



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:24 PM UTC

PDB ID : 2YIU / pdb_00002yiu
Title : X-ray structure of the dimeric cytochrome BC1 complex from the soil bacterium paracoccus denitrificans at 2.7 angstrom resolution
Authors : Kleinschroth, T.; Castellani, M.; Trinh, C.H.; Morgner, N.; Brutschy, B.; Ludwig, B.; Hunte, C.
Deposited on : 2011-05-16
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

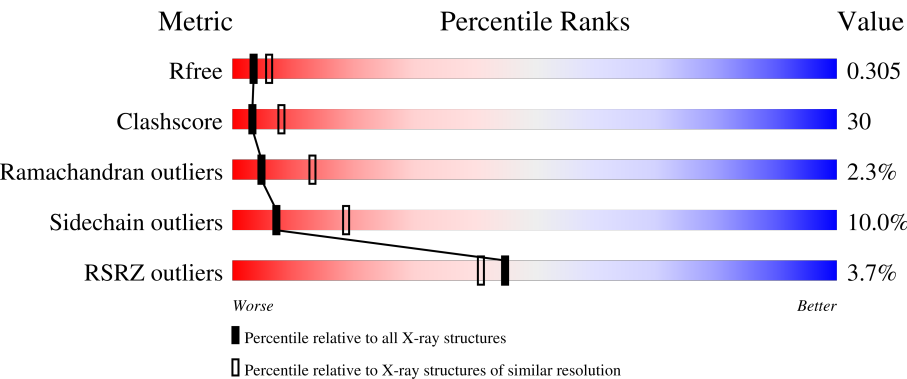
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	% 58%30%6%5%
1	D	450	% 57%31%7%5%
2	B	263	5% 38%32%8%22%
2	E	263	3% 46%26%5%22%

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Mol	Chain	Length	Quality of chain
3	C	190	6% 43% 39% 9% 8%
3	F	190	8% 46% 35% 9% 8%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12990 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 B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3439	2332	538	551	18			
1	D	428	Total	C	N	O	S	0	0	0
			3439	2332	538	551	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	HIS	-	expression tag	UNP P05418
A	442	HIS	-	expression tag	UNP P05418
A	443	HIS	-	expression tag	UNP P05418
A	444	HIS	-	expression tag	UNP P05418
A	445	HIS	-	expression tag	UNP P05418
A	446	HIS	-	expression tag	UNP P05418
A	447	HIS	-	expression tag	UNP P05418
A	448	HIS	-	expression tag	UNP P05418
A	449	HIS	-	expression tag	UNP P05418
A	450	HIS	-	expression tag	UNP P05418
D	441	HIS	-	expression tag	UNP P05418
D	442	HIS	-	expression tag	UNP P05418
D	443	HIS	-	expression tag	UNP P05418
D	444	HIS	-	expression tag	UNP P05418
D	445	HIS	-	expression tag	UNP P05418
D	446	HIS	-	expression tag	UNP P05418
D	447	HIS	-	expression tag	UNP P05418
D	448	HIS	-	expression tag	UNP P05418
D	449	HIS	-	expression tag	UNP P05418
D	450	HIS	-	expression tag	UNP P05418

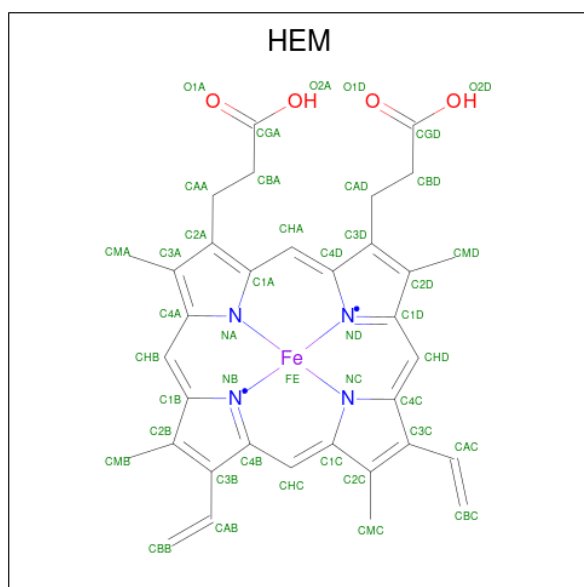
- Molecule 2 is a protein called CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total 1594	C 1020	N 264	O 301	S 9	0	0	0
2	E	206	Total 1594	C 1020	N 264	O 301	S 9	0	0	0

