:C:301:HEM:CHB	2.28	0.63
3:C:71:ASN:HB2	10:C:301:HEM:CGA	2.29	0.63
3:C:94:LEU:O	3:C:98:VAL:HG23	1.99	0.63
2:B:118:ASN:HD22	2:B:120:PHE:N	1.94	0.63
2:B:88:LEU:HD13	14:B:1201:TDS:HAI3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:HIS:HD1	3:C:154:ASN:ND2	1.97	0.63
10:C:301:HEM:HMC2	10:C:301:HEM:CBC	2.25	0.63
1:A:8:PHE:HB3	1:A:14:ILE:HG12	1.81	0.62
1:A:63:THR:O	1:A:63:THR:HG22	1.91	0.62
2:B:45:MET:CE	4:D:27:VAL:HG13	2.28	0.62
4:D:55:THR:CG2	4:D:63:ASN:OD1	2.47	0.62
7:G:2:VAL:HG13	7:G:3:GLU:N	2.09	0.62
8:H:23:VAL:O	8:H:24:TRP:C	2.33	0.62
1:A:29:HIS:CD2	1:A:213:GLY:O	2.52	0.62
3:C:180:ILE:HG12	3:C:181:THR:N	2.12	0.62
4:D:65:LYS:CB	4:D:68:LYS:NZ	2.62	0.62
7:G:17:THR:O	7:G:21:LEU:HB2	1.99	0.62
1:A:105:TYR:HD2	1:A:106:LEU:HD23	1.64	0.62
4:D:32:LEU:O	4:D:33:GLY:C	2.36	0.62
4:D:110:HIS:C	4:D:111:LEU:HD13	2.15	0.62
3:C:19:ARG:HG2	3:C:19:ARG:HH11	1.64	0.62
4:D:63:ASN:O	4:D:64:VAL:O	2.17	0.62
4:D:137:GLY:HA3	4:D:171:ARG:HH12	1.63	0.62
4:D:150:LEU:O	4:D:151:CYS:HB3	2.00	0.62
1:A:30:VAL:CG2	1:A:34:TYR:CG	2.80	0.62
2:B:95:LEU:CD2	2:B:99:LEU:CD1	2.77	0.62
3:C:225:VAL:HG12	3:C:229:GLU:HG2	1.81	0.62
7:G:29:TYR:CD2	7:G:29:TYR:C	2.66	0.62
3:C:74:ALA:H	10:C:301:HEM:HMB3	1.65	0.62
3:C:179:THR:HA	3:C:223:GLN:O	2.00	0.62
3:C:200:GLN:HE21	3:C:206:THR:HA	1.64	0.62
2:B:95:LEU:O	2:B:99:LEU:HD12	1.99	0.62
2:B:126:ARG:N	2:B:127:PRO:CD	2.63	0.62
3:C:62:ALA:HB2	3:C:68:VAL:HG12	1.81	0.62
3:C:119:LEU:HD22	3:C:124:TYR:CG	2.35	0.62
4:D:64:VAL:CG1	4:D:69:PHE:HD1	2.12	0.62
2:B:69:PHE:N	2:B:69:PHE:CD2	2.68	0.61
2:B:32:TRP:CD1	2:B:33:PRO:CD	2.84	0.61
3:C:180:ILE:HG22	3:C:223:GLN:HB3	1.83	0.61
6:F:17:PHE:O	6:F:20:TRP:HB3	2.00	0.61
2:B:57:LEU:CD1	8:H:8:TRP:CE3	2.81	0.61
3:C:270:LEU:CB	8:H:21:MET:HE2	2.30	0.61
3:C:282:VAL:HG11	4:D:16:ARG:HE	1.65	0.61
1:A:103:ARG:O	1:A:107:THR:HB	2.00	0.61
7:G:7:ASP:OD2	7:G:7:ASP:N	2.32	0.61
1:A:111:LYS:NZ	2:B:120:PHE:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD13	2:B:122:ASN:CA	2.29	0.61
1:A:215:LEU:HB3	2:B:122:ASN:HB2	1.81	0.61
4:D:9:ASP:HA	5:E:30:LYS:HZ1	1.65	0.61
4:D:90:TYR:HE1	4:D:115:VAL:O	1.84	0.61
4:D:170:PHE:CE2	4:D:171:ARG:CG	2.83	0.61
7:G:10:VAL:HG12	7:G:11:LEU:N	2.15	0.61
1:A:12:LEU:CB	1:A:14:ILE:CD1	2.79	0.61
3:C:34:VAL:HG21	3:C:151:LEU:HB2	1.82	0.61
3:C:186:GLU:HB2	3:C:194:LYS:HB2	1.83	0.61
5:E:29:ILE:O	5:E:29:ILE:CG2	2.49	0.61
1:A:32:ILE:HG23	1:A:33:PHE:N	2.14	0.61
4:D:168:THR:HA	4:D:176:PRO:HD3	1.83	0.61
2:B:134:LEU:HD13	2:B:134:LEU:N	2.14	0.61
3:C:87:GLU:C	3:C:89:ARG:H	2.04	0.61
1:A:111:LYS:CE	2:B:115:GLU:O	2.48	0.60
6:F:25:LEU:C	6:F:27:LEU:H	2.03	0.60
2:B:151:LEU:O	2:B:154:THR:CG2	2.48	0.60
3:C:93:GLU:O	3:C:97:GLU:HG3	2.01	0.60
4:D:65:LYS:HB3	4:D:68:LYS:HZ3	1.67	0.60
3:C:28:ALA:CB	3:C:239:GLY:HA3	2.25	0.60
3:C:54:TYR:HE1	3:C:70:LEU:CD2	2.13	0.60
5:E:27:LYS:O	5:E:30:LYS:HA	2.02	0.60
4:D:108:CYS:HB2	4:D:133:TYR:HH	1.65	0.60
2:B:75:ILE:HG23	2:B:75:ILE:O	2.01	0.60
3:C:62:ALA:HB2	3:C:68:VAL:CG1	2.31	0.60
3:C:173:THR:O	3:C:231:LEU:CD2	2.50	0.60
3:C:176:ALA:CB	3:C:205:LYS:HZ2	2.15	0.60
5:E:24:PHE:CE1	6:F:29:ILE:HD11	2.37	0.60
1:A:12:LEU:HB3	1:A:14:ILE:CD1	2.32	0.60
4:D:132:GLN:OE1	4:D:141:ARG:HG2	2.02	0.60
3:C:54:TYR:CE1	3:C:70:LEU:HD21	2.35	0.60
3:C:286:GLU:OE1	3:C:286:GLU:CA	2.50	0.60
4:D:105:ASN:ND2	4:D:107:VAL:HG23	2.16	0.60
1:A:105:TYR:CD2	1:A:106:LEU:HD23	2.37	0.60
10:A:302:HEM:CMB	10:A:302:HEM:HBB2	2.31	0.60
1:A:195:ILE:O	1:A:199:MET:HG3	2.02	0.59
3:C:19:ARG:HG2	3:C:19:ARG:NH1	2.17	0.59
1:A:211:ILE:CD1	1:A:212:SER:H	2.15	0.59
3:C:172:PHE:N	3:C:172:PHE:HD1	1.96	0.59
2:B:104:VAL:HB	2:B:105:PRO:CD	2.32	0.59
4:D:152:HIS:O	4:D:162:LEU:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:23:GLY:O	6:F:26:LEU:HB2	2.02	0.59
1:A:32:ILE:CG2	1:A:33:PHE:CD2	2.82	0.59
1:A:87:ARG:HH11	1:A:87:ARG:HG2	1.67	0.59
1:A:95:LEU:O	1:A:96:MET:C	2.40	0.59
3:C:80:GLU:OE2	3:C:80:GLU:HA	2.02	0.59
3:C:270:LEU:CA	8:H:21:MET:HE2	2.31	0.59
4:D:64:VAL:HG13	4:D:69:PHE:CD1	2.35	0.59
1:A:211:ILE:HG23	1:A:212:SER:O	2.02	0.59
3:C:279:VAL:C	3:C:281:LYS:H	2.05	0.59
12:A:1101:UMQ:HK2	4:D:34:ALA:HA	1.85	0.59
6:F:13:PHE:C	6:F:13:PHE:HD2	2.05	0.59
1:A:187:HIS:HE1	10:A:301:HEM:C1B	2.21	0.59
12:A:1102:UMQ:O3'	12:A:1102:UMQ:H11	2.02	0.59
1:A:112:LYS:HA	1:A:115:GLU:OE2	2.02	0.59
4:D:78:ARG:HD2	4:D:117:TRP:CD1	2.37	0.59
4:D:156:GLN:O	4:D:157:ASP:HB2	2.03	0.59
1:A:120:SER:O	1:A:123:ILE:N	2.35	0.59
3:C:171:VAL:HG23	3:C:171:VAL:O	2.01	0.59
4:D:170:PHE:CD2	4:D:171:ARG:HG3	2.38	0.59
7:G:13:LEU:O	7:G:14:VAL:C	2.41	0.59
3:C:61:VAL:HG21	3:C:214:GLY:O	2.03	0.59
7:G:24:ALA:C	7:G:26:TYR:H	2.06	0.59
2:B:25:ASN:HD22	2:B:25:ASN:N	1.87	0.58
2:B:95:LEU:HD23	2:B:99:LEU:HD12	1.84	0.58
3:C:155:ARG:O	3:C:155:ARG:HG2	2.01	0.58
2:B:134:LEU:HD21	7:G:22:PHE:CZ	2.38	0.58
5:E:4:GLY:O	5:E:8:TYR:N	2.26	0.58
1:A:32:ILE:HG22	1:A:33:PHE:CE2	2.38	0.58
1:A:211:ILE:C	1:A:212:SER:O	2.35	0.58
1:A:207:ARG:NH1	1:A:207:ARG:CG	2.61	0.58
10:A:302:HEM:HBA1	10:A:302:HEM:CHA	2.27	0.58
3:C:226:LYS:CB	3:C:226:LYS:HZ2	2.17	0.58
3:C:237:VAL:O	3:C:237:VAL:CG2	2.50	0.58
4:D:64:VAL:CG1	4:D:69:PHE:CD1	2.87	0.58
2:B:58:ASP:OD2	2:B:58:ASP:C	2.42	0.58
6:F:23:GLY:HA2	6:F:26:LEU:HD23	1.84	0.58
3:C:171:VAL:O	3:C:171:VAL:CG2	2.51	0.58
4:D:22:LEU:N	4:D:22:LEU:HD23	2.17	0.58
4:D:105:ASN:O	4:D:148:LEU:HD13	2.03	0.58
4:D:117:TRP:NE1	4:D:119:ALA:HA	2.19	0.58
3:C:34:VAL:CG2	3:C:151:LEU:CB	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:HIS:CE1	10:C:301:HEM:NA	2.72	0.58
3:C:34:VAL:HG21	3:C:151:LEU:HB3	1.84	0.58
3:C:78:LEU:HB2	3:C:112:ASN:O	2.04	0.58
3:C:270:LEU:HA	8:H:21:MET:HE2	1.84	0.58
4:D:59:LYS:H	4:D:59:LYS:HD3	1.69	0.58
6:F:27:LEU:HD11	8:H:27:ASN:HA	1.84	0.57
1:A:95:LEU:O	1:A:97:MET:N	2.36	0.57
2:B:81:LEU:HD11	14:B:1201:TDS:HAR1	1.85	0.57
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.85	0.57
3:C:60:GLN:HE22	3:C:157:ARG:H	1.52	0.57
10:C:301:HEM:HBB2	10:C:301:HEM:CMB	2.33	0.57
2:B:149:PHE:CB	2:B:150:PRO:CD	2.82	0.57
3:C:161:TYR:C	3:C:163:THR:H	2.07	0.57
4:D:133:TYR:CE2	4:D:148:LEU:CD2	2.80	0.57
6:F:27:LEU:O	6:F:30:GLN:CG	2.51	0.57
1:A:39:ILE:CD1	17:G:101:BCR:C31	2.74	0.57
1:A:87:ARG:CG	1:A:87:ARG:NH1	2.68	0.57
3:C:221:GLU:OE1	3:C:221:GLU:CA	2.52	0.57
3:C:285:ALA:O	3:C:286:GLU:OE1	2.23	0.57
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.69	0.57
1:A:103:ARG:HH21	1:A:211:ILE:HD11	1.69	0.57
3:C:79:PRO:HG2	3:C:82:PHE:CD1	2.39	0.57
3:C:183:ILE:HG22	3:C:183:ILE:O	2.05	0.57
4:D:133:TYR:HB3	4:D:137:GLY:O	2.04	0.57
1:A:127:ILE:CG2	1:A:195:ILE:CG1	2.81	0.57
4:D:102:TYR:H	4:D:102:TYR:HD2	1.52	0.57
2:B:85:PHE:HD2	14:B:1201:TDS:OAC	1.87	0.57
3:C:225:VAL:HG12	3:C:229:GLU:HG3	1.87	0.57
4:D:85:LYS:CB	4:D:85:LYS:HZ3	1.96	0.57
1:A:195:ILE:HG23	1:A:199:MET:HE3	1.87	0.57
2:B:150:PRO:O	2:B:152:ASP:N	2.38	0.57
5:E:26:ILE:HG23	5:E:32:ILE:HG13	1.85	0.57
1:A:38:GLY:HA3	10:A:303:HEM:C1C	2.40	0.57
2:B:84:VAL:HG11	2:B:101:MET:HG3	1.86	0.57
3:C:171:VAL:CG1	3:C:233:ASN:O	2.52	0.57
3:C:172:PHE:N	3:C:232:THR:OG1	2.38	0.57
7:G:34:GLU:N	7:G:34:GLU:OE2	2.38	0.57
8:H:9:VAL:O	8:H:13:VAL:HG23	2.05	0.57
1:A:27:PRO:HB2	1:A:29:HIS:CE1	2.40	0.56
1:A:44:PHE:C	1:A:44:PHE:CD2	2.79	0.56
2:B:6:LYS:O	2:B:7:PRO:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:GLY:C	2:B:159:LEU:HD23	2.25	0.56
1:A:105:TYR:CZ	13:B:201:CLA:CBB	2.88	0.56
2:B:88:LEU:HD13	14:B:1201:TDS:HAI2	1.84	0.56
3:C:171:VAL:HG12	3:C:234:ASN:HA	1.87	0.56
3:C:200:GLN:NE2	3:C:205:LYS:O	2.39	0.56
4:D:78:ARG:CD	4:D:117:TRP:CG	2.88	0.56
5:E:2:ILE:O	5:E:6:VAL:HG23	2.05	0.56
5:E:15:PHE:HA	5:E:18:ILE:HG13	1.87	0.56
1:A:168:LEU:O	1:A:182:ARG:HD3	2.05	0.56
8:H:23:VAL:HG13	8:H:28:GLY:H	1.70	0.56
2:B:122:ASN:ND2	7:G:29:TYR:HB2	2.21	0.56
3:C:40:VAL:HG12	8:H:1:MET:CE	2.35	0.56
3:C:173:THR:HB	3:C:228:GLY:C	2.26	0.56
1:A:33:PHE:CD2	1:A:33:PHE:N	2.73	0.56
2:B:97:GLY:HA2	2:B:100:LEU:HB2	1.88	0.56
2:B:123:PRO:CD	7:G:25:ALA:HB1	2.35	0.56
3:C:193:VAL:HG12	3:C:194:LYS:N	2.21	0.56
4:D:21:LEU:HD11	16:D:201:SQD:C30	2.32	0.56
6:F:10:LEU:CD1	6:F:10:LEU:C	2.74	0.56
1:A:92:MET:CG	11:A:1002:OPC:HCB1	2.35	0.56
3:C:34:VAL:HG23	3:C:151:LEU:CD2	2.36	0.56
4:D:110:HIS:O	4:D:111:LEU:HD12	2.05	0.56
1:A:33:PHE:H	1:A:33:PHE:HD2	1.51	0.56
1:A:87:ARG:HH11	1:A:87:ARG:CG	2.19	0.56
2:B:57:LEU:HD12	8:H:8:TRP:CZ3	2.41	0.56
3:C:54:TYR:HD2	3:C:125:GLN:HE22	1.53	0.56
3:C:223:GLN:O	3:C:224:ALA:HB2	2.04	0.56
4:D:139:VAL:CG2	4:D:147:SER:CA	2.66	0.56
4:D:165:TRP:HD1	4:D:165:TRP:O	1.89	0.56
8:H:23:VAL:HG12	8:H:24:TRP:N	2.13	0.56
1:A:15:GLN:O	1:A:16:ALA:C	2.43	0.56
3:C:181:THR:O	3:C:182:LYS:HG3	2.06	0.56
5:E:26:ILE:O	5:E:31:LEU:HB2	2.06	0.56
7:G:2:VAL:HG12	7:G:4:PRO:HD3	1.83	0.56
1:A:100:HIS:HE1	10:A:302:HEM:CHA	2.19	0.55
1:A:94:VAL:HG11	2:B:80:TYR:CG	2.41	0.55
4:D:21:LEU:HD11	16:D:201:SQD:H312	1.88	0.55
1:A:83:ARG:O	1:A:83:ARG:HG3	2.05	0.55
3:C:206:THR:O	3:C:206:THR:HG23	2.05	0.55
1:A:30:VAL:HG22	1:A:34:TYR:CD2	2.41	0.55
1:A:82:ILE:HD13	1:A:82:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:302:HEM:HMB1	10:A:302:HEM:CBB	2.37	0.55
3:C:14:ARG:NE	3:C:150:HIS:HD2	2.05	0.55
3:C:170:ASN:O	3:C:235:PRO:CD	2.54	0.55
1:A:155:PRO:HB2	1:A:166:SER:OG	2.06	0.55
1:A:211:ILE:HD12	1:A:212:SER:H	1.72	0.55
3:C:34:VAL:CG2	3:C:151:LEU:HB2	2.37	0.55
3:C:217:LEU:N	3:C:217:LEU:HD12	2.21	0.55
2:B:87:ILE:HG22	2:B:88:LEU:N	2.22	0.55
2:B:96:LEU:O	2:B:99:LEU:HB2	2.07	0.55
7:G:15:PHE:O	7:G:17:THR:N	2.40	0.55
1:A:44:PHE:HB2	1:A:93:MET:SD	2.46	0.55
2:B:22:MET:HA	2:B:24:HIS:CD2	2.41	0.55
2:B:123:PRO:HD2	2:B:124:PHE:H	1.72	0.55
3:C:171:VAL:HB	3:C:232:THR:HB	1.87	0.55
3:C:270:LEU:CD1	3:C:271:MET:N	2.70	0.55
1:A:143:VAL:HG13	1:A:143:VAL:O	2.07	0.55
2:B:130:THR:CG2	7:G:22:PHE:CE2	2.83	0.55
4:D:78:ARG:HD2	4:D:117:TRP:CG	2.42	0.55
1:A:35:CYS:SG	10:A:303:HEM:HMB1	2.47	0.55
1:A:72:ILE:HA	1:A:76:VAL:CG2	2.36	0.55
2:B:138:LEU:CD1	2:B:138:LEU:CB	2.76	0.55
3:C:158:GLY:C	3:C:159:GLN:NE2	2.60	0.55
1:A:6:ASP:O	1:A:9:GLN:N	2.40	0.54
2:B:124:PHE:CE1	7:G:26:TYR:CB	2.83	0.54
2:B:151:LEU:O	2:B:154:THR:HG21	2.06	0.54
3:C:176:ALA:CB	3:C:205:LYS:NZ	2.63	0.54
3:C:266:MET:CE	5:E:15:PHE:CD1	2.90	0.54
1:A:97:MET:SD	10:A:302:HEM:HAB	2.47	0.54
1:A:108:GLY:HA2	1:A:110:PHE:CD2	2.43	0.54
2:B:11:ASP:OD1	2:B:13:LYS:HB2	2.08	0.54
2:B:91:VAL:C	2:B:93:ASN:N	2.58	0.54
3:C:54:TYR:CE1	3:C:70:LEU:HG	2.43	0.54
3:C:181:THR:HG22	3:C:182:LYS:HG3	1.88	0.54
3:C:87:GLU:C	3:C:89:ARG:N	2.59	0.54
4:D:84:LEU:C	4:D:86:GLY:H	2.11	0.54
2:B:151:LEU:O	2:B:151:LEU:HD13	2.08	0.54
4:D:114:VAL:O	4:D:114:VAL:CG1	2.55	0.54
2:B:114:ILE:O	2:B:116:ASN:N	2.41	0.54
3:C:47:LYS:HD2	3:C:49:VAL:CG2	2.38	0.54
6:F:22:LEU:HD12	8:H:20:ALA:CB	2.37	0.54
1:A:7:TRP:CD2	1:A:11:ARG:NH2	2.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:C	1:A:200:LEU:HD22	2.28	0.54
4:D:34:ALA:O	4:D:37:PRO:HD2	2.08	0.54
4:D:80:LEU:O	4:D:81:VAL:HG22	2.07	0.54
1:A:110:PHE:CE1	2:B:111:VAL:HG12	2.43	0.54
2:B:159:LEU:O	2:B:160:PHE:CG	2.61	0.54
3:C:9:TYR:CE1	3:C:21:VAL:HB	2.43	0.54
3:C:180:ILE:CG2	3:C:222:GLY:O	2.56	0.54
1:A:103:ARG:NH1	1:A:104:VAL:CG2	2.65	0.54
1:A:141:ASP:C	1:A:141:ASP:OD2	2.45	0.54
1:A:145:TYR:O	1:A:145:TYR:CD1	2.61	0.54
1:A:145:TYR:O	1:A:145:TYR:CG	2.59	0.53
2:B:79:TRP:O	2:B:82:TYR:N	2.40	0.53
2:B:96:LEU:HD13	2:B:100:LEU:HD12	1.80	0.53
2:B:114:ILE:HG22	2:B:115:GLU:H	1.73	0.53
4:D:165:TRP:CD1	4:D:165:TRP:C	2.82	0.53
1:A:36:LEU:HD23	1:A:99:LEU:C	2.28	0.53
3:C:15:GLU:N	3:C:15:GLU:OE1	2.39	0.53
4:D:90:TYR:CE1	4:D:115:VAL:O	2.61	0.53
4:D:152:HIS:CE1	4:D:165:TRP:CE3	2.96	0.53
1:A:98:ILE:HD11	13:B:201:CLA:CED	2.38	0.53
2:B:81:LEU:HD23	2:B:81:LEU:N	2.14	0.53
3:C:54:TYR:HE1	3:C:70:LEU:CG	2.21	0.53
4:D:119:ALA:O	4:D:122:ASN:OD1	2.26	0.53
1:A:31:ASN:ND2	1:A:33:PHE:H	2.06	0.53
3:C:158:GLY:H	10:C:301:HEM:CAD	2.21	0.53
4:D:105:ASN:ND2	4:D:105:ASN:C	2.62	0.53
1:A:7:TRP:CD1	1:A:11:ARG:NH2	2.76	0.53
1:A:95:LEU:C	1:A:95:LEU:HD23	2.28	0.53
4:D:146:LEU:HD12	4:D:177:TRP:CE3	2.40	0.53
8:H:3:ILE:O	8:H:7:GLY:N	2.38	0.53
1:A:119:ILE:O	1:A:123:ILE:HD12	2.09	0.53
3:C:273:ILE:HG13	8:H:21:MET:CG	2.29	0.53
5:E:8:TYR:OH	5:E:12:ILE:HD11	2.09	0.53
11:A:1002:OPC:HBP2	6:F:8:ALA:HA	1.90	0.53
2:B:69:PHE:N	2:B:69:PHE:HD2	2.05	0.53
3:C:1:TYR:HB3	3:C:2:PRO:HD2	1.90	0.53
3:C:154:ASN:CG	3:C:155:ARG:N	2.62	0.53
3:C:180:ILE:HG22	3:C:222:GLY:O	2.08	0.53
3:C:188:ASP:O	3:C:190:TYR:O	2.25	0.53
1:A:31:ASN:ND2	1:A:33:PHE:HD2	2.07	0.52
1:A:80:TRP:CD2	3:C:254:ARG:NH2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:VAL:HG13	3:C:75:VAL:O	2.08	0.52
3:C:94:LEU:C	3:C:94:LEU:CD2	2.77	0.52
4:D:28:THR:O	4:D:29:GLY:C	2.45	0.52
1:A:177:GLN:O	1:A:178:ALA:C	2.39	0.52
1:A:72:ILE:HA	1:A:76:VAL:HG23	1.90	0.52
1:A:92:MET:CG	11:A:1002:OPC:CCB	2.87	0.52
2:B:119:LYS:O	2:B:119:LYS:HG2	2.10	0.52
2:B:134:LEU:HD13	2:B:134:LEU:H	1.74	0.52
3:C:171:VAL:HG11	3:C:234:ASN:ND2	2.15	0.52
8:H:2:GLU:HB2	8:H:5:VAL:CG2	2.39	0.52
2:B:118:ASN:ND2	2:B:120:PHE:HD1	2.06	0.52
1:A:12:LEU:HB2	1:A:14:ILE:CD1	2.39	0.52
2:B:134:LEU:CD2	7:G:22:PHE:CZ	2.93	0.52
4:D:165:TRP:O	4:D:165:TRP:CD1	2.62	0.52
3:C:200:GLN:CG	3:C:205:LYS:HB3	2.39	0.52
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.45	0.52
2:B:40:PHE:HZ	14:B:1202:TDS:OBD	1.93	0.52
3:C:59:GLN:HB2	3:C:67:LYS:HE3	1.92	0.52
3:C:161:TYR:C	3:C:163:THR:N	2.64	0.52
3:C:272:LEU:O	3:C:275:LYS:HB3	2.10	0.52
4:D:38:LEU:O	4:D:38:LEU:HG	2.09	0.52
6:F:25:LEU:C	6:F:27:LEU:N	2.62	0.52
2:B:154:THR:HG23	2:B:155:LEU:H	1.75	0.52
3:C:64:ASP:OD2	3:C:65:GLY:N	2.43	0.52
3:C:1:TYR:HA	10:C:301:HEM:NA	2.25	0.52
3:C:250:GLN:HE21	3:C:251:ASP:H	1.58	0.52
1:A:92:MET:HG3	11:A:1002:OPC:CCB	2.40	0.51
14:B:1202:TDS:OAO	14:B:1202:TDS:HAS1	2.09	0.51
3:C:160:ILE:O	10:C:301:HEM:HAC	2.10	0.51
1:A:18:ALA:O	1:A:21:VAL:N	2.39	0.51
3:C:200:GLN:HG2	3:C:201:THR:N	2.24	0.51
4:D:69:PHE:O	4:D:69:PHE:CD2	2.61	0.51
5:E:9:ILE:O	5:E:13:ALA:CB	2.57	0.51
1:A:103:ARG:CA	7:G:21:LEU:HD21	2.38	0.51
10:A:303:HEM:HBD1	10:A:303:HEM:HHA	1.92	0.51
2:B:57:LEU:HD13	8:H:8:TRP:CD2	2.45	0.51
3:C:210:THR:C	3:C:211:ILE:CG2	2.79	0.51
3:C:266:MET:SD	8:H:13:VAL:HG12	2.51	0.51
4:D:13:MET:O	4:D:15:ARG:N	2.43	0.51
1:A:105:TYR:CZ	13:B:201:CLA:HBB2	2.45	0.51
10:A:302:HEM:CMB	10:A:302:HEM:CBB	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:VAL:HG11	2:B:101:MET:SD	2.50	0.51
13:B:201:CLA:HMB1	13:B:201:CLA:CBB	2.20	0.51
1:A:53:ALA:HB1	4:D:41:TYR:CE2	2.45	0.51
3:C:45:VAL:HG13	3:C:85:ALA:HB2	1.93	0.51
1:A:111:LYS:O	1:A:113:PRO:CD	2.57	0.51
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.45	0.51
7:G:10:VAL:HG12	7:G:11:LEU:CD2	2.34	0.51
8:H:8:TRP:O	8:H:9:VAL:C	2.45	0.51
4:D:132:GLN:OE1	4:D:141:ARG:NH1	2.44	0.51
6:F:15:LEU:HD23	8:H:16:THR:OG1	2.10	0.51
7:G:30:LYS:C	7:G:32:PRO:HD3	2.31	0.51
1:A:88:TRP:CE3	2:B:54:LEU:HD13	2.46	0.51
1:A:103:ARG:NH2	1:A:211:ILE:HD11	2.25	0.51
2:B:57:LEU:HD21	3:C:258:MET:HE1	1.93	0.51
2:B:84:VAL:CG1	2:B:101:MET:SD	2.99	0.51
6:F:24:VAL:O	6:F:27:LEU:CB	2.55	0.51
1:A:205:MET:O	1:A:206:ILE:C	2.47	0.51
3:C:102:TYR:O	3:C:104:GLN:N	2.44	0.51
4:D:69:PHE:O	4:D:70:LEU:C	2.48	0.51
4:D:74:ASN:O	4:D:93:VAL:HG11	2.10	0.51
1:A:39:ILE:O	1:A:42:THR:N	2.43	0.50
2:B:34:ASN:O	3:C:276:LYS:HE3	2.10	0.50
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.41	0.50
3:C:180:ILE:CD1	3:C:183:ILE:CD1	2.79	0.50
3:C:232:THR:O	3:C:233:ASN:CB	2.59	0.50
7:G:34:GLU:C	7:G:35:LEU:HD23	2.31	0.50
1:A:15:GLN:O	1:A:18:ALA:N	2.45	0.50
1:A:15:GLN:O	1:A:17:LEU:N	2.44	0.50
1:A:80:TRP:CZ3	1:A:81:LEU:HG	2.45	0.50
1:A:207:ARG:HG3	1:A:207:ARG:NH1	2.05	0.50
2:B:91:VAL:C	2:B:93:ASN:H	2.15	0.50
3:C:87:GLU:O	3:C:89:ARG:N	2.44	0.50
4:D:167:GLU:O	4:D:176:PRO:HG3	2.11	0.50
6:F:4:GLU:HG2	7:G:5:LEU:HD12	1.94	0.50
8:H:5:VAL:O	8:H:6:LEU:C	2.49	0.50
1:A:93:MET:O	1:A:94:VAL:C	2.47	0.50
3:C:34:VAL:CG2	3:C:151:LEU:HD22	2.42	0.50
3:C:117:GLY:HA2	3:C:119:LEU:HD12	1.93	0.50
4:D:66:VAL:CG2	4:D:158:ASP:C	2.79	0.50
4:D:80:LEU:O	4:D:81:VAL:CG2	2.59	0.50
2:B:130:THR:HG21	7:G:22:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:271:MET:HE1	4:D:22:LEU:HD12	1.92	0.50
6:F:10:LEU:C	6:F:10:LEU:HD13	2.30	0.50
1:A:207:ARG:HH12	14:B:1202:TDS:CAI	2.18	0.50
1:A:212:SER:HB3	10:A:302:HEM:O2D	2.12	0.50
3:C:40:VAL:HG12	8:H:1:MET:HE2	1.94	0.50
3:C:229:GLU:OE1	3:C:229:GLU:CA	2.51	0.50
6:F:22:LEU:HD12	8:H:20:ALA:HB1	1.94	0.50
2:B:129:ALA:O	2:B:130:THR:C	2.49	0.50
3:C:173:THR:O	3:C:231:LEU:HD23	2.12	0.50
3:C:184:ALA:HB3	3:C:196:GLN:HB2	1.94	0.50
4:D:13:MET:HA	4:D:16:ARG:HD3	1.94	0.50
4:D:47:GLY:C	4:D:49:ALA:H	2.14	0.50
1:A:106:LEU:HD12	7:G:21:LEU:HD23	1.94	0.50
2:B:151:LEU:HD13	2:B:151:LEU:C	2.32	0.50
3:C:186:GLU:OE2	3:C:196:GLN:HG3	2.12	0.50
2:B:147:ALA:C	2:B:149:PHE:H	2.15	0.50
3:C:25:CYS:HG	10:C:301:HEM:CBC	2.23	0.50
5:E:26:ILE:HG22	5:E:32:ILE:HG13	1.91	0.50
1:A:103:ARG:HH12	1:A:104:VAL:CG2	2.18	0.50
2:B:96:LEU:C	2:B:100:LEU:HD12	2.32	0.50
1:A:147:ALA:CB	14:B:1201:TDS:HAJ3	2.32	0.49
3:C:268:ALA:HA	4:D:26:THR:OG1	2.12	0.49
1:A:124:LEU:HD21	1:A:199:MET:N	2.27	0.49
1:A:138:LEU:N	1:A:139:PRO:HD3	2.28	0.49
3:C:196:GLN:NE2	3:C:210:THR:HG23	2.28	0.49
4:D:146:LEU:CD1	4:D:177:TRP:HB2	2.42	0.49
5:E:20:VAL:HG12	5:E:21:GLY:N	2.26	0.49
3:C:80:GLU:OE2	3:C:80:GLU:CA	2.60	0.49
4:D:117:TRP:CZ2	4:D:122:ASN:CA	2.95	0.49
4:D:122:ASN:HB3	4:D:135:GLU:CD	2.24	0.49
4:D:138:LYS:HA	4:D:147:SER:CB	2.43	0.49
1:A:191:LEU:O	1:A:192:PRO:C	2.50	0.49
2:B:118:ASN:HD22	2:B:119:LYS:N	2.11	0.49
2:B:118:ASN:OD1	11:B:1001:OPC:HAH2	2.13	0.49
2:B:151:LEU:HD13	2:B:152:ASP:HB3	1.93	0.49
14:B:1202:TDS:HAA3	14:B:1202:TDS:CAG	2.38	0.49
3:C:54:TYR:OH	3:C:121:GLY:HA3	2.12	0.49
3:C:86:PRO:O	3:C:86:PRO:HG2	2.11	0.49
4:D:25:GLY:CA	16:D:201:SQD:H341	2.43	0.49
4:D:167:GLU:CD	4:D:167:GLU:H	2.15	0.49
4:D:172:THR:HG23	4:D:174:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:TYR:CD1	3:C:21:VAL:HB	2.47	0.49
3:C:101:VAL:CG1	3:C:103:PHE:CE2	2.95	0.49
3:C:151:LEU:HG	3:C:152:GLY:N	2.23	0.49
1:A:51:GLY:HA3	10:A:301:HEM:C3C	2.48	0.49
1:A:111:LYS:O	1:A:112:LYS:C	2.50	0.49
1:A:151:VAL:HG23	1:A:151:VAL:O	2.13	0.49
1:A:215:LEU:HD22	2:B:122:ASN:H	1.78	0.49
4:D:133:TYR:CD2	4:D:148:LEU:CD2	2.93	0.49
7:G:20:GLY:H	17:G:101:BCR:H363	1.77	0.49
1:A:122:VAL:O	1:A:125:ALA:HB3	2.13	0.49
2:B:159:LEU:O	2:B:160:PHE:CB	2.60	0.49
3:C:279:VAL:C	3:C:281:LYS:N	2.66	0.49
5:E:23:ILE:O	5:E:27:LYS:N	2.43	0.49
1:A:12:LEU:CB	1:A:14:ILE:HD11	2.43	0.49
6:F:28:LYS:C	6:F:30:GLN:H	2.17	0.49
7:G:6:LEU:O	7:G:9:LEU:HB2	2.12	0.49
3:C:77:MET:HB3	3:C:113:VAL:HG13	1.94	0.48
3:C:194:LYS:O	3:C:195:TYR:C	2.51	0.48
4:D:101:ASP:OD1	4:D:101:ASP:N	2.44	0.48
3:C:34:VAL:CG2	3:C:151:LEU:HB3	2.43	0.48
3:C:54:TYR:CE2	3:C:125:GLN:NE2	2.81	0.48
2:B:151:LEU:CD1	2:B:152:ASP:HB3	2.44	0.48
3:C:185:LYS:HB2	3:C:185:LYS:NZ	2.28	0.48
3:C:200:GLN:CD	3:C:205:LYS:O	2.51	0.48
4:D:21:LEU:O	4:D:21:LEU:HG	2.13	0.48
1:A:145:TYR:CD1	1:A:145:TYR:C	2.84	0.48
2:B:113:PHE:O	2:B:114:ILE:C	2.51	0.48
2:B:122:ASN:OD1	2:B:124:PHE:HB2	2.13	0.48
4:D:96:LYS:HB2	4:D:96:LYS:HZ3	1.77	0.48
7:G:23:TYR:C	7:G:23:TYR:CD2	2.87	0.48
4:D:83:GLY:HA2	4:D:162:LEU:CD1	2.43	0.48
4:D:169:ASP:O	4:D:170:PHE:C	2.51	0.48
1:A:12:LEU:CB	1:A:14:ILE:HD13	2.43	0.48
1:A:95:LEU:CD2	1:A:99:LEU:HG	2.43	0.48
2:B:40:PHE:N	2:B:41:PRO:CD	2.77	0.48
4:D:84:LEU:C	4:D:86:GLY:N	2.65	0.48
1:A:3:ASN:O	1:A:6:ASP:HB2	2.12	0.48
10:A:303:HEM:C1C	2:B:40:PHE:CZ	3.02	0.48
2:B:99:LEU:O	2:B:103:SER:OG	2.32	0.48
7:G:35:LEU:HD23	7:G:35:LEU:N	2.29	0.48
2:B:113:PHE:O	2:B:116:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:THR:O	4:D:31:ALA:N	2.47	0.48
8:H:17:TRP:O	8:H:21:MET:HB2	2.14	0.48
1:A:29:HIS:NE2	1:A:213:GLY:C	2.67	0.48
1:A:119:ILE:HD13	2:B:109:ILE:HD13	1.95	0.48
1:A:147:ALA:O	1:A:148:VAL:C	2.49	0.48
3:C:13:PRO:O	3:C:20:ILE:HA	2.14	0.48
3:C:22:CYS:C	3:C:24:ASN:H	2.16	0.48
3:C:70:LEU:N	3:C:70:LEU:HD22	2.23	0.48
3:C:159:GLN:C	3:C:160:ILE:HG13	2.34	0.48
6:F:30:GLN:HG3	6:F:31:GLY:N	2.28	0.48
1:A:95:LEU:C	1:A:97:MET:N	2.67	0.48
2:B:104:VAL:CB	2:B:105:PRO:CD	2.92	0.48
3:C:9:TYR:CD1	3:C:21:VAL:HG11	2.48	0.48
3:C:15:GLU:OE1	3:C:19:ARG:HB3	2.14	0.48
3:C:115:LEU:N	3:C:115:LEU:HD23	2.24	0.47
7:G:27:GLN:OE1	8:H:29:LEU:HD21	2.14	0.47
1:A:34:TYR:CE1	1:A:103:ARG:NE	2.75	0.47
1:A:80:TRP:CG	3:C:254:ARG:NH2	2.83	0.47
4:D:56:ALA:O	4:D:57:LYS:HG3	2.14	0.47
4:D:142:GLY:HA2	4:D:144:ALA:N	2.29	0.47
10:A:303:HEM:C3C	2:B:40:PHE:CE2	3.01	0.47
4:D:115:VAL:HG12	4:D:124:PHE:HB3	1.96	0.47
3:C:61:VAL:CG1	3:C:168:ASN:HD21	2.28	0.47
4:D:101:ASP:O	4:D:153:ALA:HB3	2.13	0.47
1:A:127:ILE:HG21	1:A:195:ILE:HG12	1.94	0.47
1:A:163:VAL:O	1:A:164:LEU:C	2.53	0.47
3:C:34:VAL:HG23	3:C:151:LEU:HD23	1.96	0.47
3:C:55:ASP:C	3:C:55:ASP:OD1	2.52	0.47
3:C:73:GLY:O	3:C:74:ALA:HB2	2.15	0.47
3:C:139:ASP:OD1	3:C:140:LYS:N	2.46	0.47
3:C:263:CYS:O	3:C:267:LEU:HB2	2.15	0.47
4:D:142:GLY:HA2	4:D:144:ALA:H	1.79	0.47
6:F:21:GLY:O	6:F:22:LEU:C	2.52	0.47
1:A:62:VAL:HG23	1:A:63:THR:N	2.29	0.47
2:B:124:PHE:CE1	7:G:26:TYR:HD1	2.31	0.47
3:C:34:VAL:O	3:C:34:VAL:HG12	2.14	0.47
6:F:21:GLY:O	6:F:24:VAL:HB	2.15	0.47
6:F:22:LEU:HD13	6:F:23:GLY:N	2.30	0.47
1:A:12:LEU:HB2	1:A:14:ILE:HD11	1.96	0.47
2:B:12:PRO:HB2	2:B:13:LYS:HD3	1.97	0.47
3:C:14:ARG:NE	3:C:150:HIS:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:MET:HG3	3:C:150:HIS:HB2	1.97	0.47
4:D:134:ASP:OD1	4:D:134:ASP:O	2.31	0.47
3:C:23:ALA:HB2	3:C:240:PHE:HE2	1.78	0.47
3:C:107:LYS:HE2	3:C:110:GLN:HE22	1.77	0.47
6:F:20:TRP:CD1	6:F:24:VAL:CG2	2.98	0.47
1:A:183:TYR:O	1:A:186:ALA:HB3	2.15	0.46
11:A:1002:OPC:HBX1	11:A:1002:OPC:HBU2	1.44	0.46
3:C:44:THR:O	3:C:132:LEU:HA	2.15	0.46
3:C:136:PRO:HG3	3:C:142:ILE:HG22	1.97	0.46
4:D:16:ARG:O	4:D:20:ASN:N	2.45	0.46
4:D:144:ALA:HA	4:D:145:PRO:HD2	1.75	0.46
1:A:7:TRP:O	1:A:11:ARG:CG	2.62	0.46
2:B:155:LEU:C	2:B:157:LEU:H	2.18	0.46
4:D:29:GLY:O	4:D:30:VAL:C	2.53	0.46
5:E:10:VAL:O	5:E:10:VAL:HG12	2.14	0.46
2:B:157:LEU:O	2:B:159:LEU:HD23	2.14	0.46
3:C:171:VAL:HG12	3:C:233:ASN:O	2.14	0.46
2:B:82:TYR:O	2:B:85:PHE:N	2.49	0.46
1:A:110:PHE:HD1	2:B:112:PRO:CB	2.13	0.46
2:B:11:ASP:HA	2:B:12:PRO:HD2	1.44	0.46
3:C:12:THR:OG1	3:C:13:PRO:CD	2.63	0.46
1:A:38:GLY:HA3	10:A:303:HEM:C4C	2.51	0.46
1:A:121:GLY:HA3	10:A:302:HEM:C3C	2.51	0.46
3:C:270:LEU:CB	8:H:21:MET:CE	2.91	0.46
4:D:115:VAL:HG13	4:D:116:PRO:HD2	1.98	0.46
4:D:126:CYS:HA	4:D:127:PRO:HD3	1.54	0.46
4:D:139:VAL:HG21	4:D:147:SER:N	2.29	0.46
2:B:109:ILE:O	2:B:112:PRO:CD	2.52	0.46
3:C:172:PHE:O	3:C:231:LEU:HG	2.16	0.46
3:C:219:VAL:HB	3:C:231:LEU:HA	1.98	0.46
1:A:14:ILE:CD1	1:A:14:ILE:N	2.78	0.46
1:A:150:ILE:HD13	14:B:1201:TDS:HAA2	1.80	0.46
1:A:195:ILE:HD13	1:A:199:MET:CE	2.45	0.46
1:A:202:HIS:HE1	10:A:302:HEM:C4C	2.33	0.46
10:A:303:HEM:HBB2	10:A:303:HEM:HMB3	1.98	0.46
2:B:84:VAL:O	2:B:87:ILE:HB	2.16	0.46
4:D:177:TRP:NE1	4:D:178:TRP:HE3	2.13	0.46
1:A:141:ASP:OD2	1:A:141:ASP:O	2.34	0.46
1:A:206:ILE:HG21	10:A:303:HEM:HBD1	1.97	0.46
2:B:124:PHE:CZ	7:G:26:TYR:HD1	2.34	0.46
2:B:130:THR:HG23	7:G:22:PHE:HE2	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LYS:NZ	2:B:153:LYS:HB3	2.30	0.46
3:C:4:TRP:HA	3:C:7:GLN:CB	2.45	0.46
3:C:153:ALA:O	3:C:240:PHE:CD1	2.69	0.46
7:G:24:ALA:C	7:G:26:TYR:N	2.68	0.46
10:A:303:HEM:C4A	14:B:1202:TDS:OAK	2.69	0.46
2:B:110:LEU:HA	2:B:110:LEU:HD23	1.16	0.46
3:C:14:ARG:NH2	3:C:150:HIS:HD2	2.11	0.46
3:C:149:ILE:HB	3:C:245:THR:HG23	1.97	0.46
4:D:150:LEU:HD11	4:D:171:ARG:NE	2.31	0.46
5:E:27:LYS:O	5:E:30:LYS:N	2.47	0.46
1:A:29:HIS:CG	1:A:214:PRO:HA	2.51	0.45
1:A:30:VAL:CG2	1:A:34:TYR:CD1	2.98	0.45
3:C:104:GLN:HA	3:C:105:PRO:HD3	1.69	0.45
2:B:4:LEU:HG	2:B:5:LYS:H	1.81	0.45
2:B:155:LEU:C	2:B:157:LEU:N	2.68	0.45
3:C:214:GLY:C	3:C:215:PRO:O	2.50	0.45
1:A:83:ARG:CD	10:A:301:HEM:O1D	2.60	0.45
2:B:137:THR:O	2:B:141:ILE:HG13	2.16	0.45
2:B:147:ALA:O	2:B:148:THR:C	2.55	0.45
3:C:273:ILE:HD12	8:H:25:GLY:HA3	1.98	0.45
4:D:21:LEU:CD1	16:D:201:SQD:C30	2.89	0.45
4:D:134:ASP:HB3	4:D:140:ILE:HD12	1.97	0.45
7:G:3:GLU:HA	7:G:4:PRO:HD2	1.72	0.45
8:H:5:VAL:C	8:H:7:GLY:N	2.68	0.45
3:C:241:GLY:O	3:C:242:GLN:HG2	2.16	0.45
1:A:94:VAL:HG11	2:B:80:TYR:CD2	2.52	0.45
3:C:101:VAL:HG11	3:C:103:PHE:CZ	2.51	0.45
3:C:171:VAL:HA	3:C:232:THR:HG21	1.98	0.45
2:B:108:LEU:HD12	2:B:108:LEU:HA	1.74	0.45
7:G:21:LEU:HD12	7:G:21:LEU:HA	1.73	0.45
1:A:71:TYR:O	1:A:72:ILE:C	2.50	0.45
2:B:18:LEU:HD23	2:B:18:LEU:HA	1.56	0.45
2:B:95:LEU:HD23	2:B:99:LEU:CD1	2.44	0.45
2:B:32:TRP:CD1	2:B:33:PRO:HD2	2.50	0.45
2:B:32:TRP:CG	2:B:33:PRO:CD	3.00	0.45
2:B:34:ASN:ND2	3:C:283:GLN:NE2	2.32	0.45
3:C:36:VAL:HG23	3:C:37:PRO:O	2.16	0.45
3:C:200:GLN:O	3:C:205:LYS:CG	2.53	0.45
2:B:85:PHE:CD2	14:B:1201:TDS:OAC	2.69	0.45
3:C:4:TRP:CG	3:C:162:PRO:HG3	2.52	0.45
4:D:141:ARG:CG	4:D:141:ARG:HH11	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:302:HEM:CBC	10:A:302:HEM:CMC	2.83	0.45
2:B:102:ALA:O	2:B:106:LEU:HG	2.16	0.45
3:C:271:MET:CE	4:D:22:LEU:HD12	2.47	0.45
4:D:59:LYS:HD3	4:D:59:LYS:N	2.32	0.45
5:E:11:PHE:HE2	5:E:15:PHE:CE1	2.35	0.45
1:A:29:HIS:CD2	1:A:213:GLY:C	2.90	0.44
1:A:112:LYS:HB3	1:A:113:PRO:HD3	1.99	0.44
2:B:16:ALA:C	2:B:19:ALA:HB3	2.38	0.44
3:C:94:LEU:CD2	3:C:98:VAL:CG2	2.95	0.44
3:C:159:GLN:CD	3:C:159:GLN:N	2.70	0.44
3:C:286:GLU:OE1	3:C:286:GLU:HA	2.17	0.44
10:C:301:HEM:CMB	10:C:301:HEM:CBB	2.94	0.44
4:D:117:TRP:HE1	4:D:119:ALA:HA	1.82	0.44
4:D:143:PRO:O	4:D:145:PRO:CD	2.58	0.44
6:F:20:TRP:CD1	6:F:24:VAL:HG21	2.52	0.44
1:A:80:TRP:CG	1:A:81:LEU:N	2.85	0.44
1:A:211:ILE:CD1	10:A:302:HEM:O2D	2.65	0.44
3:C:36:VAL:HG11	3:C:149:ILE:HD12	1.97	0.44
4:D:160:ILE:HG23	4:D:160:ILE:HD13	1.66	0.44
6:F:11:LEU:HD23	6:F:15:LEU:HD11	2.00	0.44
7:G:19:GLY:O	7:G:21:LEU:N	2.49	0.44
2:B:33:PRO:O	2:B:35:ASP:N	2.50	0.44
2:B:73:LEU:H	2:B:73:LEU:HG	1.46	0.44
14:B:1202:TDS:OAO	14:B:1202:TDS:HAS2	2.17	0.44
3:C:242:GLN:HE21	3:C:242:GLN:HB3	1.49	0.44
3:C:271:MET:O	4:D:23:ALA:HB2	2.17	0.44
4:D:163:THR:O	4:D:164:PRO:C	2.54	0.44
7:G:26:TYR:C	7:G:26:TYR:CD2	2.91	0.44
2:B:84:VAL:HG11	2:B:101:MET:CG	2.46	0.44
2:B:152:ASP:C	2:B:154:THR:N	2.60	0.44
3:C:200:GLN:CG	3:C:201:THR:N	2.81	0.44
4:D:74:ASN:O	4:D:93:VAL:CG1	2.66	0.44
1:A:95:LEU:HD22	1:A:96:MET:CE	2.43	0.44
1:A:114:ARG:CZ	1:A:212:SER:HA	2.47	0.44
2:B:40:PHE:HB3	2:B:41:PRO:HD3	1.92	0.44
2:B:134:LEU:N	2:B:134:LEU:CD1	2.70	0.44
3:C:36:VAL:HG11	3:C:149:ILE:HD13	1.99	0.44
3:C:193:VAL:CG1	3:C:194:LYS:N	2.80	0.44
7:G:11:LEU:N	7:G:11:LEU:CD2	2.58	0.44
1:A:122:VAL:HG22	10:A:302:HEM:CBC	2.48	0.44
2:B:118:ASN:ND2	2:B:119:LYS:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:VAL:HB	3:C:233:ASN:O	2.18	0.44
4:D:65:LYS:HB2	4:D:68:LYS:NZ	2.31	0.44
1:A:104:VAL:HG21	10:A:302:HEM:C2D	2.53	0.44
2:B:151:LEU:O	2:B:151:LEU:HD22	2.16	0.44
2:B:159:LEU:O	2:B:160:PHE:HD2	1.95	0.44
4:D:47:GLY:C	4:D:49:ALA:N	2.71	0.44
17:G:101:BCR:H20C	17:G:101:BCR:H361	1.34	0.44
1:A:47:GLN:CA	1:A:47:GLN:NE2	2.45	0.44
3:C:94:LEU:O	3:C:95:LYS:C	2.57	0.44
3:C:135:ASN:ND2	3:C:138:THR:HG23	2.33	0.44
4:D:81:VAL:O	4:D:83:GLY:N	2.51	0.44
5:E:27:LYS:O	5:E:30:LYS:CA	2.66	0.44
1:A:26:VAL:N	2:B:29:GLU:O	2.31	0.43
11:A:1002:OPC:CBN	7:G:5:LEU:HD11	2.48	0.43
2:B:95:LEU:C	2:B:95:LEU:CD2	2.78	0.43
2:B:124:PHE:CE1	7:G:26:TYR:CD1	3.06	0.43
3:C:73:GLY:O	3:C:74:ALA:CB	2.66	0.43
3:C:200:GLN:HG3	3:C:205:LYS:C	2.25	0.43
3:C:264:LEU:HD23	3:C:264:LEU:HA	1.46	0.43
4:D:63:ASN:HD22	4:D:63:ASN:H	1.66	0.43
1:A:31:ASN:HD22	1:A:32:ILE:N	2.15	0.43
1:A:40:THR:HG22	10:A:302:HEM:HMB1	1.98	0.43
1:A:81:LEU:O	1:A:82:ILE:C	2.57	0.43
11:A:1002:OPC:HBN1	7:G:5:LEU:HD11	1.99	0.43
2:B:131:THR:O	2:B:133:PHE:N	2.51	0.43
3:C:278:GLN:HG3	5:E:31:LEU:O	2.18	0.43
1:A:103:ARG:HG3	1:A:103:ARG:HH11	1.83	0.43
1:A:154:VAL:HB	1:A:155:PRO:CD	2.48	0.43
2:B:25:ASN:ND2	2:B:25:ASN:N	2.53	0.43
2:B:106:LEU:HG	2:B:106:LEU:H	1.64	0.43
3:C:60:GLN:HG2	3:C:70:LEU:HB3	1.99	0.43
3:C:76:LEU:HG	3:C:77:MET:N	2.34	0.43
6:F:30:GLN:HE21	6:F:30:GLN:HB2	1.68	0.43
1:A:112:LYS:HB3	1:A:113:PRO:CD	2.49	0.43
1:A:175:VAL:CG1	1:A:176:GLY:N	2.77	0.43
1:A:196:ALA:O	1:A:197:VAL:C	2.56	0.43
2:B:120:PHE:CD1	2:B:120:PHE:N	2.85	0.43
3:C:34:VAL:CG2	3:C:151:LEU:CD2	2.96	0.43
4:D:178:TRP:O	4:D:179:VAL:HG23	2.19	0.43
1:A:11:ARG:H	1:A:11:ARG:HG2	1.19	0.43
1:A:77:SER:O	1:A:78:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH1	10:A:302:HEM:O1D	2.51	0.43
2:B:41:PRO:O	2:B:42:VAL:C	2.56	0.43
3:C:4:TRP:HA	3:C:7:GLN:HB2	1.99	0.43
4:D:122:ASN:HB2	4:D:135:GLU:OE2	2.08	0.43
1:A:4:VAL:O	1:A:5:TYR:C	2.57	0.43
1:A:30:VAL:HG22	1:A:34:TYR:CB	2.49	0.43
1:A:163:VAL:O	1:A:166:SER:N	2.51	0.43
2:B:33:PRO:HB2	2:B:34:ASN:H	1.13	0.43
3:C:46:PHE:CZ	3:C:131:VAL:CG2	2.95	0.43
3:C:171:VAL:HG11	3:C:234:ASN:CA	2.41	0.43
5:E:14:LEU:C	5:E:14:LEU:HD23	2.39	0.43
1:A:32:ILE:HG22	1:A:33:PHE:N	2.32	0.43
1:A:33:PHE:C	1:A:35:CYS:H	2.22	0.43
1:A:138:LEU:N	1:A:139:PRO:CD	2.82	0.43
1:A:142:GLN:HE22	2:B:67:ASP:HB3	1.84	0.43
2:B:115:GLU:HG3	11:B:1001:OPC:OCC	2.19	0.43
3:C:171:VAL:HG12	3:C:235:PRO:HD3	1.87	0.43
4:D:65:LYS:O	4:D:67:SER:N	2.52	0.43
4:D:120:ALA:C	4:D:122:ASN:H	2.22	0.43
7:G:11:LEU:O	7:G:12:GLY:C	2.57	0.43
1:A:7:TRP:O	1:A:11:ARG:HG3	2.19	0.43
2:B:88:LEU:HD12	2:B:101:MET:SD	2.59	0.43
3:C:3:PHE:O	3:C:6:GLN:HB3	2.18	0.43
3:C:4:TRP:CE2	3:C:162:PRO:HG3	2.53	0.43
3:C:4:TRP:HZ3	10:C:301:HEM:C1D	2.37	0.43
4:D:107:VAL:HG23	4:D:107:VAL:H	1.37	0.43
1:A:95:LEU:C	1:A:95:LEU:CD2	2.87	0.42
2:B:41:PRO:O	2:B:45:MET:HB2	2.19	0.42
2:B:96:LEU:HD11	2:B:100:LEU:HD11	1.97	0.42
3:C:52:ILE:O	3:C:52:ILE:CG2	2.41	0.42
3:C:193:VAL:HG12	3:C:194:LYS:H	1.82	0.42
6:F:24:VAL:C	6:F:27:LEU:HB2	2.40	0.42
7:G:4:PRO:O	7:G:5:LEU:C	2.56	0.42
8:H:6:LEU:HD23	8:H:6:LEU:HA	1.51	0.42
2:B:87:ILE:O	2:B:88:LEU:C	2.57	0.42
3:C:34:VAL:HG23	3:C:151:LEU:HD22	2.01	0.42
10:C:301:HEM:HHA	10:C:301:HEM:HAA2	1.76	0.42
4:D:21:LEU:HD11	16:D:201:SQD:C31	2.49	0.42
4:D:78:ARG:HD3	4:D:117:TRP:CG	2.54	0.42
8:H:11:LEU:C	8:H:11:LEU:HD12	2.37	0.42
1:A:103:ARG:HB2	7:G:21:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:GLY:H	10:C:301:HEM:HAD2	1.83	0.42
6:F:10:LEU:HD13	6:F:10:LEU:HA	1.61	0.42
7:G:14:VAL:HG12	7:G:15:PHE:N	2.34	0.42
1:A:118:TRP:O	1:A:119:ILE:C	2.56	0.42
1:A:206:ILE:CG2	10:A:303:HEM:HBD1	2.50	0.42
3:C:61:VAL:CG1	3:C:168:ASN:ND2	2.82	0.42
3:C:267:LEU:HD22	3:C:267:LEU:HA	1.85	0.42
4:D:65:LYS:HD3	4:D:158:ASP:O	2.18	0.42
1:A:38:GLY:HA3	10:A:303:HEM:NC	2.35	0.42
1:A:82:ILE:HD13	1:A:82:ILE:H	1.84	0.42
1:A:88:TRP:O	1:A:92:MET:HG2	2.20	0.42
3:C:27:LEU:HA	3:C:27:LEU:HD23	1.82	0.42
3:C:36:VAL:HG23	3:C:37:PRO:N	2.34	0.42
3:C:155:ARG:HD2	3:C:239:GLY:O	2.19	0.42
8:H:3:ILE:HD12	8:H:3:ILE:HA	1.92	0.42
1:A:30:VAL:CG2	1:A:34:TYR:CD2	3.02	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.63	0.42
1:A:96:MET:CE	1:A:96:MET:HA	2.50	0.42
1:A:203:PHE:CD1	1:A:203:PHE:N	2.83	0.42
4:D:13:MET:O	4:D:16:ARG:N	2.52	0.42
1:A:103:ARG:C	1:A:103:ARG:CD	2.70	0.42
1:A:104:VAL:HG12	1:A:118:TRP:HZ3	1.83	0.42
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.39	0.42
2:B:3:THR:HG21	3:C:283:GLN:OE1	2.20	0.42
2:B:11:ASP:C	2:B:13:LYS:N	2.72	0.42
3:C:122:GLU:H	3:C:122:GLU:HG2	1.18	0.42
4:D:12:ASP:O	4:D:15:ARG:N	2.50	0.42
4:D:36:TYR:OH	4:D:40:LYS:HE3	2.19	0.42
6:F:16:ILE:HG22	6:F:17:PHE:H	1.82	0.42
1:A:44:PHE:CE1	1:A:195:ILE:HG21	2.54	0.42
1:A:127:ILE:CD1	1:A:194:LEU:HB3	2.49	0.42
1:A:150:ILE:HD11	14:B:1201:TDS:HAA2	2.00	0.42
1:A:195:ILE:HD13	1:A:199:MET:HE3	2.01	0.42
10:A:301:HEM:HBA2	10:A:301:HEM:CGD	2.46	0.42
2:B:93:ASN:OD1	2:B:96:LEU:N	2.52	0.42
2:B:156:THR:C	2:B:158:GLY:N	2.72	0.42
4:D:15:ARG:HB3	5:E:31:LEU:HD23	1.96	0.42
8:H:19:ILE:O	8:H:20:ALA:C	2.58	0.42
1:A:139:PRO:HG3	10:A:301:HEM:O2D	2.20	0.42
2:B:129:ALA:O	2:B:131:THR:N	2.53	0.42
2:B:159:LEU:HD23	2:B:159:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:ALA:O	3:C:63:ALA:C	2.57	0.42
3:C:251:ASP:OD2	3:C:251:ASP:C	2.57	0.42
4:D:146:LEU:HD12	4:D:177:TRP:CE2	2.48	0.42
2:B:36:LEU:O	2:B:37:LEU:C	2.59	0.42
2:B:130:THR:HG23	7:G:22:PHE:CE2	2.54	0.42
4:D:58:ASP:O	4:D:61:GLY:N	2.53	0.42
4:D:172:THR:O	4:D:174:GLU:OE2	2.37	0.42
10:A:303:HEM:C2C	2:B:40:PHE:CE2	3.08	0.41
2:B:87:ILE:O	2:B:89:ARG:N	2.53	0.41
4:D:22:LEU:HD22	4:D:22:LEU:HA	1.62	0.41
4:D:170:PHE:CZ	4:D:171:ARG:HG2	2.54	0.41
6:F:22:LEU:CD1	8:H:20:ALA:HB1	2.50	0.41
1:A:106:LEU:CD2	2:B:133:PHE:CE1	2.83	0.41
3:C:54:TYR:CE1	3:C:70:LEU:CG	3.01	0.41
3:C:93:GLU:OE1	3:C:93:GLU:CA	2.66	0.41
3:C:223:GLN:O	3:C:224:ALA:CB	2.68	0.41
4:D:36:TYR:N	4:D:37:PRO:HD2	2.36	0.41
2:B:134:LEU:O	2:B:135:PHE:C	2.57	0.41
2:B:152:ASP:CA	2:B:154:THR:H	2.32	0.41
3:C:94:LEU:CD2	3:C:98:VAL:HG23	2.50	0.41
3:C:157:ARG:N	10:C:301:HEM:HBA1	2.35	0.41
6:F:20:TRP:O	6:F:24:VAL:CG2	2.52	0.41
7:G:34:GLU:O	7:G:35:LEU:HG	2.21	0.41
1:A:214:PRO:HD3	2:B:24:HIS:CE1	2.55	0.41
2:B:14:LEU:HD11	2:B:18:LEU:CD1	2.47	0.41
2:B:141:ILE:O	2:B:141:ILE:HG22	2.16	0.41
3:C:215:PRO:HB3	3:C:232:THR:CG2	2.49	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.50	0.41
7:G:31:ARG:O	7:G:32:PRO:O	2.38	0.41
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.46	0.41
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.74	0.41
3:C:189:GLU:N	3:C:189:GLU:OE1	2.54	0.41
3:C:248:VAL:CG1	3:C:249:LEU:N	2.81	0.41
3:C:279:VAL:O	3:C:281:LYS:N	2.54	0.41
3:C:72:VAL:H	3:C:72:VAL:HG13	1.46	0.41
3:C:264:LEU:HD22	3:C:264:LEU:C	2.21	0.41
4:D:169:ASP:O	4:D:171:ARG:N	2.54	0.41
6:F:28:LYS:C	6:F:30:GLN:N	2.73	0.41
3:C:94:LEU:HD23	3:C:98:VAL:HG23	2.02	0.41
3:C:189:GLU:OE1	3:C:189:GLU:CA	2.68	0.41
3:C:200:GLN:HG2	3:C:201:THR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:MET:HE3	4:D:13:MET:HB3	1.53	0.41
5:E:24:PHE:CZ	6:F:29:ILE:HD11	2.55	0.41
8:H:2:GLU:C	8:H:2:GLU:OE1	2.59	0.41
3:C:33:GLU:HA	3:C:243:ASP:OD2	2.21	0.41
3:C:174:ALA:HB3	3:C:229:GLU:H	1.86	0.41
3:C:270:LEU:C	3:C:270:LEU:CD1	2.87	0.41
5:E:24:PHE:CZ	6:F:29:ILE:CD1	3.04	0.41
1:A:39:ILE:HD13	1:A:39:ILE:HG21	1.72	0.41
1:A:43:CYS:HB3	1:A:93:MET:HB2	2.02	0.41
1:A:105:TYR:OH	2:B:129:ALA:HB1	2.21	0.41
1:A:198:PHE:HA	1:A:201:LEU:HD12	2.03	0.41
10:A:303:HEM:CGA	14:B:1202:TDS:CAA	2.85	0.41
2:B:122:ASN:OD1	2:B:122:ASN:C	2.59	0.41
2:B:134:LEU:HA	2:B:134:LEU:HD12	1.12	0.41
3:C:214:GLY:N	3:C:215:PRO:CD	2.84	0.41
3:C:247:ILE:HD13	3:C:247:ILE:HG21	1.82	0.41
4:D:87:ASP:HB3	4:D:105:ASN:OD1	2.21	0.41
4:D:100:ARG:NH1	4:D:102:TYR:HH	2.19	0.41
4:D:105:ASN:HD21	4:D:107:VAL:CG2	2.23	0.41
4:D:114:VAL:O	4:D:114:VAL:HG12	2.19	0.41
7:G:18:LEU:O	7:G:22:PHE:HD1	2.03	0.41
2:B:33:PRO:O	2:B:34:ASN:C	2.57	0.41
3:C:151:LEU:CG	3:C:152:GLY:N	2.80	0.41
3:C:173:THR:O	3:C:231:LEU:HG	2.21	0.41
3:C:230:ALA:O	3:C:232:THR:N	2.53	0.41
1:A:126:VAL:H	1:A:126:VAL:HG23	1.75	0.40
11:A:1002:OPC:HBZ2	17:G:101:BCR:H333	2.03	0.40
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.56	0.40
3:C:271:MET:HE1	4:D:22:LEU:CD1	2.50	0.40
4:D:64:VAL:HG11	4:D:69:PHE:CD1	2.56	0.40
5:E:8:TYR:CD2	5:E:8:TYR:C	2.93	0.40
1:A:17:LEU:HA	1:A:17:LEU:HD13	1.67	0.40
1:A:117:THR:HG22	10:A:302:HEM:C2D	2.57	0.40
1:A:142:GLN:NE2	2:B:67:ASP:HB3	2.36	0.40
2:B:44:ILE:HG22	2:B:45:MET:N	2.35	0.40
2:B:97:GLY:HA2	2:B:100:LEU:CD1	2.51	0.40
3:C:149:ILE:HB	3:C:245:THR:CG2	2.52	0.40
3:C:218:ILE:HD12	3:C:218:ILE:H	1.86	0.40
3:C:226:LYS:O	3:C:228:GLY:N	2.54	0.40
6:F:22:LEU:HD12	8:H:20:ALA:HB2	2.02	0.40
1:A:5:TYR:O	1:A:6:ASP:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLN:HA	1:A:9:GLN:OE1	2.21	0.40
1:A:80:TRP:CD2	1:A:81:LEU:N	2.89	0.40
3:C:72:VAL:O	3:C:72:VAL:HG22	2.20	0.40
3:C:79:PRO:HD3	3:C:149:ILE:HG12	2.03	0.40
3:C:178:GLY:O	3:C:224:ALA:HB1	2.20	0.40
3:C:285:ALA:HB2	4:D:10:VAL:CG2	2.46	0.40
4:D:76:GLY:C	4:D:77:ASP:O	2.60	0.40
1:A:26:VAL:HA	1:A:27:PRO:HD2	1.56	0.40
1:A:211:ILE:O	1:A:212:SER:O	2.40	0.40
10:A:302:HEM:HBB2	10:A:302:HEM:HMB1	2.00	0.40
10:A:303:HEM:HBA2	14:B:1202:TDS:HAA2	2.02	0.40
2:B:149:PHE:CB	2:B:150:PRO:HD3	2.50	0.40
3:C:274:LEU:HA	3:C:274:LEU:HD23	1.58	0.40
1:A:195:ILE:CD1	1:A:199:MET:CE	3.00	0.40
1:A:215:LEU:HB2	7:G:28:GLN:OE1	2.21	0.40
2:B:85:PHE:HE1	2:B:147:ALA:CB	2.34	0.40
2:B:156:THR:C	2:B:158:GLY:H	2.25	0.40
3:C:115:LEU:HD23	3:C:115:LEU:HA	1.59	0.40
3:C:146:LYS:HG3	3:C:248:VAL:HG23	2.02	0.40
7:G:27:GLN:OE1	8:H:29:LEU:CD2	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:GLU:OE2	7:G:33:ASN:CB[8_565]	2.09	0.11