- Molecule 3 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

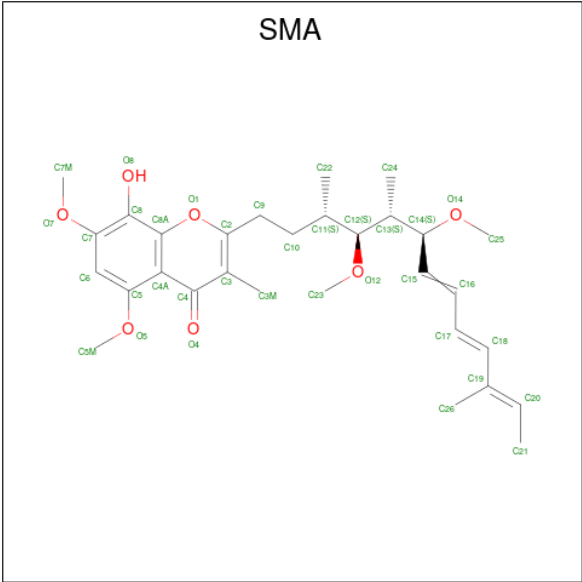
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	174	Total 1289	C 804	N 230	O 248	S 7	0	0	0
3	F	174	Total 1289	C 804	N 230	O 248	S 7	0	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



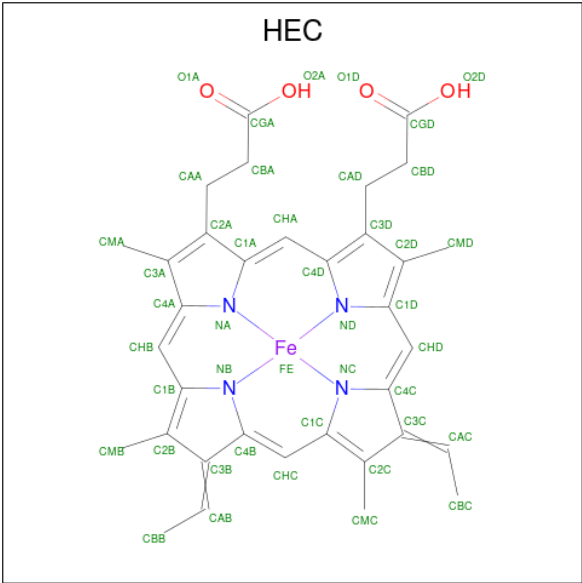
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is STIGMATELLIN A (CCD ID: SMA) (formula: $\text{C}_{30}\text{H}_{42}\text{O}_7$).



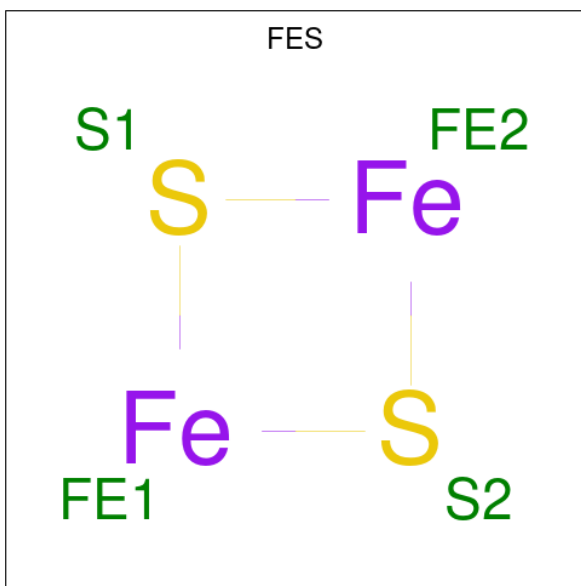
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			37	30	7			
5	D	1	Total	C	O		0	0
			37	30	7			