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%)	154 (72%)	41 (19%)	18 (8%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	158/160 (99%)	89 (56%)	43 (27%)	26 (16%)	0	1
3	C	286/289 (99%)	204 (71%)	51 (18%)	31 (11%)	0	5
4	D	164/179 (92%)	114 (70%)	28 (17%)	22 (13%)	0	3
5	E	30/32 (94%)	15 (50%)	11 (37%)	4 (13%)	0	3
6	F	30/35 (86%)	15 (50%)	8 (27%)	7 (23%)	0	0
7	G	35/37 (95%)	11 (31%)	15 (43%)	9 (26%)	0	0
8	H	27/29 (93%)	15 (56%)	6 (22%)	6 (22%)	0	1
All	All	943/976 (97%)	617 (65%)	203 (22%)	123 (13%)	0	3

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ALA
1	A	36	LEU
1	A	73	MET
1	A	74	ASN
1	A	112	LYS
1	A	162	GLY
2	B	22	MET
2	B	33	PRO
2	B	34	ASN
2	B	37	LEU
2	B	87	ILE
2	B	88	LEU
2	B	113	PHE
2	B	114	ILE
2	B	115	GLU
2	B	125	ARG
3	C	23	ALA
3	C	63	ALA
3	C	66	SER
3	C	74	ALA
3	C	173	THR
3	C	186	GLU
3	C	189	GLU
3	C	192	ASN
3	C	200	GLN
3	C	201	THR
3	C	202	ASP
3	C	212	PRO

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Mol	Chain	Res	Type
3	C	224	ALA
3	C	226	LYS
3	C	227	ALA
3	C	230	ALA
4	D	13	MET
4	D	14	GLY
4	D	49	ALA
4	D	63	ASN
4	D	64	VAL
4	D	70	LEU
4	D	71	GLU
4	D	77	ASP
4	D	135	GLU
4	D	139	VAL
4	D	145	PRO
4	D	167	GLU
6	F	9	ALA
6	F	10	LEU
6	F	29	ILE
7	G	16	ALA
7	G	20	GLY
7	G	27	GLN
7	G	32	PRO
7	G	34	GLU
8	H	2	GLU
8	H	4	ASP
1	A	2	ALA
1	A	3	ASN
1	A	114	ARG
1	A	132	GLY
1	A	136	TYR
1	A	150	ILE
2	B	146	GLY
3	C	34	VAL
3	C	174	ALA
3	C	191	GLY
3	C	278	GLN
4	D	21	LEU
4	D	56	ALA
4	D	81	VAL
4	D	97	GLU
4	D	110	HIS

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Mol	Chain	Res	Type
6	F	24	VAL
7	G	19	GLY
1	A	32	ILE
1	A	131	PHE
2	B	94	LYS
2	B	95	LEU
3	C	20	ILE
3	C	91	PRO
3	C	184	ALA
3	C	195	TYR
4	D	82	GLN
4	D	138	LYS
4	D	174	GLU
5	E	13	ALA
6	F	17	PHE
7	G	4	PRO
7	G	14	VAL
1	A	96	MET
2	B	78	GLU
2	B	134	LEU
2	B	145	ILE
3	C	175	SER
3	C	187	GLU
3	C	231	LEU
4	D	122	ASN
8	H	7	GLY
8	H	20	ALA
1	A	60	PRO
1	A	155	PRO
2	B	2	ALA
2	B	36	LEU
2	B	86	GLN
2	B	102	ALA
2	B	124	PHE
2	B	137	THR
2	B	141	ILE
3	C	194	LYS
5	E	17	GLY
5	E	19	ALA
6	F	6	LEU
7	G	31	ARG
2	B	92	PRO

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Mol	Chain	Res	Type
2	B	105	PRO
2	B	122	ASN
3	C	88	GLU
3	C	215	PRO
1	A	206	ILE
5	E	18	ILE
6	F	16	ILE
8	H	19	ILE
8	H	23	VAL
3	C	69	GLY
4	D	143	PRO

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%)	135 (73%)	49 (27%)	0 2
2	B	137/137 (100%)	95 (69%)	42 (31%)	0 2
3	C	242/243 (100%)	164 (68%)	78 (32%)	0 1
4	D	139/146 (95%)	100 (72%)	39 (28%)	0 2
5	E	25/25 (100%)	18 (72%)	7 (28%)	0 2
6	F	24/27 (89%)	14 (58%)	10 (42%)	0 0
7	G	28/28 (100%)	15 (54%)	13 (46%)	0 0
8	H	24/24 (100%)	18 (75%)	6 (25%)	0 2
All	All	803/814 (99%)	559 (70%)	244 (30%)	0 2

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	TYR
1	A	11	ARG
1	A	12	LEU

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Mol	Chain	Res	Type
1	A	14	ILE
1	A	17	LEU
1	A	30	VAL
1	A	31	ASN
1	A	32	ILE
1	A	36	LEU
1	A	47	GLN
1	A	52	PHE
1	A	61	THR
1	A	62	VAL
1	A	72	ILE
1	A	77	SER
1	A	81	LEU
1	A	82	ILE
1	A	83	ARG
1	A	84	SER
1	A	87	ARG
1	A	97	MET
1	A	103	ARG
1	A	106	LEU
1	A	107	THR
1	A	110	PHE
1	A	112	LYS
1	A	114	ARG
1	A	123	ILE
1	A	130	SER
1	A	142	GLN
1	A	143	VAL
1	A	148	VAL
1	A	151	VAL
1	A	152	SER
1	A	155	PRO
1	A	161	VAL
1	A	163	VAL
1	A	164	LEU
1	A	169	LEU
1	A	170	ARG
1	A	173	SER
1	A	182	ARG
1	A	195	ILE
1	A	200	LEU
1	A	201	LEU

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Mol	Chain	Res	Type
1	A	207	ARG
1	A	208	LYS
1	A	211	ILE
2	B	4	LEU
2	B	5	LYS
2	B	8	ASP
2	B	13	LYS
2	B	15	ARG
2	B	20	LYS
2	B	25	ASN
2	B	35	ASP
2	B	39	VAL
2	B	40	PHE
2	B	44	ILE
2	B	51	ILE
2	B	55	SER
2	B	69	PHE
2	B	73	LEU
2	B	74	GLU
2	B	76	LEU
2	B	79	TRP
2	B	81	LEU
2	B	86	GLN
2	B	88	LEU
2	B	90	SER
2	B	94	LYS
2	B	96	LEU
2	B	100	LEU
2	B	101	MET
2	B	103	SER
2	B	115	GLU
2	B	119	LYS
2	B	120	PHE
2	B	127	PRO
2	B	132	ILE
2	B	134	LEU
2	B	138	LEU
2	B	140	THR
2	B	141	ILE
2	B	153	LYS
2	B	154	THR
2	B	155	LEU

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Mol	Chain	Res	Type
2	B	156	THR
2	B	157	LEU
2	B	159	LEU
3	C	3	PHE
3	C	7	GLN
3	C	12	THR
3	C	14	ARG
3	C	19	ARG
3	C	21	VAL
3	C	22	CYS
3	C	30	LYS
3	C	35	GLU
3	C	36	VAL
3	C	40	VAL
3	C	47	LYS
3	C	54	TYR
3	C	56	THR
3	C	58	LEU
3	C	59	GLN
3	C	60	GLN
3	C	70	LEU
3	C	77	MET
3	C	80	GLU
3	C	88	GLU
3	C	92	GLU
3	C	93	GLU
3	C	95	LYS
3	C	96	LYS
3	C	100	ASP
3	C	101	VAL
3	C	110	GLN
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	137	THR
3	C	141	ASN
3	C	150	HIS
3	C	154	ASN
3	C	155	ARG

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Mol	Chain	Res	Type
3	C	165	GLU
3	C	172	PHE
3	C	175	SER
3	C	179	THR
3	C	180	ILE
3	C	185	LYS
3	C	186	GLU
3	C	188	ASP
3	C	189	GLU
3	C	198	SER
3	C	199	ILE
3	C	203	SER
3	C	205	LYS
3	C	206	THR
3	C	207	VAL
3	C	208	VAL
3	C	210	THR
3	C	211	ILE
3	C	212	PRO
3	C	216	GLU
3	C	218	ILE
3	C	221	GLU
3	C	223	GLN
3	C	226	LYS
3	C	232	THR
3	C	233	ASN
3	C	242	GLN
3	C	249	LEU
3	C	251	ASP
3	C	256	LYS
3	C	259	ILE
3	C	262	ILE
3	C	264	LEU
3	C	267	LEU
3	C	270	LEU
3	C	276	LYS
3	C	282	VAL
3	C	286	GLU
3	C	288	ASN
4	D	9	ASP
4	D	13	MET
4	D	16	ARG

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Mol	Chain	Res	Type
4	D	22	LEU
4	D	35	LEU
4	D	60	LEU
4	D	65	LYS
4	D	66	VAL
4	D	67	SER
4	D	68	LYS
4	D	69	PHE
4	D	72	SER
4	D	77	ASP
4	D	78	ARG
4	D	79	VAL
4	D	84	LEU
4	D	85	LYS
4	D	95	SER
4	D	96	LYS
4	D	97	GLU
4	D	99	ILE
4	D	101	ASP
4	D	105	ASN
4	D	109	THR
4	D	111	LEU
4	D	114	VAL
4	D	134	ASP
4	D	139	VAL
4	D	140	ILE
4	D	141	ARG
4	D	146	LEU
4	D	148	LEU
4	D	154	THR
4	D	160	ILE
4	D	161	VAL
4	D	170	PHE
4	D	172	THR
4	D	174	GLU
4	D	179	VAL
5	E	7	PHE
5	E	11	PHE
5	E	12	ILE
5	E	14	LEU
5	E	18	ILE
5	E	26	ILE

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Mol	Chain	Res	Type
5	E	29	ILE
6	F	6	LEU
6	F	10	LEU
6	F	11	LEU
6	F	12	SER
6	F	15	LEU
6	F	22	LEU
6	F	25	LEU
6	F	27	LEU
6	F	29	ILE
6	F	30	GLN
7	G	1	MET
7	G	2	VAL
7	G	3	GLU
7	G	4	PRO
7	G	5	LEU
7	G	6	LEU
7	G	9	LEU
7	G	23	TYR
7	G	28	GLN
7	G	29	TYR
7	G	30	LYS
7	G	34	GLU
7	G	35	LEU
8	H	2	GLU
8	H	6	LEU
8	H	14	VAL
8	H	18	SER
8	H	21	MET
8	H	27	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	31	ASN
1	A	47	GLN
2	B	25	ASN
2	B	34	ASN
2	B	118	ASN
3	C	59	GLN
3	C	60	GLN

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Mol	Chain	Res	Type
3	C	110	GLN
3	C	141	ASN
3	C	154	ASN
3	C	200	GLN
3	C	223	GLN
3	C	234	ASN
3	C	242	GLN
3	C	250	GLN
3	C	288	ASN
4	D	105	ASN
4	D	152	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\#\|Z\| > 2$
12	UMQ	A	1104	-	35,35,35	1.58	3 (8%)	46,46,46	3.04	19 (41%)
14	TDS	B	1202	10	27,31,31	3.15	11 (40%)	33,40,40	6.63	19 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	HEM	A	302	1	42,50,50	2.40	15 (35%)	46,82,82	2.26	13 (28%)
12	UMQ	A	1102	-	35,35,35	2.17	9 (25%)	46,46,46	3.03	18 (39%)
11	OPC	A	1002	-	53,53,54	2.05	14 (26%)	59,61,64	2.88	20 (33%)
10	HEM	A	301	1	42,50,50	2.20	13 (30%)	46,82,82	3.65	29 (63%)
14	TDS	B	1201	-	27,31,31	3.12	10 (37%)	33,40,40	6.12	20 (60%)
16	SQD	D	201	-	52,54,54	2.93	25 (48%)	62,65,65	5.06	31 (50%)
10	HEM	A	303	14,1,18	42,50,50	2.53	11 (26%)	46,82,82	2.54	15 (32%)
13	CLA	B	201	18	63,73,73	2.22	20 (31%)	74,113,113	3.03	34 (45%)
17	BCR	G	101	-	41,41,41	3.48	23 (56%)	56,56,56	6.82	27 (48%)
11	OPC	B	1001	-	53,53,54	2.28	23 (43%)	59,61,64	2.71	25 (42%)
10	HEM	C	301	3	42,50,50	2.29	11 (26%)	46,82,82	2.13	14 (30%)
15	FES	D	200	4	0,4,4	-	-	-		
12	UMQ	A	1101	-	35,35,35	1.75	5 (14%)	46,46,46	3.05	24 (52%)
12	UMQ	A	1103	-	35,35,35	1.98	5 (14%)	46,46,46	2.59	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	UMQ	A	1104	-	2/2/10/10	13/20/60/60	0/2/2/2
14	TDS	B	1202	10	-	11/16/17/17	0/2/2/2
10	HEM	A	302	1	-	6/12/54/54	-
12	UMQ	A	1102	-	2/2/10/10	12/20/60/60	0/2/2/2
11	OPC	A	1002	-	-	32/57/57/60	-
16	SQD	D	201	-	3/3/9/9	27/49/69/69	0/1/1/1
10	HEM	A	301	1	-	5/12/54/54	-
14	TDS	B	1201	-	-	11/16/17/17	0/2/2/2
10	HEM	A	303	14,1,18	-	2/12/54/54	-
13	CLA	B	201	18	2/2/15/20	13/37/115/115	-
17	BCR	G	101	-	-	12/29/63/63	0/2/2/2
11	OPC	B	1001	-	-	23/57/57/60	-
10	HEM	C	301	3	-	4/12/54/54	-
15	FES	D	200	4	-	-	0/1/1/1
12	UMQ	A	1101	-	2/2/10/10	11/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	UMQ	A	1103	-	2/2/10/10	11/20/60/60	0/2/2/2

All (198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	101	BCR	C8-C9	-10.35	1.23	1.46
14	B	1202	TDS	CAD-CAL	-10.08	1.21	1.38
14	B	1201	TDS	CAD-CAL	-9.07	1.23	1.38
10	A	302	HEM	C3C-C2C	-8.82	1.28	1.40
10	A	303	HEM	C3C-C2C	-8.76	1.28	1.40
17	G	101	BCR	C26-C25	7.64	1.47	1.34
10	C	301	HEM	C3D-C2D	7.42	1.52	1.36
17	G	101	BCR	C23-C22	-7.34	1.30	1.46
12	A	1102	UMQ	O1'-C1'	7.32	1.52	1.40
12	A	1101	UMQ	C1'-C2'	-7.15	1.31	1.52
11	B	1001	OPC	OBJ-CBK	7.13	1.54	1.33
10	A	303	HEM	C3D-C2D	7.04	1.52	1.36
16	D	201	SQD	C4-C3	6.70	1.69	1.52
12	A	1103	UMQ	O1'-C1'	6.63	1.51	1.40
16	D	201	SQD	O47-C7	6.40	1.52	1.34
16	D	201	SQD	C17-C16	-6.40	1.20	1.51
10	C	301	HEM	C3C-C2C	-6.35	1.31	1.40
17	G	101	BCR	C30-C25	6.33	1.61	1.53
14	B	1201	TDS	OAB-CAE	6.01	1.47	1.36
10	A	301	HEM	C3D-C2D	6.00	1.49	1.36
14	B	1202	TDS	CAD-CAE	-5.94	1.20	1.37
13	B	201	CLA	C3C-C2C	5.86	1.49	1.36
12	A	1103	UMQ	C1'-C2'	-5.76	1.35	1.52
17	G	101	BCR	C38-C26	5.68	1.60	1.50
11	A	1002	OPC	OAN-CAO	5.55	1.50	1.34
16	D	201	SQD	O6-C1	5.49	1.49	1.40
16	D	201	SQD	C12-C11	-5.44	1.24	1.51
14	B	1201	TDS	CAD-CAE	-5.38	1.22	1.37
13	B	201	CLA	CHC-C1C	5.30	1.47	1.34
11	B	1001	OPC	CAG-CAH	-5.24	1.35	1.51
10	A	302	HEM	C3D-C2D	5.19	1.48	1.36
14	B	1201	TDS	CAR-CAQ	-5.17	1.27	1.52
10	A	303	HEM	C3B-C2B	-5.11	1.26	1.37
12	A	1102	UMQ	C1'-C2'	-5.10	1.37	1.52
13	B	201	CLA	OBD-CAD	5.02	1.31	1.22
14	B	1202	TDS	CAR-CAQ	-5.00	1.28	1.52
13	B	201	CLA	C3B-C2B	5.00	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C16-C15	-4.92	1.27	1.51
13	B	201	CLA	O2D-CGD	4.86	1.45	1.33
17	G	101	BCR	C7-C6	-4.85	1.28	1.45
16	D	201	SQD	O48-C23	4.84	1.47	1.33
10	C	301	HEM	CMB-C2B	4.83	1.60	1.50
17	G	101	BCR	C8-C7	-4.81	1.18	1.33
12	A	1104	UMQ	O1'-C1'	4.81	1.48	1.40
12	A	1104	UMQ	C1'-C2'	-4.76	1.38	1.52
16	D	201	SQD	C18-C17	-4.76	1.28	1.51
10	A	301	HEM	CMB-C2B	4.71	1.60	1.50
11	A	1002	OPC	CBP-CBQ	-4.66	1.32	1.52
14	B	1201	TDS	CAR-CAS	-4.64	1.28	1.51
14	B	1202	TDS	CAR-CAS	-4.62	1.28	1.51
14	B	1201	TDS	OAK-CAL	4.59	1.44	1.37
12	A	1102	UMQ	O5'-C1'	4.59	1.53	1.41
10	A	303	HEM	C3C-C4C	4.58	1.48	1.41
16	D	201	SQD	C13-C12	-4.55	1.29	1.51
14	B	1202	TDS	OAB-CAE	4.54	1.44	1.36
10	A	301	HEM	FE-NB	-4.45	1.73	1.98
13	B	201	CLA	O2A-CGA	4.41	1.46	1.33
10	A	301	HEM	CMC-C2C	4.37	1.62	1.51
11	B	1001	OPC	CAV-CAW	4.33	1.56	1.31
11	B	1001	OPC	CAQ-CAP	-4.30	1.36	1.52
11	A	1002	OPC	CAV-CAW	4.25	1.55	1.31
11	A	1002	OPC	CAQ-CAP	-4.24	1.36	1.52
13	B	201	CLA	C3D-C4D	-4.22	1.34	1.44
16	D	201	SQD	C11-C10	-4.21	1.30	1.51
11	A	1002	OPC	CBP-CBO	-4.20	1.30	1.51
11	A	1002	OPC	CAG-CAH	-4.03	1.39	1.51
16	D	201	SQD	C21-C20	-4.01	1.26	1.51
10	A	301	HEM	CAD-C3D	3.89	1.61	1.51
17	G	101	BCR	C19-C18	-3.80	1.37	1.46
12	A	1101	UMQ	O1'-C1'	3.78	1.46	1.40
13	B	201	CLA	CHD-C4C	3.75	1.47	1.39
11	A	1002	OPC	OBJ-CBK	3.71	1.44	1.33
10	A	303	HEM	O1A-CGA	3.58	1.33	1.22
11	B	1001	OPC	OAN-CAO	3.58	1.44	1.34
17	G	101	BCR	C1-C6	-3.56	1.49	1.53
10	A	302	HEM	C1B-C2B	3.55	1.51	1.44
11	A	1002	OPC	CAQ-CAR	-3.53	1.34	1.51
17	G	101	BCR	C24-C25	-3.53	1.33	1.45
11	A	1002	OPC	CAR-CAS	-3.45	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C22-C21	-3.43	1.25	1.50
14	B	1201	TDS	CAE-CAF	3.41	1.49	1.42
10	A	302	HEM	C3C-CAC	3.38	1.55	1.47
10	A	302	HEM	O1A-CGA	3.37	1.33	1.22
16	D	201	SQD	C20-C19	-3.37	1.35	1.51
16	D	201	SQD	C19-C18	-3.34	1.35	1.51
10	A	302	HEM	O1D-CGD	3.34	1.33	1.22
10	A	303	HEM	C1B-NB	-3.34	1.34	1.40
17	G	101	BCR	C27-C26	3.32	1.57	1.51
12	A	1103	UMQ	O5'-C1'	3.29	1.50	1.41
10	A	302	HEM	CHD-C1D	-3.29	1.31	1.40
17	G	101	BCR	C12-C13	-3.27	1.38	1.46
10	C	301	HEM	C3C-CAC	3.27	1.55	1.47
17	G	101	BCR	C36-C18	3.26	1.57	1.50
14	B	1202	TDS	OAK-CAL	3.23	1.42	1.37
10	A	301	HEM	C1A-CHA	-3.18	1.32	1.41
17	G	101	BCR	C24-C23	-3.17	1.23	1.33
12	A	1104	UMQ	O2'-C2'	-3.14	1.35	1.43
12	A	1101	UMQ	O2'-C2'	-3.11	1.35	1.43
14	B	1201	TDS	OBD-CAM	3.11	1.45	1.35
10	A	301	HEM	C3C-CAC	3.10	1.54	1.47
10	C	301	HEM	CMA-C3A	3.10	1.57	1.51
16	D	201	SQD	C36-C35	-3.08	1.36	1.51
11	B	1001	OPC	CBL-CBK	3.07	1.59	1.50
11	A	1002	OPC	CBC-CBD	-3.06	1.36	1.51
12	A	1103	UMQ	O2'-C2'	-3.05	1.35	1.43
11	B	1001	OPC	CAG-NAF	-3.05	1.42	1.51
11	A	1002	OPC	CBT-CBS	-3.04	1.33	1.50
11	A	1002	OPC	CBQ-CBR	-3.01	1.33	1.50
11	B	1001	OPC	CAQ-CAR	-2.99	1.36	1.51
13	B	201	CLA	C4C-C3C	2.98	1.50	1.45
11	B	1001	OPC	CAR-CAS	-2.95	1.37	1.51
16	D	201	SQD	C15-C14	-2.94	1.37	1.51
10	A	301	HEM	C4A-CHB	-2.92	1.32	1.41
17	G	101	BCR	C39-C30	2.92	1.59	1.53
11	B	1001	OPC	CBC-CBD	-2.92	1.37	1.51
13	B	201	CLA	C3D-C2D	2.89	1.46	1.39
11	B	1001	OPC	CBB-CBC	-2.88	1.37	1.51
10	A	302	HEM	C3B-C2B	-2.88	1.31	1.37
10	C	301	HEM	C1B-NB	-2.86	1.35	1.40
10	A	301	HEM	CBD-CGD	2.85	1.57	1.50
16	D	201	SQD	C14-C13	-2.85	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	302	HEM	CMB-C2B	2.82	1.56	1.50
12	A	1102	UMQ	C1-C2	2.82	1.60	1.52
12	A	1101	UMQ	O5'-C1'	2.80	1.49	1.41
11	A	1002	OPC	CBB-CBC	-2.79	1.37	1.51
14	B	1202	TDS	OBD-CAM	2.78	1.44	1.35
10	A	302	HEM	CHC-C4B	-2.77	1.33	1.40
10	A	301	HEM	C2A-C3A	-2.73	1.29	1.37
13	B	201	CLA	C1D-ND	-2.68	1.34	1.37
10	C	301	HEM	CMD-C2D	2.68	1.56	1.50
16	D	201	SQD	C34-C33	-2.68	1.38	1.51
14	B	1202	TDS	CAE-CAF	2.68	1.48	1.42
10	A	302	HEM	C1A-CHA	-2.67	1.33	1.41
12	A	1102	UMQ	C3'-C4'	2.67	1.59	1.52
10	C	301	HEM	C4A-CHB	-2.64	1.33	1.41
13	B	201	CLA	CHB-C4A	2.63	1.35	1.33
10	A	301	HEM	C2C-C1C	2.63	1.48	1.42
11	A	1002	OPC	PAJ-OAI	2.60	1.69	1.59
10	A	302	HEM	CAB-C3B	2.59	1.54	1.47
10	A	303	HEM	CAD-C3D	2.56	1.57	1.51
10	A	301	HEM	C3C-C2C	-2.54	1.36	1.40
16	D	201	SQD	C35-C34	-2.54	1.39	1.51
17	G	101	BCR	C20-C19	2.53	1.41	1.34
11	B	1001	OPC	CBP-CBQ	-2.51	1.41	1.52
16	D	201	SQD	C37-C36	-2.50	1.36	1.51
10	A	303	HEM	C3C-CAC	2.48	1.53	1.47
16	D	201	SQD	C32-C31	-2.47	1.39	1.51
16	D	201	SQD	C1-C2	2.47	1.59	1.52
13	B	201	CLA	MG-NA	-2.47	2.00	2.06
16	D	201	SQD	C33-C32	-2.46	1.39	1.51
17	G	101	BCR	C17-C18	2.45	1.41	1.35
17	G	101	BCR	C40-C30	2.43	1.58	1.53
10	A	303	HEM	O1D-CGD	2.43	1.30	1.22
14	B	1202	TDS	CAH-CAG	-2.41	1.33	1.41
17	G	101	BCR	C11-C10	-2.40	1.35	1.43
13	B	201	CLA	C1C-C2C	2.40	1.49	1.44
11	B	1001	OPC	CBZ-CBY	2.40	1.63	1.51
13	B	201	CLA	CHD-C1D	2.40	1.43	1.38
16	D	201	SQD	C38-C37	-2.39	1.33	1.50
13	B	201	CLA	C4-C3	2.37	1.56	1.50
12	A	1101	UMQ	C4-C5	2.35	1.58	1.53
10	A	303	HEM	FE-ND	2.34	2.11	1.98
12	A	1102	UMQ	O2'-C2'	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	101	BCR	C21-C22	2.32	1.41	1.35
11	B	1001	OPC	CBP-CBO	-2.32	1.40	1.51
10	C	301	HEM	CAB-C3B	2.31	1.53	1.47
13	B	201	CLA	CBD-CGD	-2.30	1.45	1.52
11	B	1001	OPC	CBX-CBW	2.30	1.63	1.51
12	A	1102	UMQ	O2-C2	2.29	1.48	1.43
11	B	1001	OPC	CBG-NAF	-2.28	1.43	1.50
10	C	301	HEM	O1A-CGA	2.26	1.29	1.22
17	G	101	BCR	C16-C17	-2.21	1.36	1.43
10	A	303	HEM	C2A-C3A	-2.20	1.31	1.37
12	A	1103	UMQ	O5-C1	2.19	1.47	1.41
10	A	301	HEM	C4D-C3D	2.19	1.48	1.45
13	B	201	CLA	C1B-CHB	2.19	1.47	1.41
10	A	302	HEM	CHB-C1B	2.18	1.39	1.34
17	G	101	BCR	C29-C28	2.17	1.57	1.52
11	B	1001	OPC	CBW-CBV	2.17	1.62	1.51
14	B	1201	TDS	CBC-CBB	-2.16	1.34	1.50
10	C	301	HEM	CHD-C1D	-2.15	1.34	1.40
14	B	1202	TDS	CAH-CAP	-2.15	1.36	1.39
11	B	1001	OPC	CBY-CBX	2.14	1.62	1.51
11	B	1001	OPC	CBI-CAM	2.13	1.57	1.50
13	B	201	CLA	C2-C3	2.11	1.37	1.33
14	B	1202	TDS	CAF-CAN	2.11	1.43	1.41
17	G	101	BCR	C2-C1	2.10	1.58	1.54
12	A	1102	UMQ	O1-C1	2.09	1.47	1.41
11	B	1001	OPC	CBM-CBL	2.06	1.59	1.52
12	A	1102	UMQ	C4'-C5'	2.06	1.58	1.52
14	B	1201	TDS	CAF-CAN	2.06	1.43	1.41
11	B	1001	OPC	CCA-CBZ	2.05	1.64	1.51
13	B	201	CLA	C6-C5	2.04	1.59	1.52
10	A	302	HEM	CBA-CGA	2.04	1.55	1.50
16	D	201	SQD	C4-C5	-2.03	1.48	1.53
10	A	302	HEM	CMC-C2C	2.03	1.56	1.51
11	B	1001	OPC	OCC-CBK	2.01	1.28	1.22
11	B	1001	OPC	CBV-CBU	2.00	1.61	1.51