- Molecule 6 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



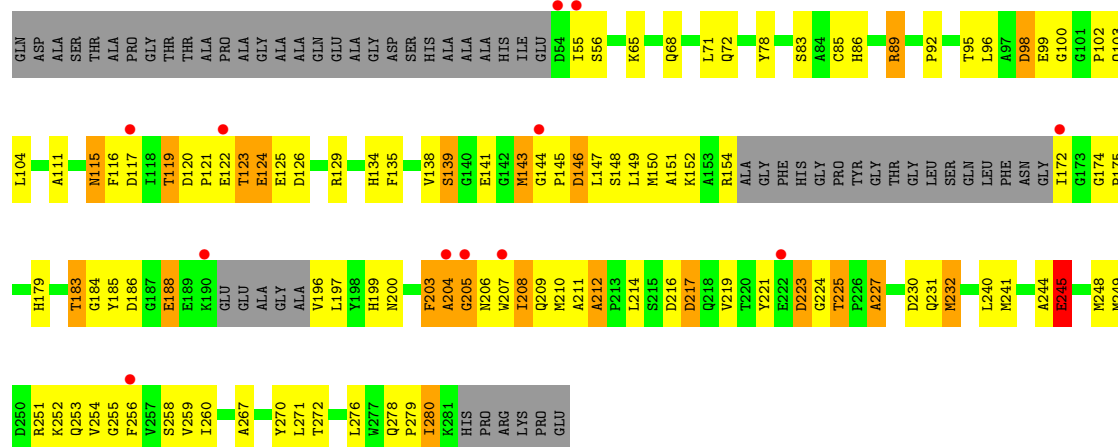
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is water.

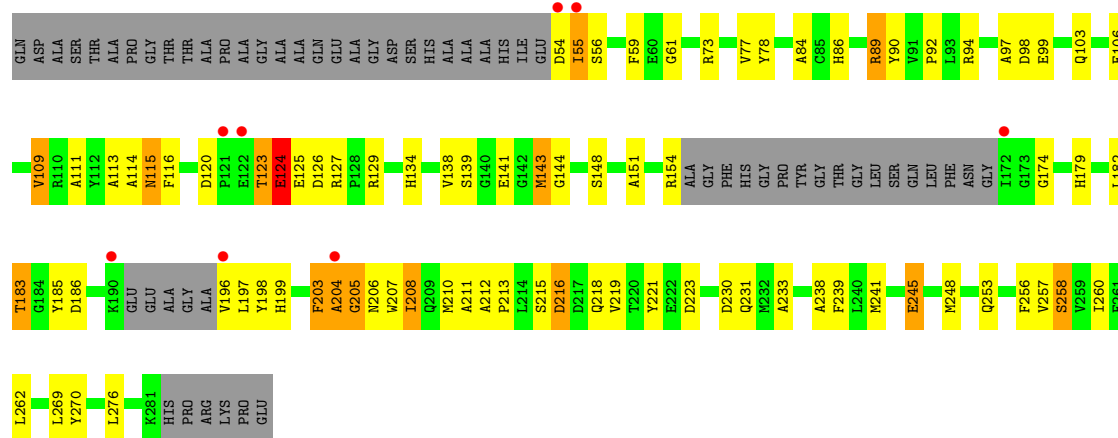
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		
8	B	1	Total	O	0	0
			1	1		
8	D	1	Total	O	0	0
			1	1		
8	F	1	Total	O	0	0
			1	1		