All (321) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	101	BCR	C24-C23-C22	28.08	167.78	126.23
17	G	101	BCR	C7-C8-C9	26.41	165.30	126.23
14	B	1202	TDS	CAE-CAD-CAL	23.04	155.92	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1201	TDS	CAE-CAD-CAL	21.50	153.53	119.98
17	G	101	BCR	C8-C7-C6	18.66	176.84	127.00
16	D	201	SQD	O3-C3-C4	-16.36	71.81	110.38
17	G	101	BCR	C23-C24-C25	15.79	169.18	127.00
16	D	201	SQD	O4-C4-C3	15.48	146.87	110.38
14	B	1202	TDS	CAL-CAM-CAN	-14.66	107.79	120.05
14	B	1202	TDS	OAK-CAL-CAM	13.31	128.44	114.53
14	B	1201	TDS	CAD-CAL-CAM	-12.35	108.90	120.59
16	D	201	SQD	C17-C16-C15	11.93	174.66	114.37
16	D	201	SQD	C18-C17-C16	11.78	173.90	114.37
14	B	1201	TDS	CAL-CAM-CAN	-11.77	110.20	120.05
14	B	1201	TDS	OAK-CAL-CAM	11.76	126.82	114.53
16	D	201	SQD	C12-C11-C10	11.00	169.96	114.37
11	A	1002	OPC	CAA-NAF-CAE	-10.84	80.51	108.98
14	B	1202	TDS	CAD-CAL-CAM	-10.45	110.70	120.59
12	A	1104	UMQ	O1'-C1'-C2'	10.19	123.75	108.27
17	G	101	BCR	C32-C1-C6	-9.77	94.91	110.24
16	D	201	SQD	C13-C12-C11	9.76	163.68	114.37
17	G	101	BCR	C33-C5-C6	-9.58	114.03	124.48
14	B	1201	TDS	CAD-CAE-CAF	-9.44	103.06	120.83
16	D	201	SQD	C22-C21-C20	9.42	177.00	113.36
14	B	1202	TDS	CAD-CAE-CAF	-9.33	103.27	120.83
10	A	301	HEM	C3B-C2B-C1B	-9.25	99.46	106.41
16	D	201	SQD	O6-C1-C2	8.91	121.80	108.27
12	A	1103	UMQ	CA-O1'-C1'	8.62	128.41	113.68
14	B	1202	TDS	OAO-CAP-CAQ	8.51	124.04	112.07
11	B	1001	OPC	CAA-NAF-CBG	-8.34	87.07	108.98
16	D	201	SQD	O47-C7-C8	8.26	129.35	111.48
14	B	1202	TDS	OAB-CAE-CAF	8.04	127.37	115.91
10	A	301	HEM	CAD-C3D-C4D	8.00	138.64	124.70
12	A	1104	UMQ	CA-O1'-C1'	7.70	126.84	113.68
12	A	1101	UMQ	O2'-C2'-C3'	7.65	128.42	110.38
10	A	301	HEM	C4B-C3B-C2B	7.54	114.21	107.28
12	A	1102	UMQ	CA-O1'-C1'	7.52	126.53	113.68
10	A	303	HEM	CBA-CAA-C2A	-7.33	100.21	112.54
12	A	1103	UMQ	O1'-C1'-C2'	7.19	119.19	108.27
17	G	101	BCR	C8-C9-C10	7.09	130.17	119.01
17	G	101	BCR	C20-C21-C22	7.06	137.18	127.28
13	B	201	CLA	C4-C3-C5	7.06	127.48	115.23
10	A	301	HEM	CHC-C4B-NB	7.00	131.96	124.44
10	A	303	HEM	C4C-CHD-C1D	6.87	131.63	122.56
16	D	201	SQD	O5-C5-C4	6.79	121.94	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	1101	UMQ	O5'-C1'-O1'	6.75	125.99	110.04
14	B	1201	TDS	OAB-CAE-CAF	6.71	125.47	115.91
13	B	201	CLA	C4A-NA-C1A	6.61	109.69	106.68
13	B	201	CLA	C1D-ND-C4D	-6.56	101.71	106.31
12	A	1103	UMQ	O5'-C1'-O1'	6.39	125.14	110.04
11	A	1002	OPC	CAA-NAF-CBG	-6.25	92.56	108.98
14	B	1202	TDS	CAQ-CAP-CAH	-6.23	111.75	120.40
10	A	301	HEM	C4D-C3D-C2D	-6.21	97.85	106.89
11	B	1001	OPC	CBU-CBT-CBS	6.16	147.12	112.60
10	A	303	HEM	CAD-C3D-C4D	6.10	135.33	124.70
13	B	201	CLA	CMD-C2D-C1D	6.08	135.44	124.73
16	D	201	SQD	C15-C14-C13	5.99	144.65	114.37
11	A	1002	OPC	CAA-NAF-CAG	-5.95	86.24	109.91
11	B	1001	OPC	CAM-OAN-CAO	-5.93	103.60	117.80
10	A	301	HEM	C2C-C3C-C4C	5.91	111.02	106.90
12	A	1102	UMQ	C1'-O5'-C5'	5.89	125.23	113.72
13	B	201	CLA	C3C-C4C-NC	5.86	117.94	110.43
13	B	201	CLA	O2D-CGD-CBD	5.86	121.47	111.23
12	A	1104	UMQ	O5-C5-C4	5.82	120.19	109.70
11	A	1002	OPC	OAN-CAO-CAP	5.76	123.93	111.48
14	B	1202	TDS	CAJ-OAK-CAL	-5.70	109.14	117.51
14	B	1201	TDS	CAA-OAB-CAE	5.68	127.13	117.67
12	A	1101	UMQ	O1-C4'-C5'	5.67	124.35	109.48
11	A	1002	OPC	CAH-CAG-NAF	5.62	133.85	115.82
12	A	1102	UMQ	O5-C5-C4	5.61	119.81	109.70
12	A	1103	UMQ	O2'-C2'-C3'	5.59	123.55	110.38
10	A	301	HEM	C3D-C4D-ND	5.58	116.29	110.17
12	A	1102	UMQ	O5'-C1'-O1'	5.55	123.15	110.04
13	B	201	CLA	C2D-C1D-ND	5.52	115.59	110.13
12	A	1102	UMQ	O1'-C1'-C2'	5.47	116.58	108.27
11	B	1001	OPC	CBG-NAF-CAG	5.44	131.52	109.91
14	B	1201	TDS	OAO-CAP-CAQ	5.39	119.66	112.07
10	A	302	HEM	CBA-CAA-C2A	-5.37	103.52	112.54
10	A	302	HEM	CMB-C2B-C1B	5.35	133.40	125.03
12	A	1104	UMQ	O5'-C1'-C2'	5.34	121.34	110.37
13	B	201	CLA	C2C-C1C-NC	5.32	115.57	109.98
10	A	302	HEM	C3B-C4B-NB	5.31	113.28	109.47
12	A	1101	UMQ	CA-O1'-C1'	5.29	122.72	113.68
10	C	301	HEM	C4C-CHD-C1D	5.20	129.43	122.56
11	A	1002	OPC	CBI-CAM-CAL	-5.16	99.75	111.78
13	B	201	CLA	CHD-C4C-C3C	-5.16	117.25	124.77
10	A	302	HEM	CAD-CBD-CGD	-5.14	100.02	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	101	BCR	C36-C18-C17	5.14	131.14	122.82
16	D	201	SQD	C14-C13-C12	5.13	140.32	114.37
11	B	1001	OPC	CAR-CAQ-CAP	5.12	131.93	113.13
12	A	1102	UMQ	O2'-C2'-C3'	5.10	122.39	110.38
13	B	201	CLA	C4C-C3C-C2C	-5.08	99.50	106.89
10	A	301	HEM	CBB-CAB-C3B	-5.03	102.37	127.53
12	A	1102	UMQ	C3-C4-C5	5.01	119.31	110.23
12	A	1104	UMQ	O2'-C2'-C1'	5.00	122.00	110.08
12	A	1102	UMQ	O1-C1-C2	5.00	120.38	108.09
11	A	1002	OPC	OAI-CAH-CAG	4.98	133.63	109.65
13	B	201	CLA	C5-C3-C2	-4.96	110.04	121.17
12	A	1101	UMQ	O2'-C2'-C1'	4.95	121.87	110.08
10	A	301	HEM	CMB-C2B-C1B	4.93	132.73	125.03
14	B	1201	TDS	CAE-CAF-CAG	-4.91	117.82	124.97
17	G	101	BCR	C34-C9-C8	-4.90	110.60	118.09
12	A	1101	UMQ	O5-C5-C4	4.88	118.50	109.70
13	B	201	CLA	C6-C5-C3	-4.88	101.58	113.47
12	A	1102	UMQ	O5'-C1'-C2'	4.82	120.28	110.37
13	B	201	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
12	A	1102	UMQ	O2-C2-C1	4.71	121.31	110.08
14	B	1202	TDS	CAE-CAF-CAG	-4.70	118.13	124.97
10	A	303	HEM	CMB-C2B-C1B	4.67	132.33	125.03
17	G	101	BCR	C2-C1-C6	4.63	117.16	110.44
12	A	1102	UMQ	C1'-C2'-C3'	4.63	119.74	110.01
12	A	1104	UMQ	C1'-C2'-C3'	4.62	119.74	110.01
12	A	1101	UMQ	O1-C1-C2	4.54	119.27	108.09
16	D	201	SQD	C16-C15-C14	4.52	137.22	114.37
12	A	1101	UMQ	O5'-C1'-C2'	4.49	119.58	110.37
13	B	201	CLA	CHD-C1D-ND	-4.47	118.50	124.80
13	B	201	CLA	CED-O2D-CGD	-4.45	105.83	115.92
11	B	1001	OPC	OAN-CAO-OAD	-4.43	113.34	123.70
10	A	301	HEM	C2B-C1B-NB	4.39	114.89	109.84
12	A	1101	UMQ	C2'-C3'-C4'	-4.38	99.73	109.68
11	A	1002	OPC	CAR-CAS-CAT	4.37	136.45	114.37
12	A	1103	UMQ	O2'-C2'-C1'	4.32	120.37	110.08
10	A	301	HEM	CHD-C1D-ND	4.32	129.08	124.44
12	A	1101	UMQ	O5-C1-C2	-4.32	101.50	110.37
10	C	301	HEM	CBD-CAD-C3D	-4.31	100.60	112.53
14	B	1202	TDS	OAO-CAN-CAM	4.24	121.27	116.11
11	B	1001	OPC	CBP-CBO-CBN	4.24	135.80	114.37
10	C	301	HEM	C2C-C3C-C4C	4.22	109.84	106.90
13	B	201	CLA	O2A-CGA-CBA	4.21	124.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	301	HEM	CBB-CAB-C3B	-4.16	106.72	127.53
10	A	301	HEM	O2D-CGD-O1D	-4.15	112.67	123.33
17	G	101	BCR	C36-C18-C19	-4.12	111.79	118.09
16	D	201	SQD	C35-C34-C33	4.12	135.19	114.37
13	B	201	CLA	C3D-C4D-ND	4.10	116.66	109.99
14	B	1201	TDS	CAQ-CAP-CAH	-4.08	114.74	120.40
13	B	201	CLA	C3B-C4B-NB	4.08	114.48	109.21
10	C	301	HEM	C3B-C4B-NB	-4.08	106.54	109.47
12	A	1101	UMQ	O1'-C1'-C2'	3.99	114.33	108.27
12	A	1104	UMQ	C3'-C4'-C5'	-3.96	102.15	110.93
12	A	1102	UMQ	C3'-C4'-C5'	3.95	119.69	110.93
12	A	1101	UMQ	C1-O1-C4'	-3.94	108.65	117.98
11	B	1001	OPC	OAN-CAO-CAP	3.91	119.94	111.48
11	A	1002	OPC	CAQ-CAR-CAS	3.88	134.00	114.37
16	D	201	SQD	O4-C4-C5	-3.88	99.77	109.32
11	B	1001	OPC	CBI-OBJ-CBK	3.86	131.21	117.12
16	D	201	SQD	O6-C44-C45	3.83	120.14	110.82
14	B	1201	TDS	OAB-CAE-CAD	3.81	130.06	123.27
13	B	201	CLA	CAA-CBA-CGA	-3.81	102.39	113.21
11	B	1001	OPC	CAA-NAF-CAG	-3.79	94.86	109.91
13	B	201	CLA	CHB-C4A-NA	3.74	129.80	124.40
10	C	301	HEM	CAD-CBD-CGD	3.73	123.57	113.67
11	B	1001	OPC	CAR-CAS-CAT	3.72	133.19	114.37
17	G	101	BCR	C32-C1-C2	3.72	123.24	108.95
10	A	301	HEM	C1D-C2D-C3D	3.68	110.85	106.98
12	A	1102	UMQ	C1-O5-C5	3.68	120.90	113.72
10	A	301	HEM	O1A-CGA-CBA	-3.61	111.63	123.09
12	A	1104	UMQ	O3'-C3'-C2'	3.61	118.88	110.38
17	G	101	BCR	C33-C5-C4	3.60	121.28	113.60
10	A	302	HEM	CMB-C2B-C3B	-3.60	119.72	128.43
10	A	302	HEM	C2D-C1D-ND	3.60	114.06	109.90
17	G	101	BCR	C29-C28-C27	3.60	119.19	111.28
12	A	1104	UMQ	O1-C4'-C5'	3.59	118.90	109.48
14	B	1201	TDS	CAU-CAV-CAW	-3.59	96.24	114.37
14	B	1201	TDS	CAS-CAT-CAU	-3.57	96.32	114.37
13	B	201	CLA	CMB-C2B-C1B	3.56	133.67	128.46
12	A	1104	UMQ	C3-C4-C5	3.53	116.64	110.23
10	A	303	HEM	CMB-C2B-C3B	-3.52	119.91	128.43
10	A	303	HEM	CHA-C4D-ND	-3.51	120.02	124.37
13	B	201	CLA	O1D-CGD-CBD	-3.48	117.66	124.52
16	D	201	SQD	C32-C31-C30	3.47	131.92	114.37
17	G	101	BCR	C3-C4-C5	-3.46	107.88	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	302	HEM	CHB-C1B-NB	-3.46	120.08	124.37
16	D	201	SQD	O47-C45-C44	3.46	120.76	108.34
10	C	301	HEM	CHC-C4B-NB	3.46	128.16	124.44
12	A	1104	UMQ	O1-C1-C2	3.42	116.51	108.09
10	C	301	HEM	C4D-ND-C1D	3.41	109.25	105.21
10	A	302	HEM	CAA-CBA-CGA	3.40	123.00	113.83
11	A	1002	OPC	CBP-CBQ-CBR	3.38	131.51	112.60
14	B	1202	TDS	OAB-CAE-CAD	3.36	129.26	123.27
11	A	1002	OPC	CAS-CAT-CAU	-3.35	97.74	113.86
10	C	301	HEM	CMD-C2D-C1D	3.35	130.27	125.03
10	A	301	HEM	CHC-C4B-C3B	-3.35	119.44	124.57
12	A	1104	UMQ	O2'-C2'-C3'	3.35	118.26	110.38
10	A	301	HEM	O2A-CGA-CBA	3.33	124.51	114.00
10	A	302	HEM	CHC-C4B-C3B	-3.29	119.53	124.57
12	A	1101	UMQ	O2-C2-C3	3.29	118.12	110.38
14	B	1201	TDS	CAT-CAU-CAV	3.27	130.88	114.37
12	A	1102	UMQ	O2'-C2'-C1'	3.26	117.85	110.08
14	B	1201	TDS	CAV-CAW-CAX	3.24	130.72	114.37
11	B	1001	OPC	CBO-CBP-CBQ	3.23	129.39	113.86
10	C	301	HEM	C4B-C3B-C2B	3.22	110.24	107.28
17	G	101	BCR	C23-C22-C21	-3.21	113.96	119.01
16	D	201	SQD	O9-S-C6	3.19	111.52	106.76
12	A	1104	UMQ	C2'-C3'-C4'	-3.17	102.49	109.68
12	A	1102	UMQ	O5-C1-C2	3.16	116.86	110.37
11	A	1002	OPC	PAJ-OAI-CAH	3.16	136.28	121.26
16	D	201	SQD	C36-C35-C34	3.14	130.23	114.37
11	A	1002	OPC	OBJ-CBK-OCC	-3.13	115.81	123.63
13	B	201	CLA	CAC-C3C-C4C	3.12	128.85	124.79
10	A	301	HEM	CHA-C4D-ND	-3.12	120.50	124.37
10	A	301	HEM	CMD-C2D-C1D	3.12	129.90	125.03
16	D	201	SQD	O2-C2-C1	3.11	117.50	110.08
17	G	101	BCR	C39-C30-C25	3.11	115.11	110.24
12	A	1104	UMQ	O2-C2-C3	3.10	117.69	110.38
16	D	201	SQD	C1-C2-C3	3.10	116.53	110.01
10	A	303	HEM	CHD-C1D-ND	3.09	127.76	124.44
14	B	1201	TDS	CAF-CAG-CAH	-3.08	117.58	120.60
12	A	1101	UMQ	C1-O5-C5	3.06	119.69	113.72
10	A	303	HEM	CAD-C3D-C2D	-3.06	122.14	127.87
11	B	1001	OPC	CCB-CCA-CBZ	3.05	133.99	113.36
17	G	101	BCR	C20-C19-C18	-3.03	118.07	126.36
11	A	1002	OPC	CAE-NAF-CAG	3.02	121.93	109.91
10	A	302	HEM	C4B-CHC-C1C	3.02	126.55	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	201	SQD	O5-C1-O6	3.02	117.19	110.04
10	A	303	HEM	C4D-C3D-C2D	-3.02	102.50	106.89
12	A	1102	UMQ	C2'-C3'-C4'	3.00	116.48	109.68
12	A	1101	UMQ	O2-C2-C1	2.95	117.09	110.08
10	A	303	HEM	C3B-C4B-NB	2.94	111.58	109.47
11	A	1002	OPC	CBA-CBB-CBC	2.94	129.25	114.37
10	A	301	HEM	CMA-C3A-C4A	-2.93	124.16	128.46
11	B	1001	OPC	OBJ-CBI-CAM	2.93	116.83	108.40
10	A	302	HEM	C1D-C2D-C3D	-2.92	103.91	106.98
14	B	1202	TDS	CAP-CAH-CAG	2.92	119.88	116.64
10	C	301	HEM	C4B-CHC-C1C	-2.92	118.71	122.56
13	B	201	CLA	C6-C7-C8	2.92	125.66	115.97
16	D	201	SQD	C33-C32-C31	2.92	129.11	114.37
14	B	1202	TDS	CAF-CAG-CAH	-2.90	117.75	120.60
11	B	1001	OPC	CBP-CBQ-CBR	2.89	128.81	112.60
12	A	1103	UMQ	O1-C1-C2	2.88	115.18	108.09
12	A	1103	UMQ	C1'-C2'-C3'	2.88	116.07	110.01
14	B	1202	TDS	CAT-CAU-CAV	2.84	128.71	114.37
10	A	303	HEM	CAA-CBA-CGA	2.82	121.42	113.83
12	A	1103	UMQ	C1-O5-C5	2.81	119.20	113.72
13	B	201	CLA	O2A-C1-C2	2.81	118.91	108.11
11	A	1002	OPC	CBG-NAF-CAE	2.79	116.31	108.98
10	A	303	HEM	C4D-ND-C1D	2.79	108.51	105.21
12	A	1103	UMQ	O3'-C3'-C4'	2.78	117.07	109.94
16	D	201	SQD	O49-C7-C8	-2.78	112.92	123.78
10	A	301	HEM	C4C-CHD-C1D	2.77	126.22	122.56
12	A	1101	UMQ	C1'-O5'-C5'	2.75	119.10	113.72
11	B	1001	OPC	CBW-CBV-CBU	2.74	128.22	114.37
11	A	1002	OPC	CBG-NAF-CAG	2.68	120.58	109.91
10	A	302	HEM	CBD-CAD-C3D	2.66	119.89	112.53
16	D	201	SQD	O47-C7-O49	-2.58	117.67	123.70
12	A	1103	UMQ	O5'-C1'-C2'	2.58	115.67	110.37
11	B	1001	OPC	CBY-CBX-CBW	2.57	127.36	114.37
12	A	1101	UMQ	O3'-C3'-C2'	2.56	116.40	110.38
10	A	301	HEM	CMC-C2C-C3C	2.55	129.78	124.68
10	A	301	HEM	CMD-C2D-C3D	-2.55	119.25	126.15
10	A	302	HEM	CHC-C4B-NB	2.54	127.17	124.44
10	C	301	HEM	C1B-NB-C4B	2.54	108.21	105.21
12	A	1101	UMQ	C3'-C4'-C5'	-2.53	105.32	110.93
14	B	1202	TDS	CAR-CAQ-CAP	2.50	118.79	112.85
16	D	201	SQD	C19-C18-C17	2.50	127.02	114.37
10	A	301	HEM	O2D-CGD-CBD	2.50	121.89	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1202	TDS	CBC-CBB-CBA	2.50	130.21	113.36
16	D	201	SQD	C46-O48-C23	2.49	126.22	117.12
10	A	303	HEM	CHD-C1D-C2D	-2.49	121.10	125.03
11	A	1002	OPC	CBY-CBX-CBW	-2.49	101.80	114.37
12	A	1101	UMQ	O4-C4-C3	-2.47	104.56	110.38
12	A	1102	UMQ	O6'-C6'-C5'	2.46	119.71	111.33
16	D	201	SQD	C34-C33-C32	2.46	126.79	114.37
10	A	301	HEM	CAB-C3B-C2B	-2.46	120.44	128.43
13	B	201	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
11	B	1001	OPC	CBZ-CBY-CBX	2.45	126.78	114.37
11	B	1001	OPC	OAI-CAH-CAG	2.42	121.28	109.65
17	G	101	BCR	C15-C16-C17	2.40	128.44	123.52
14	B	1201	TDS	CAR-CAS-CAT	2.40	126.49	114.37
17	G	101	BCR	C34-C9-C10	-2.40	118.93	122.82
14	B	1201	TDS	CAE-CAF-CAN	2.39	120.09	115.08
12	A	1103	UMQ	O2-C2-C1	2.38	115.74	110.08
14	B	1201	TDS	CAS-CAR-CAQ	-2.37	103.85	113.74
12	A	1104	UMQ	O3-C3-C2	2.37	115.95	110.38
10	A	303	HEM	O2A-CGA-O1A	2.37	129.41	123.33
16	D	201	SQD	O8-S-C6	2.36	110.52	105.97
12	A	1104	UMQ	C6'-C5'-C4'	2.35	120.00	113.38
11	A	1002	OPC	CBU-CBT-CBS	2.35	125.74	112.60
14	B	1202	TDS	CAV-CAW-CAX	2.33	126.16	114.37
10	A	301	HEM	CAD-C3D-C2D	-2.33	123.51	127.87
10	A	303	HEM	O1A-CGA-CBA	-2.31	115.75	123.09
12	A	1101	UMQ	C4-C3-C2	-2.31	106.78	110.83
12	A	1102	UMQ	C4-C3-C2	2.29	114.85	110.83
13	B	201	CLA	C7-C6-C5	-2.28	107.18	113.26
10	C	301	HEM	C1D-C2D-C3D	-2.28	104.58	106.98
11	B	1001	OPC	CBA-CBB-CBC	2.28	125.89	114.37
10	A	301	HEM	C4B-CHC-C1C	2.28	125.56	122.56
16	D	201	SQD	C45-O47-C7	-2.27	112.36	117.80
11	B	1001	OPC	CBM-CBL-CBK	2.25	121.95	113.69
11	A	1002	OPC	CAQ-CAP-CAO	2.25	121.93	113.69
17	G	101	BCR	C37-C22-C23	2.25	121.52	118.09
12	A	1104	UMQ	O1-C4'-C3'	2.24	112.92	107.23
14	B	1202	TDS	CAY-CAZ-CBA	2.24	125.69	114.37
11	B	1001	OPC	CBT-CBS-CBR	2.24	141.61	124.83
12	A	1101	UMQ	C1-C2-C3	-2.22	105.33	110.01
13	B	201	CLA	CAC-C3C-C2C	2.22	131.64	127.56
13	B	201	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
13	B	201	CLA	C3A-C2A-C1A	2.21	104.64	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	301	HEM	CHB-C1B-C2B	-2.19	120.74	126.94
13	B	201	CLA	CBA-CAA-C2A	-2.18	107.29	113.79
12	A	1103	UMQ	O5-C5-C6	2.17	111.81	106.44
12	A	1104	UMQ	C1-O5-C5	2.16	117.94	113.72
12	A	1103	UMQ	C3-C4-C5	2.16	114.15	110.23
12	A	1101	UMQ	C3-C4-C5	2.14	114.12	110.23
14	B	1201	TDS	CAP-CAH-CAG	2.14	119.02	116.64
11	B	1001	OPC	CBO-CBN-CBM	2.14	125.17	114.37
17	G	101	BCR	C31-C1-C6	-2.14	106.89	110.24
12	A	1101	UMQ	O6-C6-C5	2.13	118.58	111.33
17	G	101	BCR	C30-C25-C26	2.12	125.53	122.64
13	B	201	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
17	G	101	BCR	C32-C1-C31	-2.10	102.61	108.63
13	B	201	CLA	C1C-C2C-C3C	-2.10	104.77	106.98
17	G	101	BCR	C7-C6-C5	2.09	126.37	121.56
12	A	1101	UMQ	CI-CH-CG	-2.09	103.81	114.37
10	A	301	HEM	CMA-C3A-C2A	2.08	128.87	124.94
10	C	301	HEM	C3B-C2B-C1B	-2.07	104.86	106.41
13	B	201	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
11	B	1001	OPC	CAY-CAZ-CBA	2.07	124.82	114.37
17	G	101	BCR	C27-C26-C25	-2.06	119.92	122.70
12	A	1104	UMQ	O5'-C1'-O1'	2.06	114.91	110.04
11	B	1001	OPC	CBX-CBW-CBV	2.03	124.62	114.37
10	A	301	HEM	C1B-NB-C4B	-2.01	102.83	105.21

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1101	UMQ	C1'
12	A	1101	UMQ	C2'
12	A	1102	UMQ	C1'
12	A	1102	UMQ	C2'
12	A	1103	UMQ	C1'
12	A	1103	UMQ	C2'
12	A	1104	UMQ	C1'
12	A	1104	UMQ	C2'
13	B	201	CLA	ND
13	B	201	CLA	C8
16	D	201	SQD	C4
16	D	201	SQD	C5
16	D	201	SQD	C3

All (193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	301	HEM	C1A-C2A-CAA-CBA
10	A	301	HEM	C3A-C2A-CAA-CBA
10	A	302	HEM	C1A-C2A-CAA-CBA
10	A	302	HEM	C2D-C3D-CAD-CBD
10	A	302	HEM	C4D-C3D-CAD-CBD
10	A	303	HEM	C2D-C3D-CAD-CBD
10	A	303	HEM	C4D-C3D-CAD-CBD
11	A	1002	OPC	OAN-CAM-CBI-OBJ
11	A	1002	OPC	CAM-CAL-OAK-PAJ
11	A	1002	OPC	CAL-OAK-PAJ-OBH
11	A	1002	OPC	CAL-OAK-PAJ-OAB
11	A	1002	OPC	CAL-OAK-PAJ-OAI
11	A	1002	OPC	CAH-OAI-PAJ-OBH
11	A	1002	OPC	CAH-OAI-PAJ-OAB
11	A	1002	OPC	NAF-CAG-CAH-OAI
11	A	1002	OPC	CBO-CBP-CBQ-CBR
11	B	1001	OPC	CAH-OAI-PAJ-OAK
11	B	1001	OPC	CAH-OAI-PAJ-OBH
11	B	1001	OPC	NAF-CAG-CAH-OAI
11	B	1001	OPC	CBO-CBP-CBQ-CBR
12	A	1101	UMQ	O5'-C1'-O1'-CA
12	A	1102	UMQ	C2'-C1'-O1'-CA
12	A	1103	UMQ	O5'-C1'-O1'-CA
12	A	1104	UMQ	C3'-C4'-O1-C1
12	A	1104	UMQ	O5'-C1'-O1'-CA
13	B	201	CLA	O2A-C1-C2-C3
14	B	1202	TDS	CAP-CAQ-CAR-CAS
14	B	1202	TDS	CAF-CAE-OAB-CAA
16	D	201	SQD	O5-C1-O6-C44
16	D	201	SQD	O5-C5-C6-S
16	D	201	SQD	C5-C6-S-O7
16	D	201	SQD	C5-C6-S-O8
16	D	201	SQD	C5-C6-S-O9
17	G	101	BCR	C1-C6-C7-C8
17	G	101	BCR	C5-C6-C7-C8
17	G	101	BCR	C6-C7-C8-C9
17	G	101	BCR	C7-C8-C9-C34
17	G	101	BCR	C23-C24-C25-C26
12	A	1104	UMQ	O5-C1-O1-C4'
12	A	1104	UMQ	C2-C1-O1-C4'
14	B	1201	TDS	CAD-CAL-OAK-CAJ
12	A	1102	UMQ	C3'-C4'-O1-C1

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Mol	Chain	Res	Type	Atoms
14	B	1201	TDS	CAM-CAL-OAK-CAJ
14	B	1201	TDS	CAD-CAE-OAB-CAA
14	B	1202	TDS	CAD-CAE-OAB-CAA
16	D	201	SQD	C24-C23-O48-C46
13	B	201	CLA	CBD-CGD-O2D-CED
16	D	201	SQD	C8-C7-O47-C45
16	D	201	SQD	O10-C23-O48-C46
11	A	1002	OPC	CAQ-CAR-CAS-CAT
16	D	201	SQD	C33-C34-C35-C36
16	D	201	SQD	C31-C32-C33-C34
16	D	201	SQD	C12-C13-C14-C15
12	A	1102	UMQ	O5'-C5'-C6'-O6'
16	D	201	SQD	C13-C14-C15-C16
12	A	1103	UMQ	O5'-C5'-C6'-O6'
12	A	1104	UMQ	O5-C5-C6-O6
14	B	1201	TDS	CAF-CAE-OAB-CAA
16	D	201	SQD	O49-C7-O47-C45
14	B	1202	TDS	CAS-CAT-CAU-CAV
12	A	1103	UMQ	C4'-C5'-C6'-O6'
17	G	101	BCR	C37-C22-C23-C24
17	G	101	BCR	C7-C8-C9-C10
17	G	101	BCR	C21-C22-C23-C24
11	A	1002	OPC	CBM-CBN-CBO-CBP
11	B	1001	OPC	CAZ-CBA-CBB-CBC
13	B	201	CLA	C8-C10-C11-C12
12	A	1101	UMQ	O5'-C5'-C6'-O6'
12	A	1104	UMQ	C4-C5-C6-O6
12	A	1101	UMQ	O1'-CA-CB-CC
12	A	1104	UMQ	O1'-CA-CB-CC
13	B	201	CLA	C10-C11-C12-C13
17	G	101	BCR	C22-C23-C24-C25
11	A	1002	OPC	CBU-CBV-CBW-CBX
12	A	1101	UMQ	C4'-C5'-C6'-O6'
12	A	1102	UMQ	C4'-C5'-C6'-O6'
11	B	1001	OPC	CAP-CAO-OAN-CAM
16	D	201	SQD	C10-C11-C12-C13
11	A	1002	OPC	CAH-CAG-NAF-CAA
13	B	201	CLA	O1D-CGD-O2D-CED
13	B	201	CLA	C15-C16-C17-C18
12	A	1102	UMQ	C4-C5-C6-O6
12	A	1102	UMQ	O5-C5-C6-O6
12	A	1104	UMQ	CB-CC-CD-CF

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Mol	Chain	Res	Type	Atoms
11	B	1001	OPC	CAY-CAZ-CBA-CBB
12	A	1102	UMQ	C5'-C4'-O1-C1
11	A	1002	OPC	CBL-CBM-CBN-CBO
11	A	1002	OPC	CBV-CBW-CBX-CBY
13	B	201	CLA	C3A-C2A-CAA-CBA
11	B	1001	OPC	CBT-CBU-CBV-CBW
11	A	1002	OPC	CBY-CBZ-CCA-CCB
12	A	1103	UMQ	CG-CH-CI-CJ
16	D	201	SQD	C29-C30-C31-C32
11	A	1002	OPC	CBT-CBU-CBV-CBW
14	B	1202	TDS	CAY-CAZ-CBA-CBB
16	D	201	SQD	C15-C16-C17-C18
11	B	1001	OPC	CAH-CAG-NAF-CAE
11	A	1002	OPC	CBW-CBX-CBY-CBZ
17	G	101	BCR	C23-C24-C25-C30
12	A	1102	UMQ	CI-CJ-CK-CL
11	B	1001	OPC	OAD-CAO-OAN-CAM
16	D	201	SQD	C11-C12-C13-C14
11	A	1002	OPC	CAZ-CBA-CBB-CBC
11	B	1001	OPC	CBC-CBD-CBE-CBF
12	A	1101	UMQ	CF-CG-CH-CI
16	D	201	SQD	C28-C29-C30-C31
12	A	1103	UMQ	CF-CG-CH-CI
14	B	1201	TDS	CAT-CAU-CAV-CAW
11	B	1001	OPC	CBU-CBV-CBW-CBX
14	B	1201	TDS	CAR-CAS-CAT-CAU
12	A	1103	UMQ	C4-C5-C6-O6
12	A	1101	UMQ	CA-CB-CC-CD
14	B	1201	TDS	CAW-CAX-CAY-CAZ
13	B	201	CLA	C1A-C2A-CAA-CBA
11	B	1001	OPC	CBK-CBL-CBM-CBN
14	B	1202	TDS	CAU-CAV-CAW-CAX
12	A	1102	UMQ	CC-CD-CF-CG
11	A	1002	OPC	CAW-CAX-CAY-CAZ
13	B	201	CLA	C4-C3-C5-C6
12	A	1104	UMQ	CH-CI-CJ-CK
12	A	1104	UMQ	CI-CJ-CK-CL
11	A	1002	OPC	CBC-CBD-CBE-CBF
12	A	1104	UMQ	CG-CH-CI-CJ
14	B	1202	TDS	CAR-CAS-CAT-CAU
14	B	1202	TDS	CAM-CAL-OAK-CAJ
16	D	201	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
16	D	201	SQD	C2-C1-O6-C44
13	B	201	CLA	C2-C3-C5-C6
16	D	201	SQD	C25-C26-C27-C28
12	A	1101	UMQ	CC-CD-CF-CG
16	D	201	SQD	C16-C17-C18-C19
14	B	1201	TDS	CAV-CAW-CAX-CAY
11	B	1001	OPC	CAS-CAT-CAU-CAV
11	B	1001	OPC	CAR-CAS-CAT-CAU
10	A	301	HEM	C2A-CAA-CBA-CGA
11	B	1001	OPC	CBL-CBM-CBN-CBO
10	A	302	HEM	C3A-C2A-CAA-CBA
11	A	1002	OPC	CAS-CAT-CAU-CAV
11	A	1002	OPC	CBX-CBY-CBZ-CCA
13	B	201	CLA	C11-C10-C8-C9
11	B	1001	OPC	CAH-CAG-NAF-CAA
12	A	1103	UMQ	CA-CB-CC-CD
12	A	1101	UMQ	O5-C1-O1-C4'
12	A	1101	UMQ	CB-CC-CD-CF
12	A	1102	UMQ	O1'-CA-CB-CC
12	A	1103	UMQ	CD-CF-CG-CH
14	B	1202	TDS	CAX-CAY-CAZ-CBA
11	A	1002	OPC	CBP-CBQ-CBR-CBS
11	A	1002	OPC	CBK-CBL-CBM-CBN
11	A	1002	OPC	CAL-CAM-CBI-OBJ
16	D	201	SQD	O6-C44-C45-C46
11	A	1002	OPC	CAH-OAI-PAJ-OAK
11	B	1001	OPC	CAH-OAI-PAJ-OAB
11	B	1001	OPC	CBP-CBQ-CBR-CBS
16	D	201	SQD	O6-C44-C45-O47
16	D	201	SQD	C14-C15-C16-C17
12	A	1102	UMQ	CB-CA-O1'-C1'
14	B	1201	TDS	CAX-CAY-CAZ-CBA
11	A	1002	OPC	CAT-CAU-CAV-CAW
10	A	301	HEM	CAA-CBA-CGA-O2A
12	A	1104	UMQ	CC-CD-CF-CG
17	G	101	BCR	C11-C10-C9-C34
10	C	301	HEM	C3D-CAD-CBD-CGD
12	A	1102	UMQ	CF-CG-CH-CI
11	B	1001	OPC	CAL-CAM-CBI-OBJ
11	B	1001	OPC	CBS-CBT-CBU-CBV
11	B	1001	OPC	CBM-CBN-CBO-CBP
10	A	301	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	G	101	BCR	C11-C10-C9-C8
14	B	1201	TDS	CAU-CAV-CAW-CAX
13	B	201	CLA	C12-C13-C15-C16
12	A	1103	UMQ	CH-CI-CJ-CK
10	A	302	HEM	CAD-CBD-CGD-O2D
12	A	1101	UMQ	CG-CH-CI-CJ
11	A	1002	OPC	CAY-CAZ-CBA-CBB
10	C	301	HEM	CAD-CBD-CGD-O2D
12	A	1104	UMQ	CD-CF-CG-CH
10	C	301	HEM	CAD-CBD-CGD-O1D
10	A	302	HEM	CAD-CBD-CGD-O1D
11	A	1002	OPC	OAK-CAL-CAM-OAN
11	A	1002	OPC	CAH-CAG-NAF-CBG
16	D	201	SQD	C44-C45-C46-O48
12	A	1103	UMQ	O5-C5-C6-O6
14	B	1202	TDS	CAT-CAU-CAV-CAW
14	B	1201	TDS	CAS-CAT-CAU-CAV
12	A	1103	UMQ	CB-CA-O1'-C1'
16	D	201	SQD	O47-C7-C8-C9
11	A	1002	OPC	OAK-CAL-CAM-CBI
14	B	1202	TDS	CAD-CAL-OAK-CAJ
12	A	1101	UMQ	C2-C1-O1-C4'
10	C	301	HEM	CAA-CBA-CGA-O2A
13	B	201	CLA	C2-C1-O2A-CGA
11	B	1001	OPC	OAD-CAO-CAP-CAQ

There are no ring outliers.

15 monomers are involved in 175 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1104	UMQ	3	0
14	B	1202	TDS	20	0
10	A	302	HEM	22	0
12	A	1102	UMQ	1	0
11	A	1002	OPC	18	0
10	A	301	HEM	17	0
14	B	1201	TDS	21	0
16	D	201	SQD	9	0
10	A	303	HEM	25	0
13	B	201	CLA	5	0
17	G	101	BCR	9	0
11	B	1001	OPC	2	0

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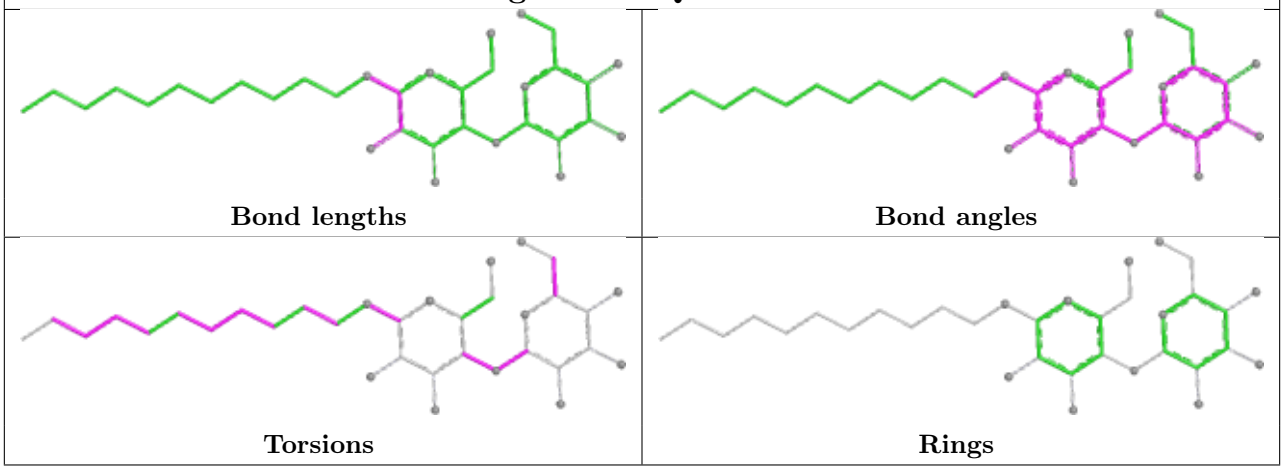
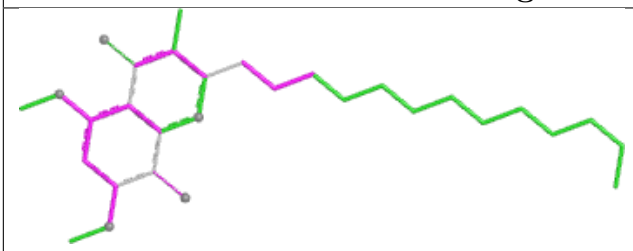
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	301	HEM	29	0
15	D	200	FES	1	0
12	A	1101	UMQ	2	0

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 then 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.

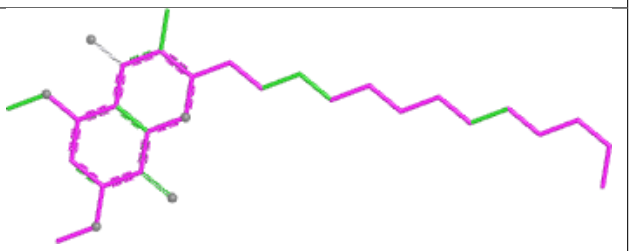
Ligand UMQ A 1104



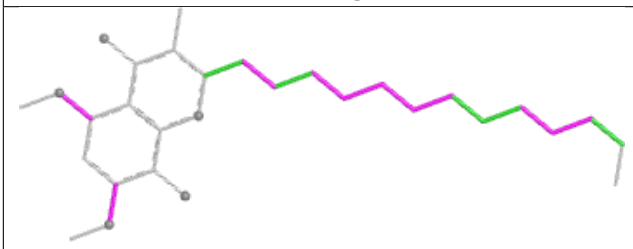
Ligand TDS B 1202



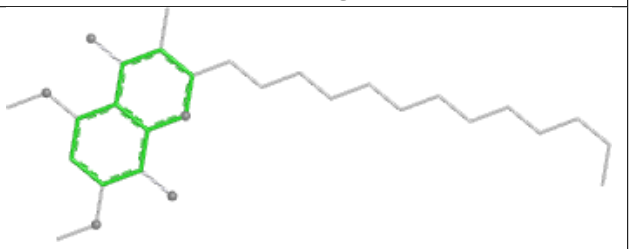
Bond lengths



Bond angles

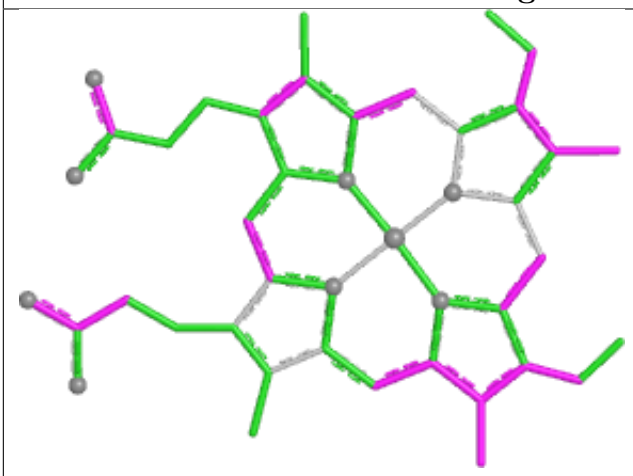


Torsions

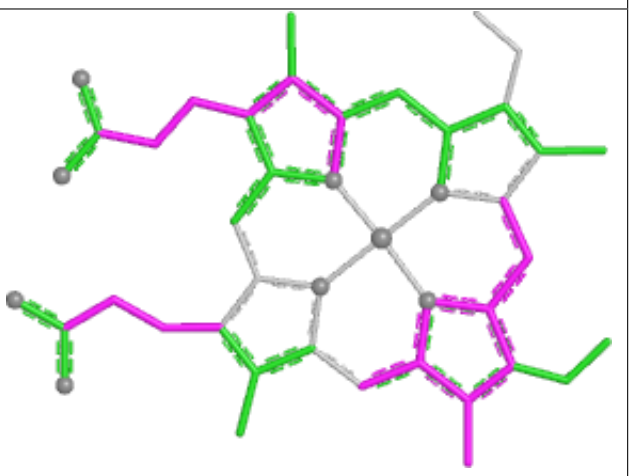


Rings

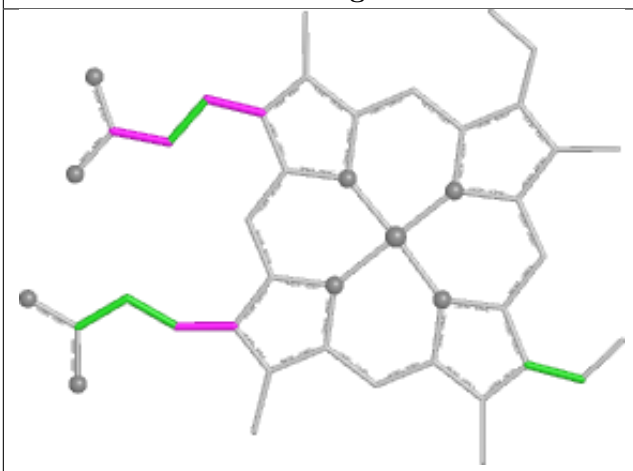
Ligand HEM A 302



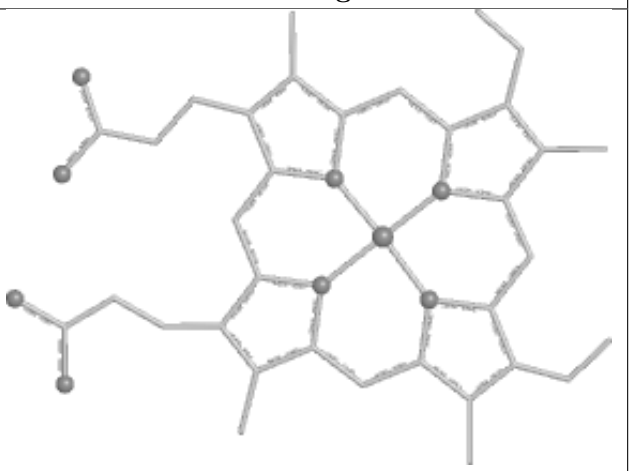
Bond lengths



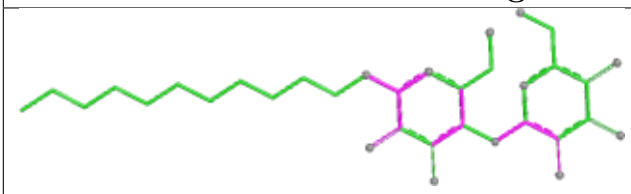
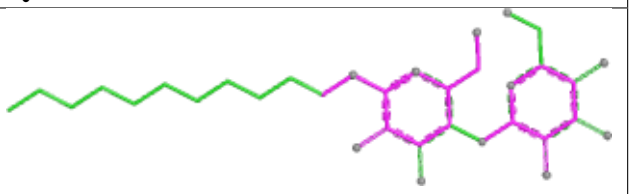
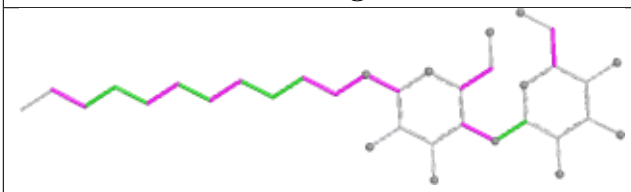
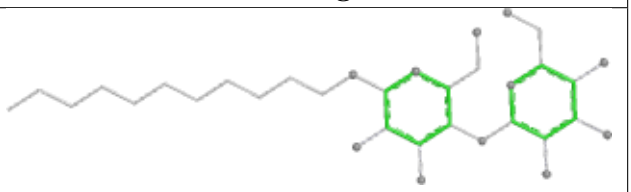
Bond angles

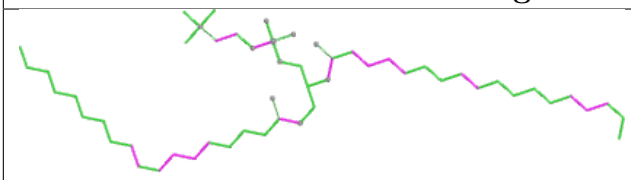
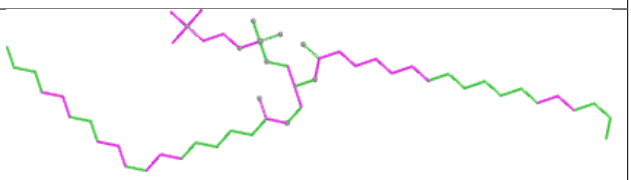
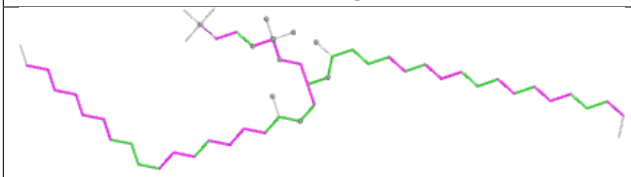
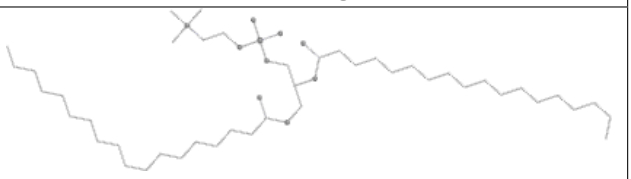


Torsions

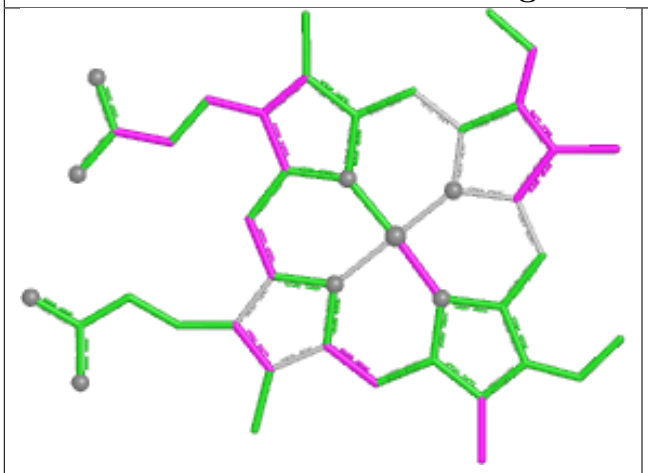


Rings

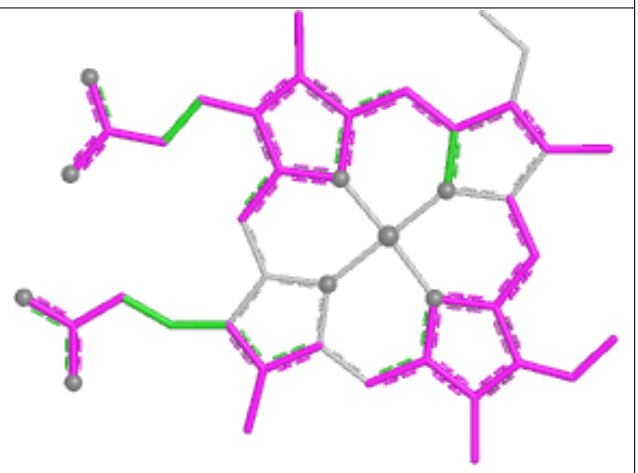
Ligand UMQ A 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OPC A 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

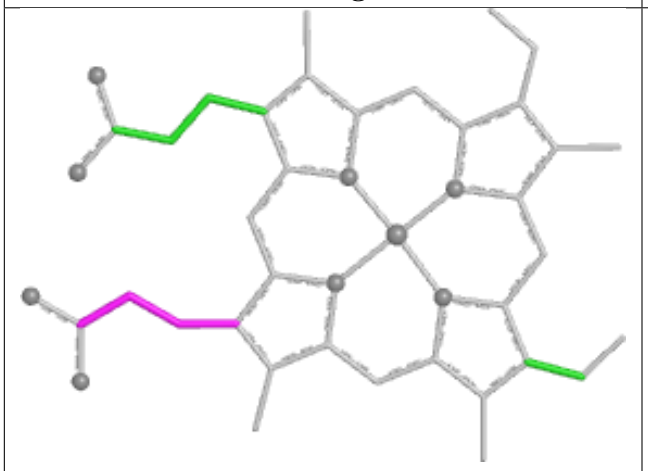
Ligand HEM A 301



Bond lengths



Bond angles



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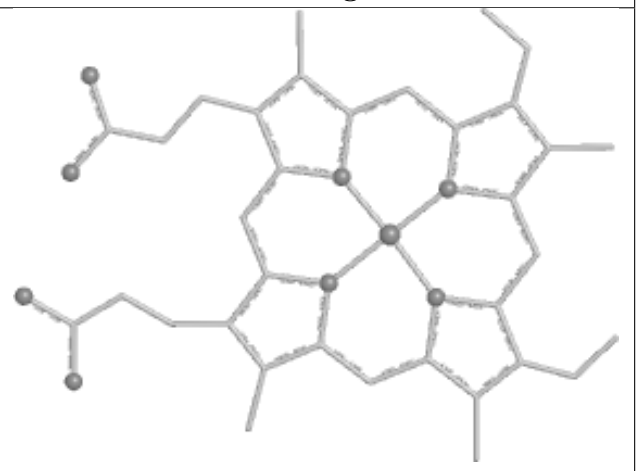
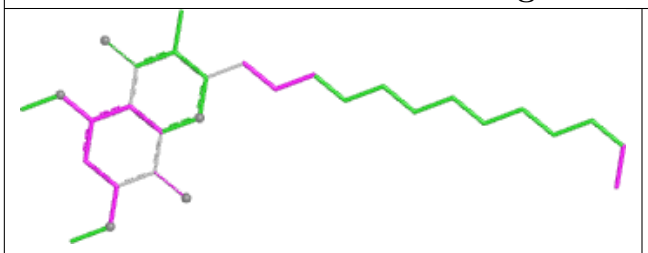


Rings

Ligand TDS B 1201



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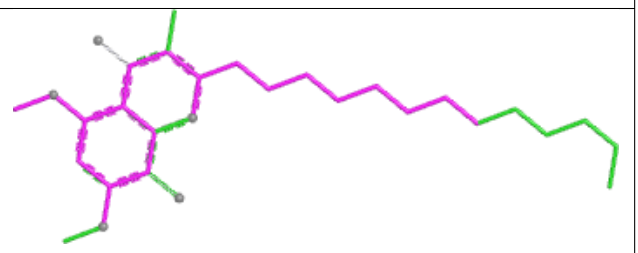
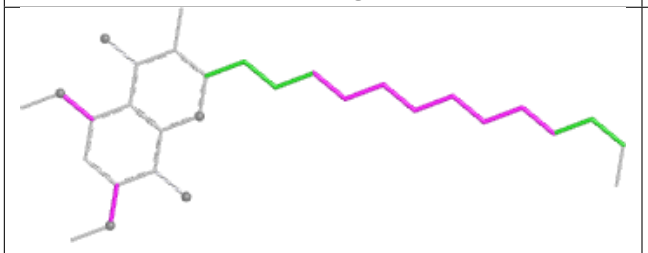