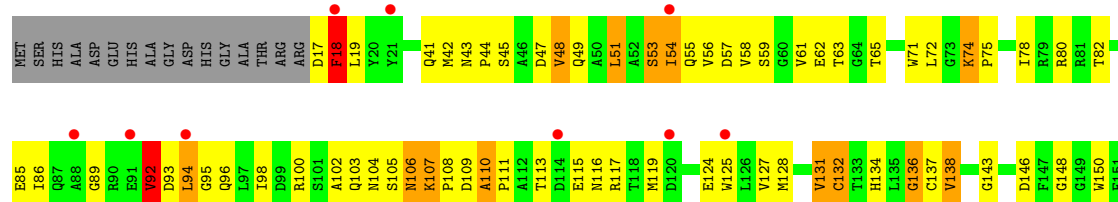
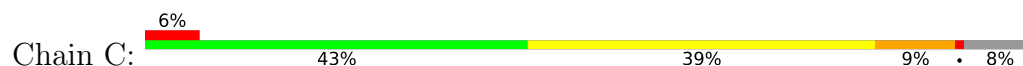
• Molecule 2: CYTOCHROME C1, HEME PROTEIN

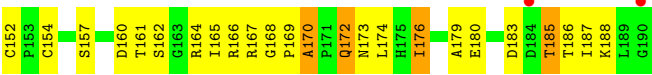


• Molecule 2: CYTOCHROME C1, HEME PROTEIN

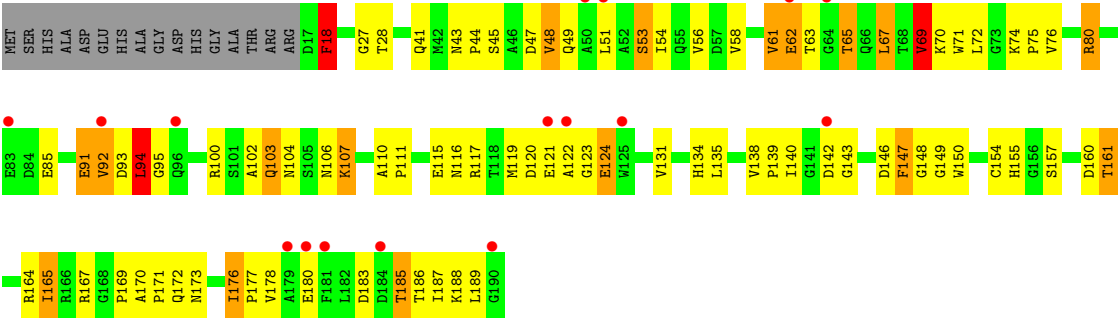


• Molecule 3: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT





● Molecule 3: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.30Å 164.91Å 100.61Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	97.96 – 2.70 97.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (97.96-2.70) 94.3 (97.96-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.238 , 0.290 (Not available) , 0.305	Depositor DCC
R_{free} test set	3535 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12990	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7952e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, SMA, HEM, HEC

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	1.00	1/3573 (0.0%)	1.20	21/4904 (0.4%)
1	D	0.92	1/3573 (0.0%)	1.13	21/4904 (0.4%)
2	B	0.91	0/1634	1.20	10/2223 (0.4%)
2	E	0.80	0/1634	1.06	8/2223 (0.4%)
3	C	0.93	0/1317	1.30	14/1796 (0.8%)
3	F	0.83	1/1317 (0.1%)	1.17	10/1796 (0.6%)
All	All	0.92	3/13048 (0.0%)	1.17	84/17846 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	138	VAL	CA-C	-6.01	1.47	1.52
1	D	281	ILE	CA-CB	5.76	1.61	1.54
1	A	129	TRP	N-CA	-5.21	1.39	1.46