Bond angles



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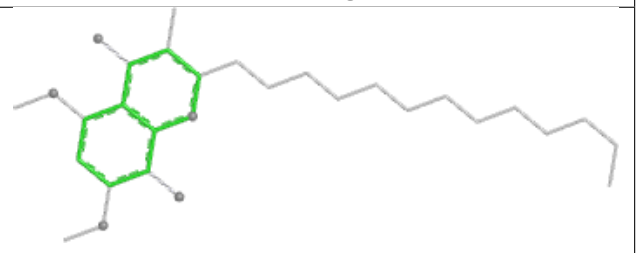
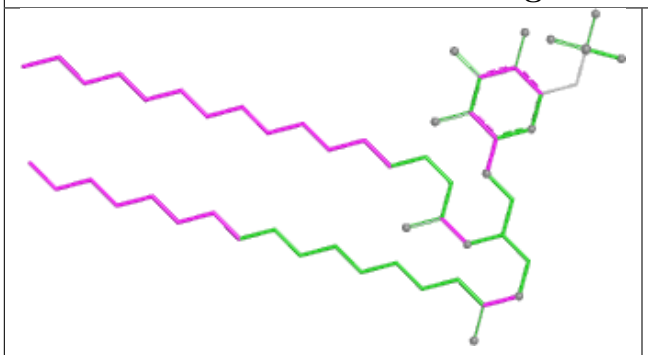


Rings

Ligand SQD D 201



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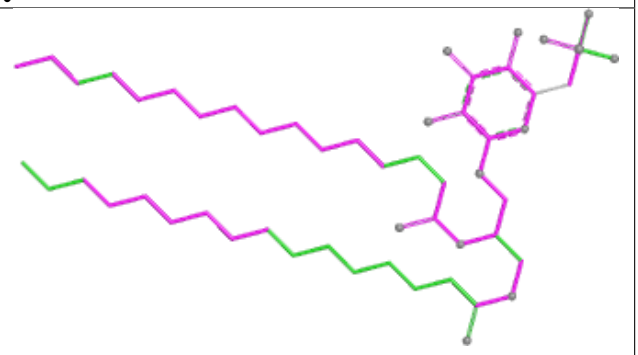

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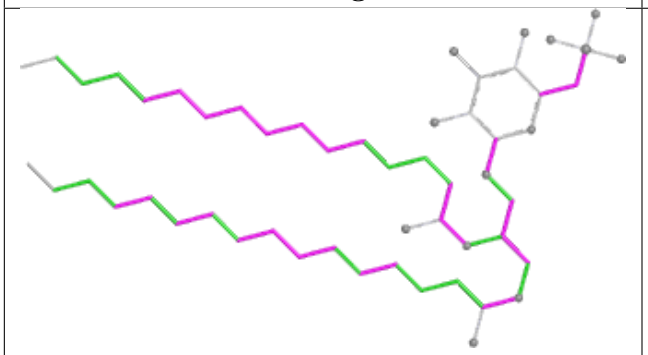

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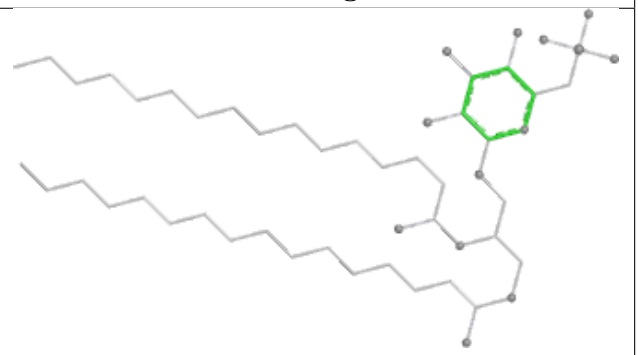
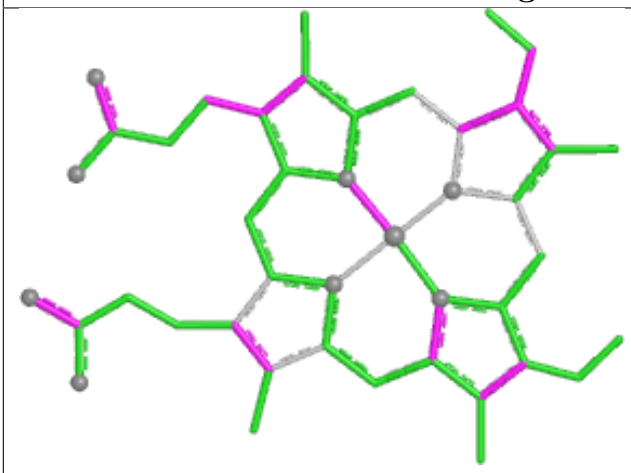


Rings

Ligand HEM A 303



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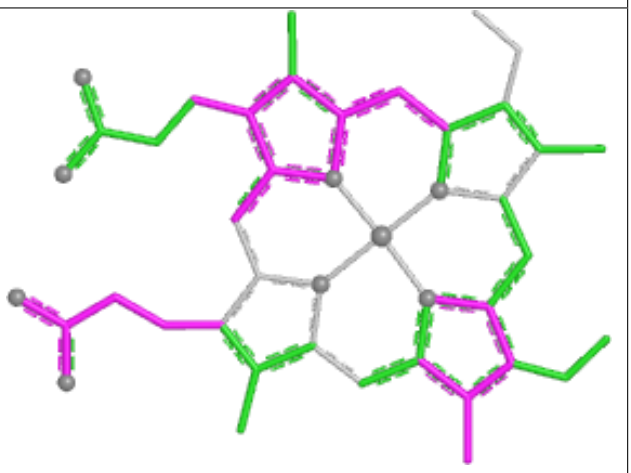
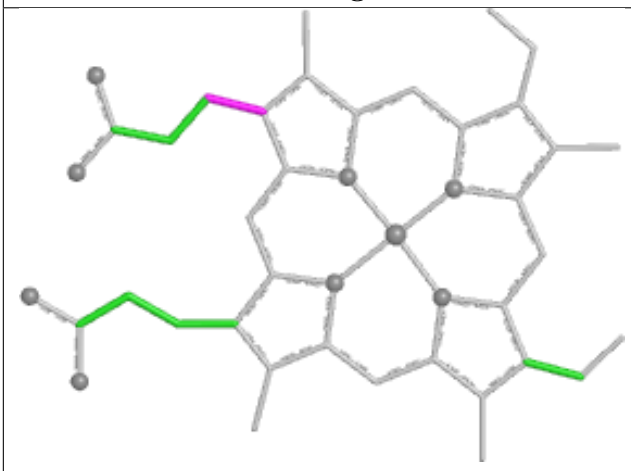


Bond angles



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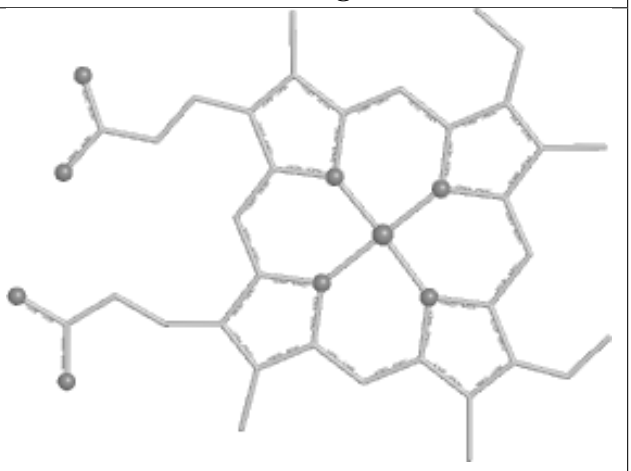
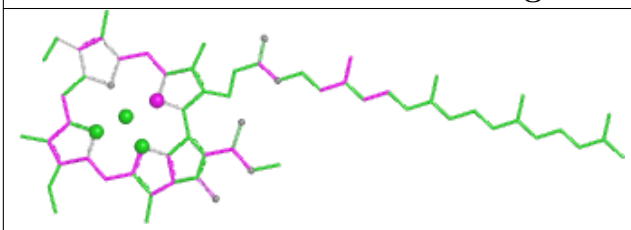
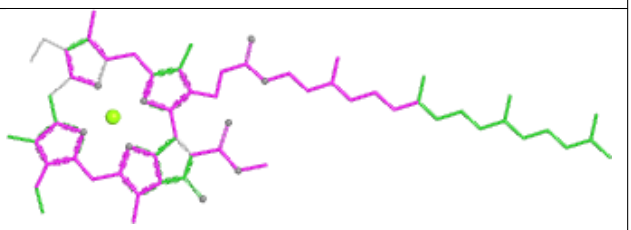


Rings

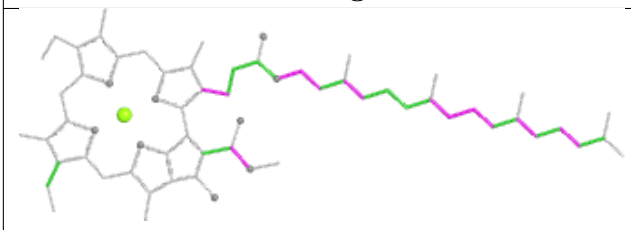
Ligand CLA B 201



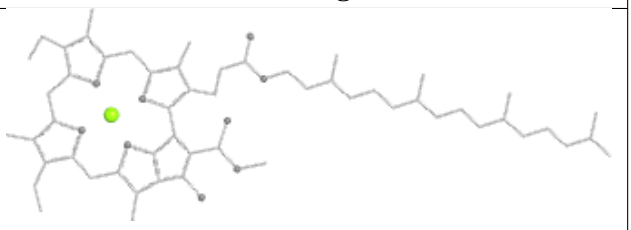
Bond lengths



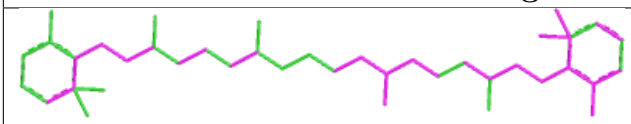
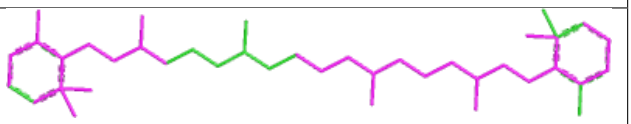
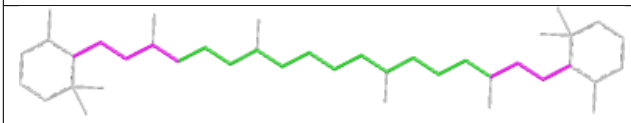
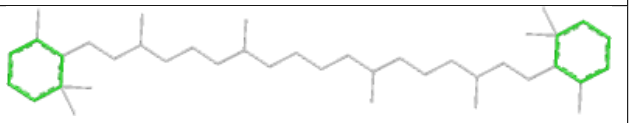
Bond angles

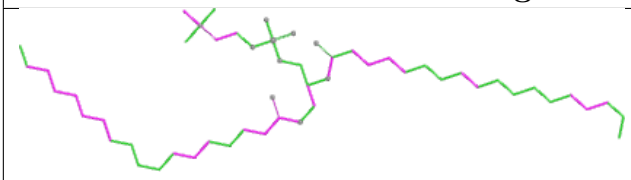
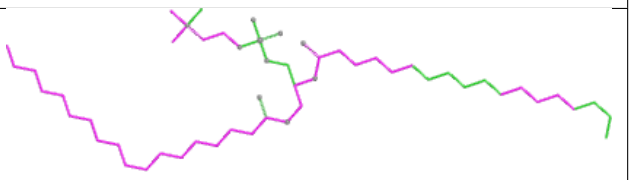
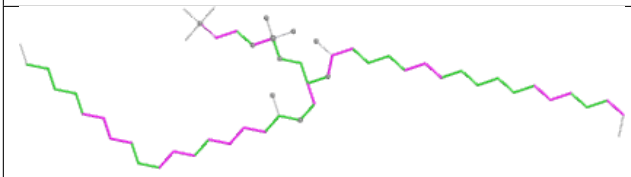
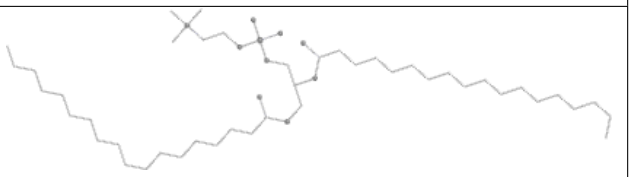


Torsions

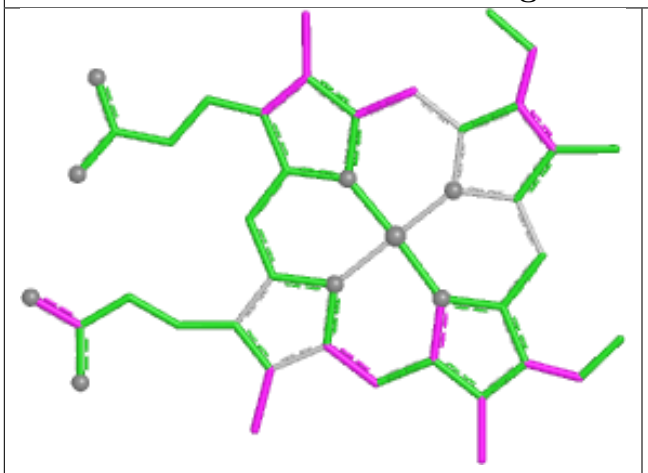


Rings

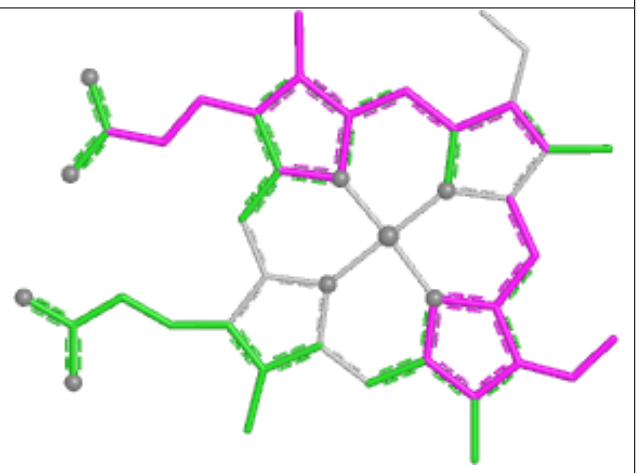
Ligand BCR G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OPC B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

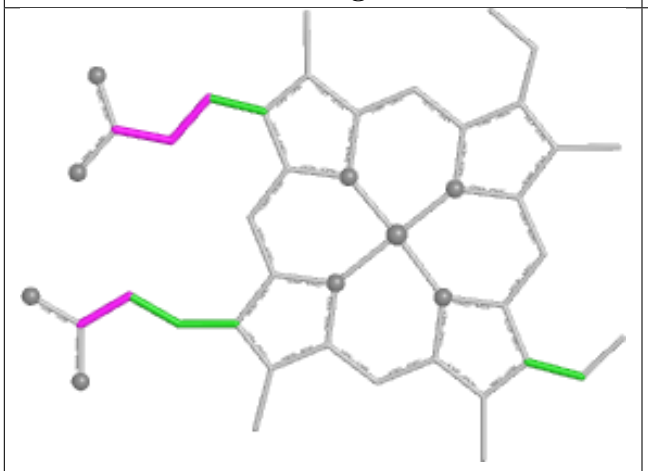
Ligand HEM C 301



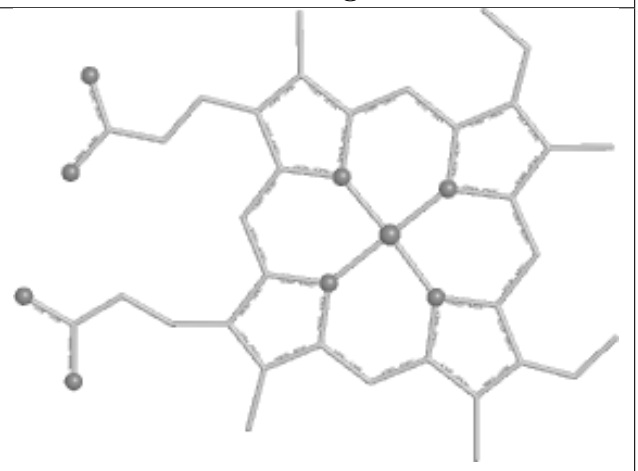
Bond lengths



Bond angles

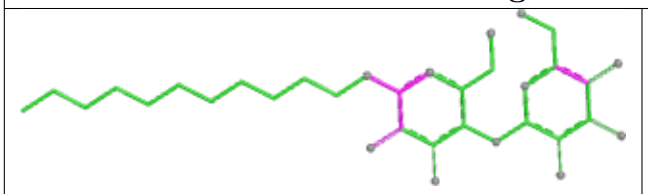


Torsions



Rings

Ligand UMQ A 1101



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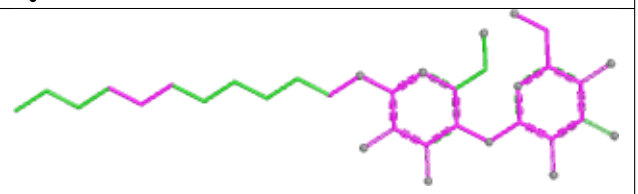
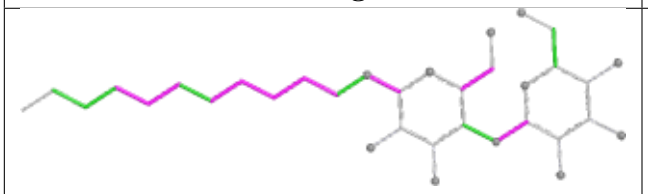


Bond angles



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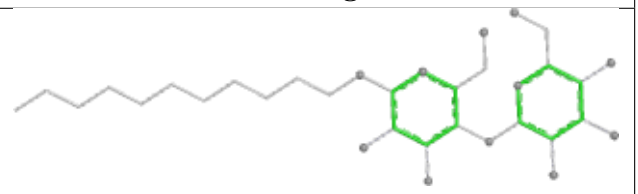
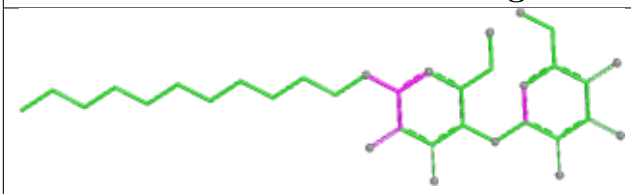
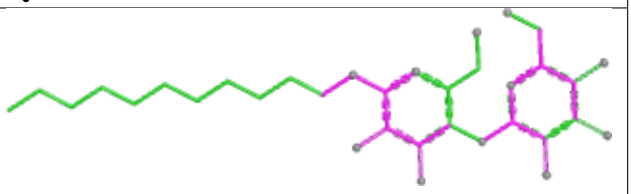
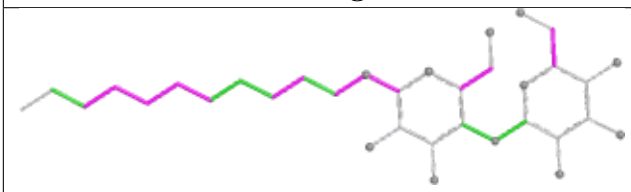
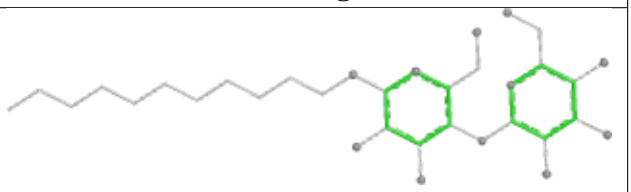


Rings

Ligand UMQ A 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	215/215 (100%)	-0.60	1 (0%) 91 90	5, 31, 72, 170	0
2	B	160/160 (100%)	-0.44	5 (3%) 49 48	22, 50, 97, 146	0
3	C	288/289 (99%)	0.10	16 (5%) 24 25	7, 55, 142, 159	1 (0%)
4	D	168/179 (93%)	0.73	18 (10%) 6 8	24, 90, 140, 156	0
5	E	32/32 (100%)	-0.17	2 (6%) 20 21	39, 63, 93, 110	0
6	F	32/35 (91%)	-0.59	0 100 100	35, 50, 112, 121	0
7	G	37/37 (100%)	-0.42	0 100 100	29, 44, 119, 138	0
8	H	29/29 (100%)	-0.62	0 100 100	31, 42, 72, 95	0
All	All	961/976 (98%)	-0.11	42 (4%) 34 34	5, 52, 132, 170	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	95	SER	13.5
4	D	96	LYS	12.6
3	C	220	SER	4.9
4	D	75	ALA	4.9
4	D	179	VAL	4.7
4	D	50	VAL	4.4
4	D	141	ARG	4.4
4	D	157	ASP	4.2
4	D	159	ASN	4.1
2	B	160	PHE	4.0
3	C	197	VAL	3.8
4	D	97	GLU	3.7
3	C	206	THR	3.6
4	D	156	GLN	3.6
4	D	67	SER	3.4
4	D	158	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	32	ILE	3.2
3	C	183	ILE	3.1
2	B	74	GLU	3.1
3	C	196	GLN	2.9
3	C	207	VAL	2.8
4	D	55	THR	2.7
4	D	161	VAL	2.7
3	C	287	MET	2.6
3	C	221	GLU	2.6
3	C	191	GLY	2.5
2	B	159	LEU	2.5
2	B	28	GLY	2.5
4	D	165	TRP	2.4
3	C	288	ASN	2.4
3	C	184	ALA	2.3
2	B	1	MET	2.3
3	C	181	THR	2.3
4	D	93	VAL	2.3
5	E	1	MET	2.2
3	C	208	VAL	2.2
3	C	73	GLY	2.2
1	A	1	MET	2.2
4	D	174	GLU	2.2
3	C	182	LYS	2.1
4	D	162	LEU	2.1
3	C	219	VAL	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

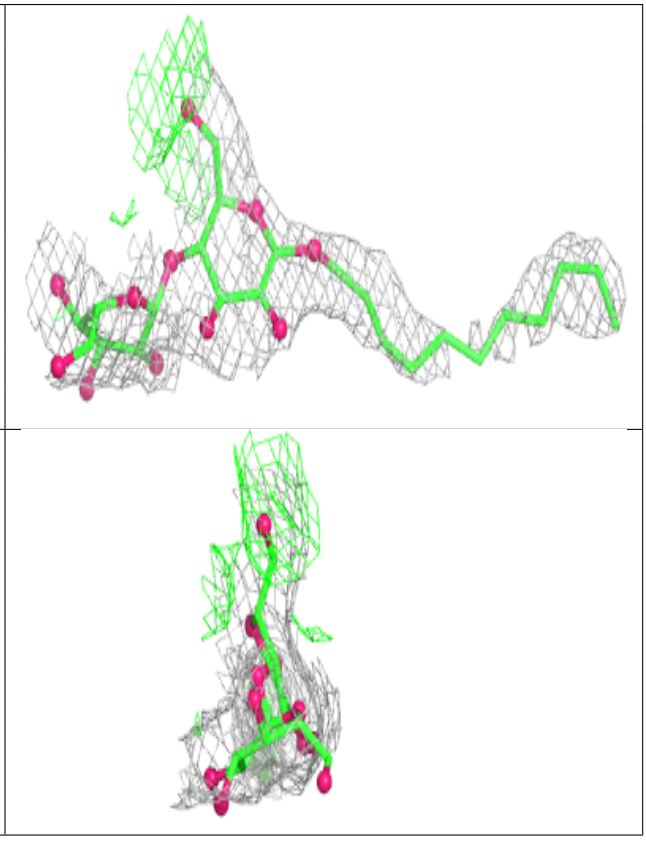
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	UMQ	A	1102	34/34	0.78	0.39	47,118,166,176	0
12	UMQ	A	1103	34/34	0.84	0.46	58,109,133,141	0
12	UMQ	A	1104	34/34	0.84	0.35	61,129,164,178	0
17	BCR	G	101	40/40	0.84	0.35	24,63,149,159	0
16	SQD	D	201	54/54	0.85	0.58	44,147,189,215	0
11	OPC	A	1002	54/55	0.88	0.39	19,84,180,191	0
12	UMQ	A	1101	34/34	0.91	0.31	18,110,147,150	0
14	TDS	B	1201	30/30	0.91	0.26	46,83,113,127	0
11	OPC	B	1001	54/55	0.94	0.39	28,80,117,123	0
13	CLA	B	201	65/65	0.95	0.20	23,51,105,119	0
14	TDS	B	1202	30/30	0.97	0.18	32,78,98,120	0
10	HEM	C	301	43/43	0.98	0.25	3,35,79,104	0
9	CD	A	216	1/1	0.99	0.08	63,63,63,63	0
10	HEM	A	301	43/43	0.99	0.16	2,21,41,74	0
15	FES	D	200	4/4	0.99	0.06	59,69,70,72	0
10	HEM	A	302	43/43	0.99	0.17	6,26,45,63	0
10	HEM	A	303	43/43	0.99	0.16	21,48,67,87	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.

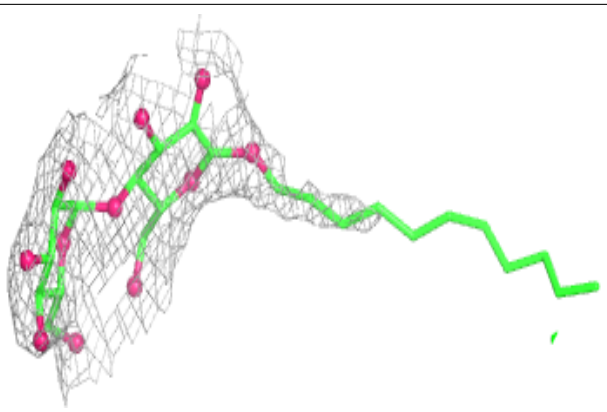
Electron density around UMQ A 1102:

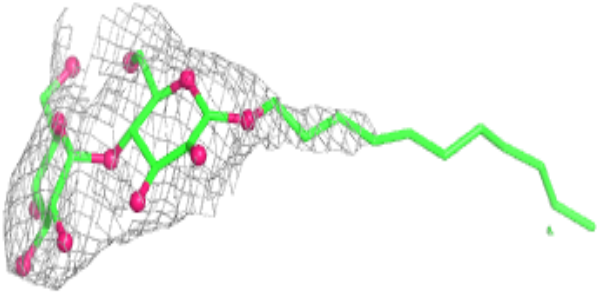
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

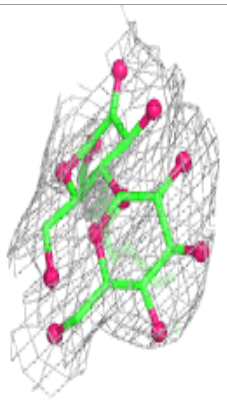


Electron density around UMQ A 1103:

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

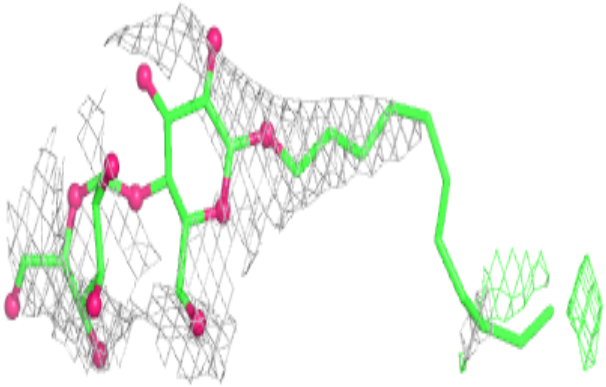


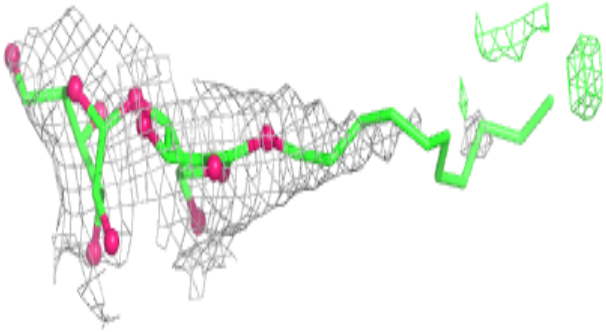




Electron density around UMQ A 1104:

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





Electron density around BCR G 101:

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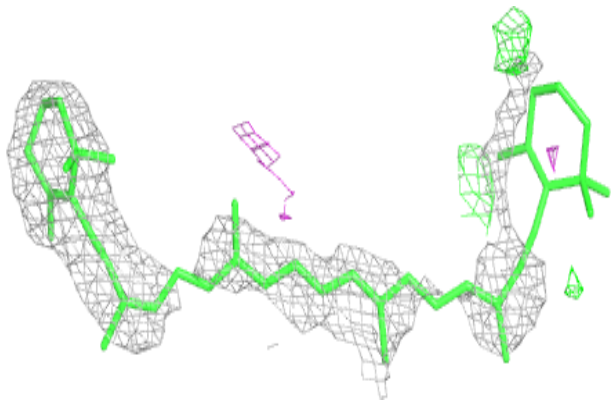
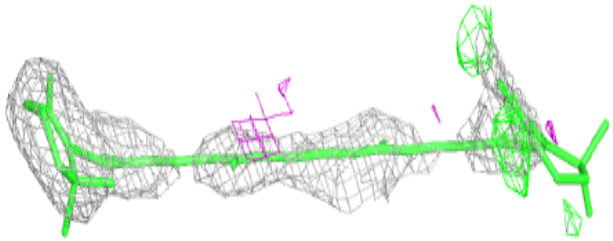
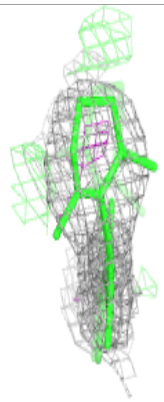
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

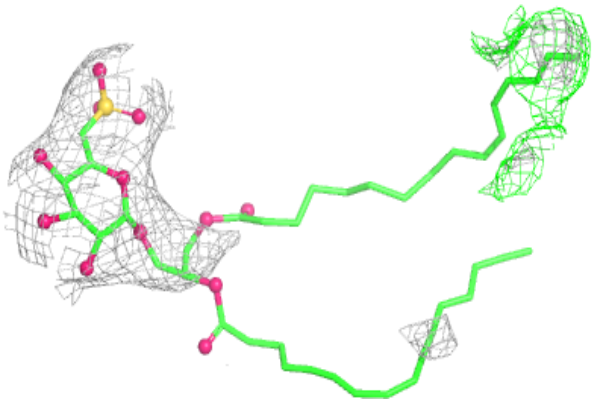


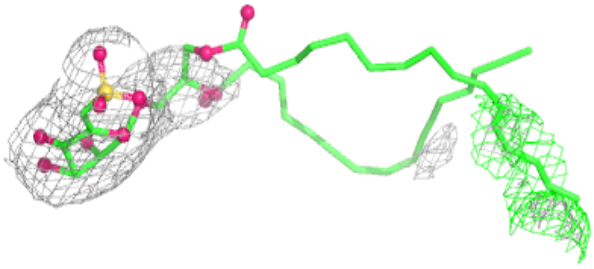


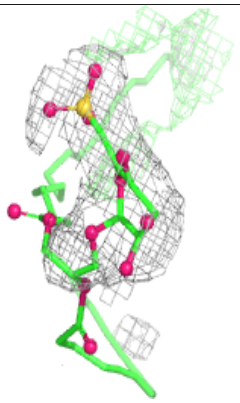


Electron density around SQD D 201:

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

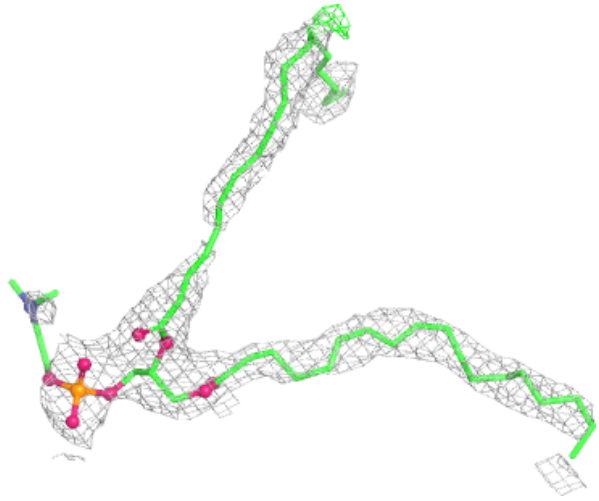


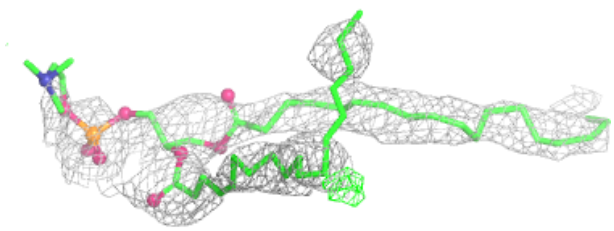


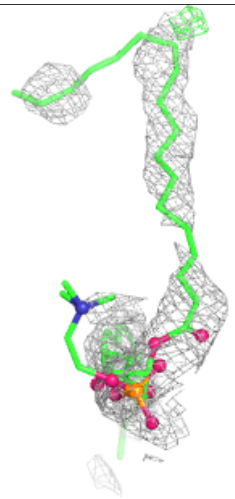


Electron density around OPC A 1002:

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

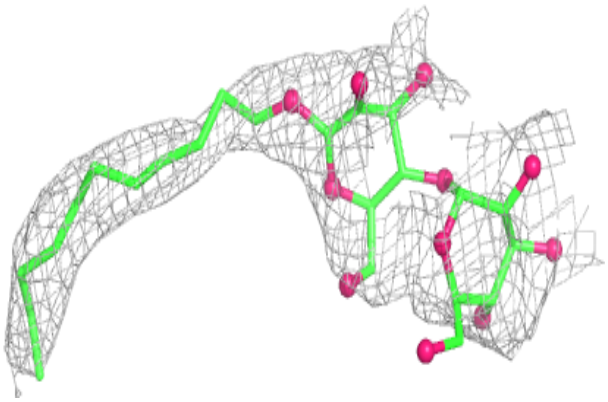


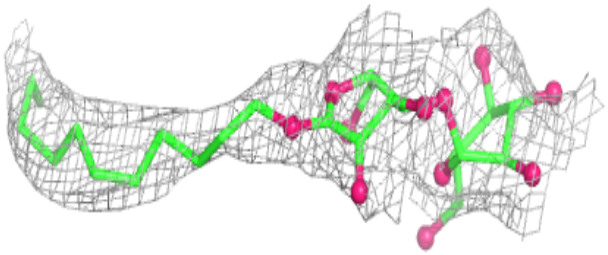


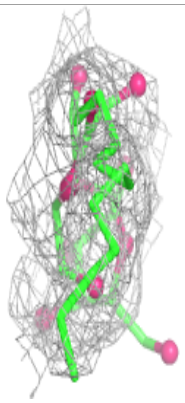


Electron density around UMQ A 1101:

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

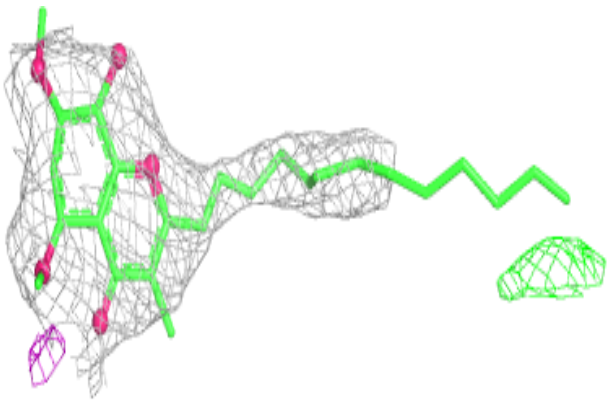


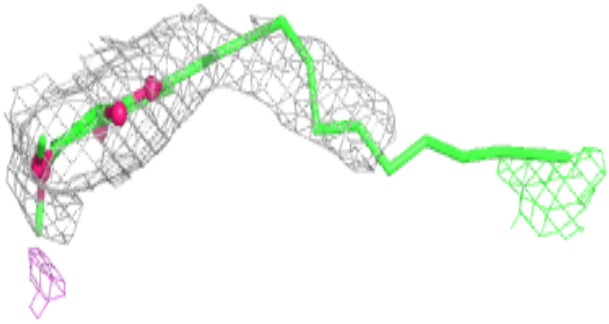


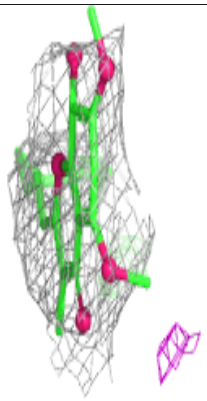


Electron density around TDS B 1201:

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

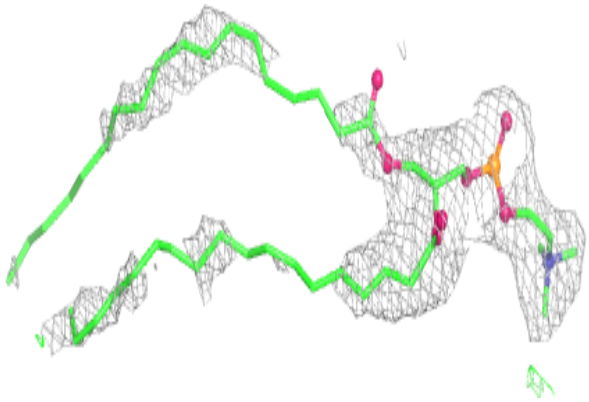


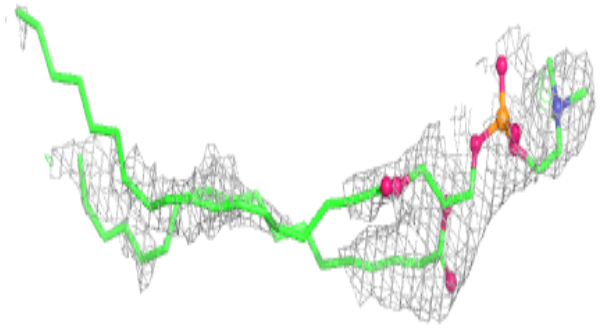


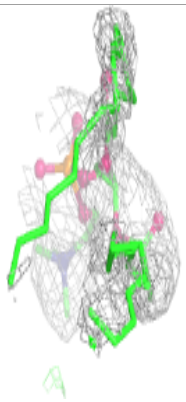


Electron density around OPC B 1001:

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

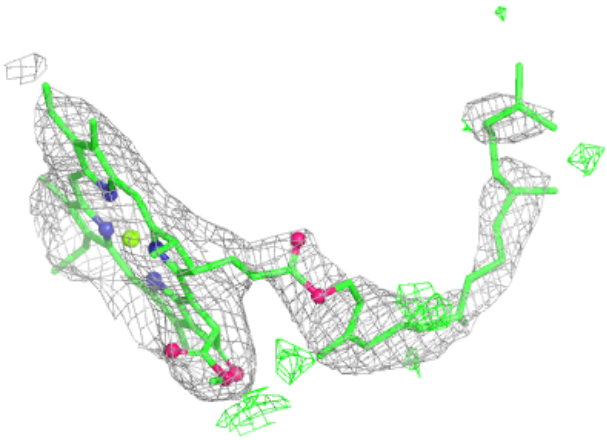


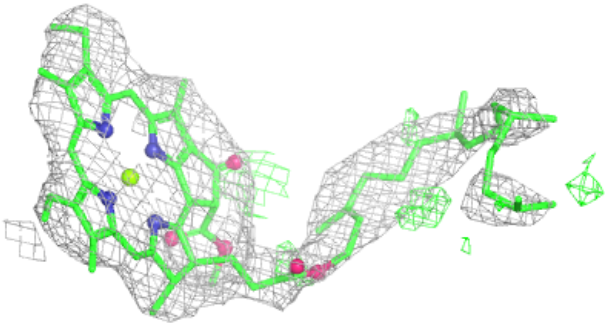


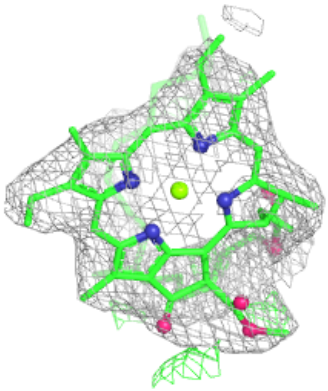


Electron density around CLA B 201:

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







Electron density around TDS B 1202:

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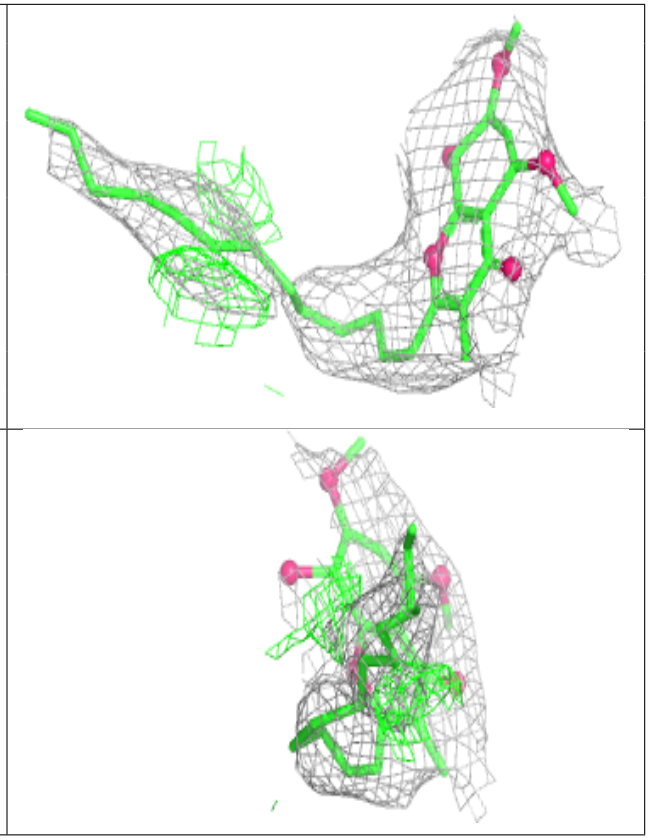
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 301:

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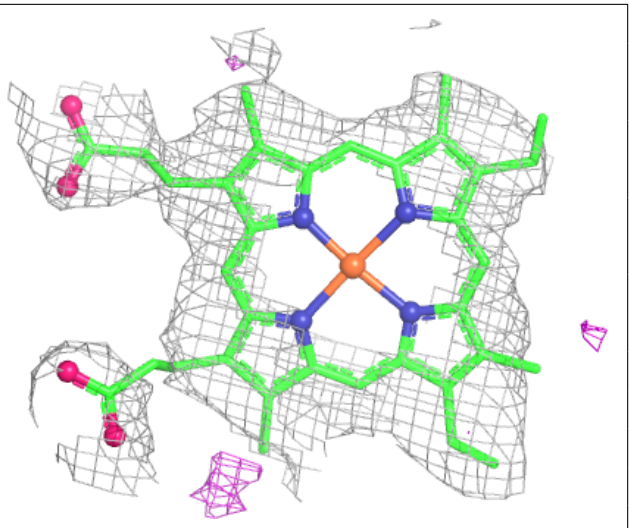
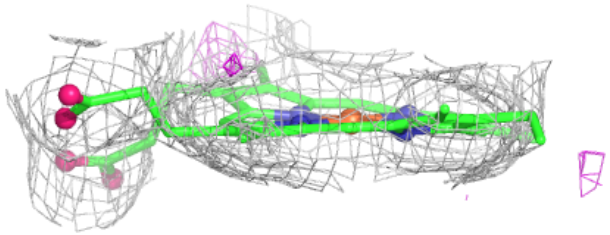
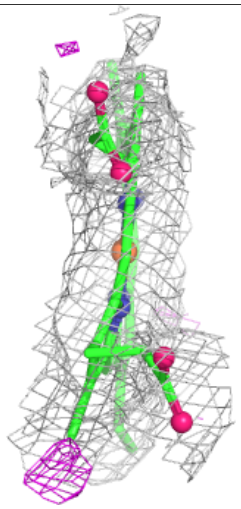
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM A 301:

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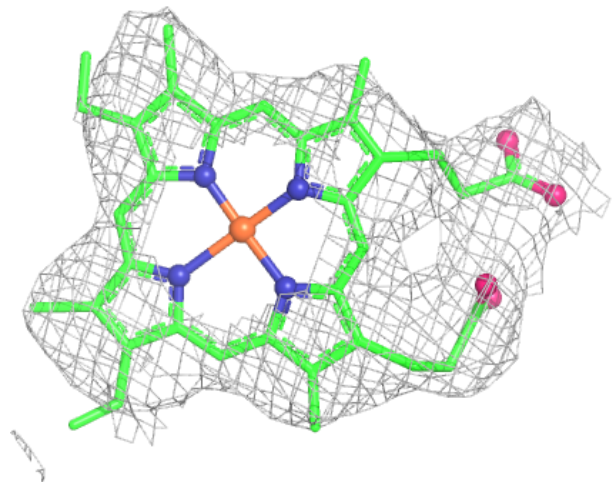
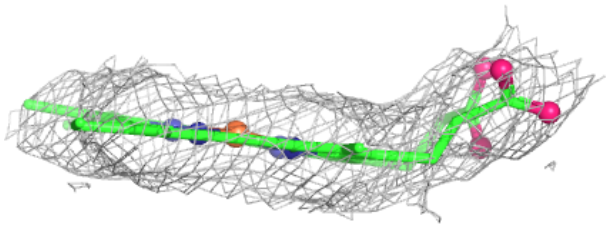
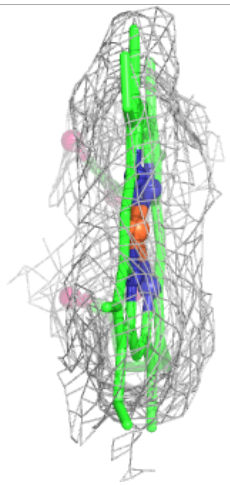
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

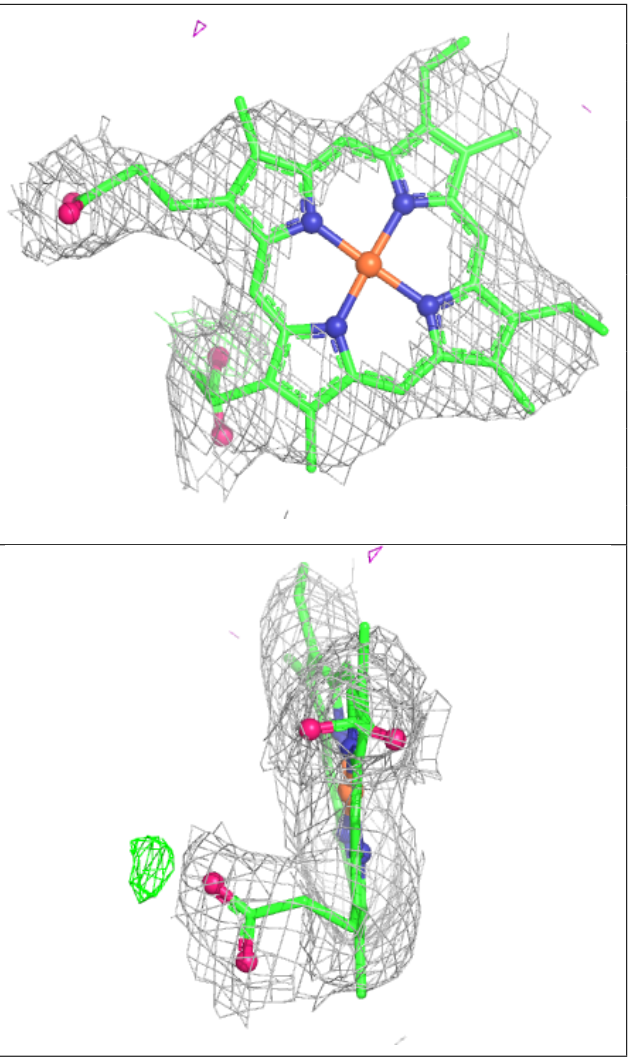






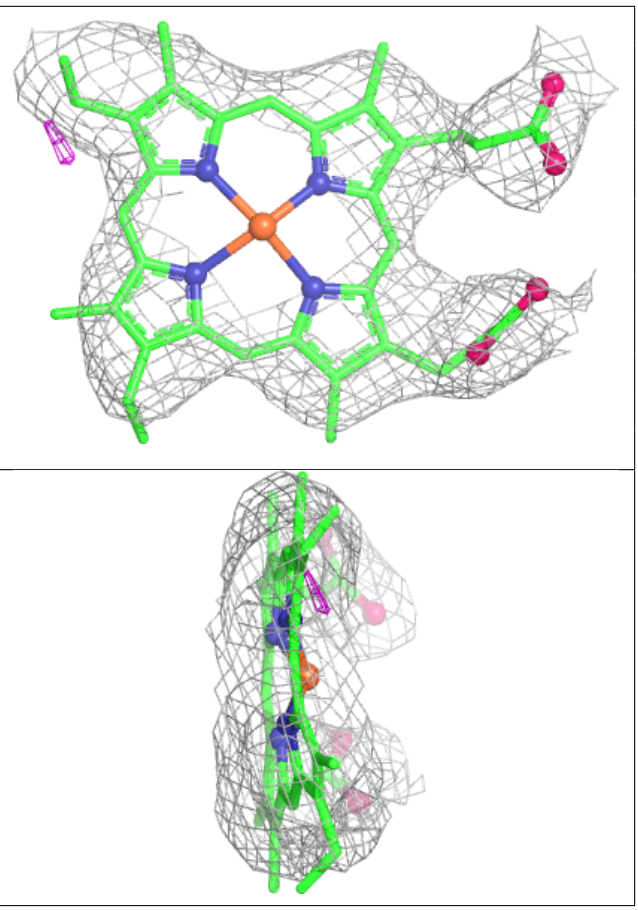
Electron density around HEM A 302:

$2mF_o$-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 A 303:

$2mF_o$-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.