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	18	PHE	N-CA-C	-10.19	101.34	113.88
1	A	398	ALA	N-CA-C	-9.13	101.23	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	74	LYS	CA-C-N	8.66	128.43	119.76
3	C	74	LYS	C-N-CA	8.66	128.43	119.76
2	B	139	SER	N-CA-C	8.56	119.20	107.73
1	A	288	THR	CA-C-N	8.51	128.55	119.78
1	A	288	THR	C-N-CA	8.51	128.55	119.78
3	C	138	VAL	CA-C-N	-8.39	111.09	119.90
3	C	138	VAL	C-N-CA	-8.39	111.09	119.90
1	A	389	TYR	CA-C-N	-8.36	109.79	119.32
1	A	389	TYR	C-N-CA	-8.36	109.79	119.32
3	F	18	PHE	N-CA-C	-8.35	103.61	113.88
1	D	346	VAL	CA-C-N	-7.47	111.28	119.19
1	D	346	VAL	C-N-CA	-7.47	111.28	119.19
3	C	136	GLY	N-CA-C	7.42	125.56	115.32
2	B	212	ALA	CA-C-N	7.29	128.95	119.84
2	B	212	ALA	C-N-CA	7.29	128.95	119.84
1	A	346	VAL	CA-C-N	-7.27	112.22	119.56
1	A	346	VAL	C-N-CA	-7.27	112.22	119.56
1	D	414	ILE	CB-CA-C	-7.21	101.48	111.65
3	F	69	VAL	CB-CA-C	-6.96	100.22	110.81
2	E	61	GLY	CA-C-N	6.81	126.77	119.28
2	E	61	GLY	C-N-CA	6.81	126.77	119.28
3	F	176	ILE	CA-C-N	6.80	127.34	119.99
3	F	176	ILE	C-N-CA	6.80	127.34	119.99
1	A	293	VAL	CB-CA-C	-6.54	103.32	110.85
3	C	110	ALA	N-CA-C	6.54	117.65	110.13
3	C	82	THR	N-CA-C	-6.49	102.16	110.53
2	E	245	GLU	CA-C-N	-6.48	113.13	119.87
2	E	245	GLU	C-N-CA	-6.48	113.13	119.87
1	D	108	VAL	N-CA-C	6.43	116.58	110.53
1	A	349	LEU	N-CA-C	-6.40	105.36	113.43
1	D	339	ALA	N-CA-C	-6.22	104.50	111.28
1	D	188	ASN	CA-C-N	-6.21	112.24	119.32
1	D	188	ASN	C-N-CA	-6.21	112.24	119.32
1	A	414	ILE	CB-CA-C	-6.20	104.04	111.97
3	C	170	ALA	CA-C-N	-6.14	113.90	120.47
3	C	170	ALA	C-N-CA	-6.14	113.90	120.47
1	A	415	GLU	N-CA-C	6.10	118.79	110.55
1	A	374	PHE	N-CA-C	-6.03	104.63	111.14
2	B	245	GLU	CA-C-N	-6.03	113.47	119.56
2	B	245	GLU	C-N-CA	-6.03	113.47	119.56
1	A	414	ILE	N-CA-C	5.96	116.14	110.42
1	A	32	THR	N-CA-C	-5.95	106.05	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	GLY	N-CA-C	-5.79	105.79	112.73
1	D	288	THR	CA-C-N	5.75	125.71	119.78
1	D	288	THR	C-N-CA	5.75	125.71	119.78
3	C	176	ILE	CA-C-N	5.74	125.72	120.03
3	C	176	ILE	C-N-CA	5.74	125.72	120.03
1	D	389	TYR	CA-C-N	-5.70	112.83	119.32
1	D	389	TYR	C-N-CA	-5.70	112.83	119.32
1	D	276	HIS	CA-C-N	5.68	126.94	119.84
1	D	276	HIS	C-N-CA	5.68	126.94	119.84
1	D	159	ALA	N-CA-C	-5.68	105.17	111.36
3	F	147	PHE	N-CA-C	-5.67	104.60	112.03
1	D	105	PHE	N-CA-C	5.66	117.53	111.36
3	F	138	VAL	CB-CA-C	-5.66	104.24	110.52
2	B	98	ASP	N-CA-C	5.57	118.72	110.48
1	D	114	ARG	N-CA-C	-5.54	105.24	111.28
3	C	61	VAL	N-CA-C	5.47	115.46	108.12
1	D	293	VAL	N-CA-C	5.47	113.89	107.77
3	F	67	LEU	N-CA-C	-5.43	101.42	110.17
2	B	104	LEU	CA-C-N	-5.43	114.74	120.66
2	B	104	LEU	C-N-CA	-5.43	114.74	120.66
2	E	198	TYR	CB-CA-C	-5.41	104.02	110.94
1	D	125	ARG	N-CA-C	5.36	118.93	112.93
1	A	305	LEU	N-CA-C	5.35	117.55	111.02
1	D	146	GLY	N-CA-C	-5.34	106.32	112.73
3	F	172	GLN	N-CA-C	5.31	117.75	109.52
1	A	276	HIS	CA-C-N	5.27	126.43	119.84
1	A	276	HIS	C-N-CA	5.27	126.43	119.84
1	A	23	LEU	CA-C-N	-5.22	111.89	120.88
1	A	23	LEU	C-N-CA	-5.22	111.89	120.88
3	F	124	GLU	N-CA-C	5.17	117.00	111.36
2	E	233	ALA	N-CA-C	-5.17	105.73	111.36
1	D	194	PHE	N-CA-C	-5.14	105.86	111.82
1	A	46	ILE	N-CA-C	5.14	120.06	113.07
3	F	173	ASN	N-CA-C	-5.11	103.30	110.50
3	C	172	GLN	N-CA-C	5.08	116.91	109.24
2	E	109	VAL	N-CA-C	-5.07	105.55	110.42
1	A	387	GLY	N-CA-C	-5.05	101.21	113.18
2	E	182	LEU	N-CA-C	-5.05	106.63	112.89
2	B	253	GLN	N-CA-C	5.04	117.16	111.11
2	B	146	ASP	N-CA-C	-5.03	103.51	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	17	ASP	Peptide
3	F	107	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3439	0	3402	190	0
1	D	3439	0	3402	174	0
2	B	1594	0	1530	140	0
2	E	1594	0	1530	98	0
3	C	1289	0	1231	103	0
3	F	1289	0	1231	89	0
4	A	86	0	60	18	0
4	D	86	0	60	18	0
5	A	37	0	42	2	0
5	D	37	0	41	2	0
6	B	43	0	30	3	0
6	E	43	0	30	5	0
7	C	4	0	0	1	0
7	F	4	0	0	1	0
8	A	3	0	0	1	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
All	All	12990	0	12589	780	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (780) 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)
2:E:123:THR:CG2	2:E:125:GLU:H	1.37	1.37
2:B:99:GLU:HA	2:B:103:GLN:NE2	1.43	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:GLY:HA2	2:E:206:ASN:OD1	1.26	1.30
2:B:123:THR:HG22	2:B:124:GLU:N	1.32	1.18
3:F:183:ASP:OD1	3:F:186:THR:HB	1.46	1.16
2:B:123:THR:CG2	2:B:125:GLU:H	1.59	1.15
1:A:385:ALA:O	1:A:390:PRO:HD3	1.47	1.13
3:C:95:GLY:HA2	3:C:100:ARG:HH21	1.16	1.10
2:B:214:LEU:HD22	2:B:232:MET:HE3	1.15	1.09
1:A:311:ASP:O	1:A:316:MET:HE2	1.51	1.09
1:A:154:MET:HE1	1:A:292:ILE:HD12	1.24	1.09
2:B:123:THR:CG2	2:B:124:GLU:N	2.07	1.09
2:B:123:THR:CG2	2:B:124:GLU:H	1.59	1.08
2:E:123:THR:HG22	2:E:124:GLU:N	1.52	1.07
2:E:123:THR:HG22	2:E:124:GLU:H	0.98	1.07
1:A:46:ILE:HD12	1:A:46:ILE:C	1.80	1.07
2:B:203:PHE:CE2	2:B:204:ALA:HB2	1.88	1.06
2:E:123:THR:HG22	2:E:125:GLU:H	0.92	1.06
2:E:123:THR:HG22	2:E:125:GLU:N	1.69	1.05
2:E:123:THR:CG2	2:E:125:GLU:N	2.22	1.02
3:C:95:GLY:HA2	3:C:100:ARG:NH2	1.71	1.02
2:B:85:CYS:HA	2:B:143:MET:HE2	1.05	1.02
2:E:123:THR:CG2	2:E:124:GLU:N	2.19	1.01
1:A:350:ASP:HB2	1:A:408:LEU:HD13	1.43	1.01
2:E:208:ILE:HG23	2:E:210:MET:H	1.19	1.01
3:F:94:LEU:HD23	3:F:100:ARG:NH1	1.75	1.01
3:F:183:ASP:OD2	3:F:185:THR:HG22	1.61	1.00
3:C:59:SER:HB3	3:C:185:THR:OG1	1.62	0.99
2:E:123:THR:O	2:E:124:GLU:HB2	1.59	0.99
1:A:46:ILE:HD12	1:A:47:TRP:N	1.79	0.97
3:F:120:ASP:OD1	3:F:120:ASP:O	1.82	0.97
3:C:119:MET:CE	3:C:180:GLU:HA	1.93	0.97
2:B:123:THR:HG22	2:B:125:GLU:N	1.79	0.97
3:C:94:LEU:HD23	3:C:100:ARG:NH1	1.79	0.96
1:A:114:ARG:C	1:A:114:ARG:HD2	1.90	0.96
3:F:95:GLY:HA2	3:F:100:ARG:NH2	1.80	0.96
2:B:115:ASN:N	2:B:115:ASN:HD22	1.59	0.96
2:E:205:GLY:CA	2:E:206:ASN:OD1	2.13	0.95
2:B:123:THR:HG22	2:B:124:GLU:H	0.78	0.95
1:D:385:ALA:O	1:D:390:PRO:HD3	1.65	0.95
2:E:115:ASN:N	2:E:115:ASN:HD22	1.66	0.94
1:A:387:GLY:HA2	1:A:390:PRO:HD2	1.49	0.94
2:E:55:ILE:HG22	2:E:56:SER:N	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:LEU:CD2	2:B:232:MET:HE3	1.98	0.92
2:B:99:GLU:HA	2:B:103:GLN:HE21	1.33	0.92
2:B:205:GLY:HA2	2:B:206:ASN:OD1	1.69	0.92
3:C:119:MET:HE3	3:C:180:GLU:HA	1.50	0.91
1:D:387:GLY:HA2	1:D:390:PRO:HD2	1.52	0.91
2:B:203:PHE:CD2	2:B:204:ALA:N	2.38	0.91
1:D:114:ARG:HD2	1:D:114:ARG:C	1.95	0.91
1:A:154:MET:CE	1:A:292:ILE:HD12	2.02	0.90
2:B:85:CYS:HA	2:B:143:MET:CE	1.98	0.90
1:D:62:GLY:O	4:D:500:HEM:HBC2	1.70	0.90
1:A:46:ILE:C	1:A:46:ILE:CD1	2.42	0.90
1:A:278:ASP:OD1	1:A:281:ILE:HD12	1.72	0.89
1:A:66:VAL:HG23	4:A:500:HEM:CBC	2.03	0.89
2:B:55:ILE:HD11	2:B:179:HIS:NE2	1.87	0.89
3:F:85:GLU:O	3:F:161:THR:HG21	1.72	0.88
1:D:385:ALA:O	1:D:390:PRO:CD	2.21	0.88
3:F:183:ASP:OD1	3:F:186:THR:CB	2.20	0.88
1:A:242:LEU:HD21	2:B:280:ILE:HD12	1.53	0.88
1:D:154:MET:HE3	1:D:278:ASP:HB3	1.55	0.87
2:B:123:THR:O	2:B:124:GLU:HB2	1.73	0.87
4:A:501:HEM:HMC2	4:A:501:HEM:HBC2	1.56	0.87
2:B:183:THR:CG2	2:B:183:THR:O	2.22	0.86
2:B:85:CYS:CA	2:B:143:MET:HE2	2.00	0.86
1:D:122:LYS:HE2	1:D:350:ASP:OD2	1.74	0.86
3:C:58:VAL:HG11	3:C:187:ILE:HD12	1.56	0.86
1:A:317:LEU:HD21	1:A:321:LEU:HD11	1.58	0.86
2:B:99:GLU:CA	2:B:103:GLN:NE2	2.36	0.86
1:A:311:ASP:O	1:A:316:MET:CE	2.24	0.86
1:A:350:ASP:HB2	1:A:408:LEU:CD1	2.06	0.86
1:A:319:ASN:HD22	1:A:319:ASN:C	1.84	0.85
2:E:115:ASN:HD22	2:E:115:ASN:H	1.24	0.85
1:A:317:LEU:HD21	1:A:321:LEU:CD1	2.06	0.85
1:A:66:VAL:HG23	4:A:500:HEM:HBC2	1.56	0.85
1:A:66:VAL:CG2	4:A:500:HEM:CBC	2.54	0.85
3:F:185:THR:O	3:F:185:THR:HG23	1.75	0.85
1:A:154:MET:HE2	1:A:154:MET:HA	1.57	0.84
1:D:66:VAL:CG2	4:D:500:HEM:CBC	2.56	0.84
2:B:98:ASP:O	2:B:103:GLN:HG2	1.78	0.83
4:D:501:HEM:HBC2	4:D:501:HEM:HMC2	1.58	0.83
1:D:8:HIS:H	1:D:8:HIS:CD2	1.95	0.83
1:D:422:GLN:HA	1:D:422:GLN:NE2	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:THR:HG21	2:E:125:GLU:HB2	1.61	0.83
3:F:119:MET:HE3	3:F:180:GLU:HA	1.60	0.83
1:A:121:TYR:CE2	1:A:346:VAL:HG22	2.14	0.82
3:F:53:SER:O	3:F:54:ILE:HG23	1.78	0.82
1:D:319:ASN:C	1:D:319:ASN:HD22	1.87	0.81
2:E:55:ILE:CG2	2:E:56:SER:N	2.41	0.81
1:D:376:VAL:O	1:D:380:VAL:HG22	1.79	0.81
3:F:94:LEU:HD23	3:F:100:ARG:HH11	1.44	0.81
1:A:122:LYS:HE3	1:A:350:ASP:OD2	1.80	0.81
2:E:208:ILE:HG23	2:E:210:MET:N	1.94	0.81
2:B:214:LEU:HD22	2:B:232:MET:CE	2.06	0.81
3:C:71:TRP:O	3:C:72:LEU:HB2	1.81	0.81
1:A:108:VAL:O	1:A:112:ILE:HD12	1.79	0.81
3:C:168:GLY:C	1:D:309:THR:HG22	2.06	0.80
1:D:366:TRP:CE3	1:D:407:ILE:HD13	2.16	0.80
1:D:66:VAL:HG23	4:D:500:HEM:CBC	2.11	0.80
1:D:12:LYS:HA	1:D:17:ARG:HH12	1.47	0.80
1:D:66:VAL:HG23	4:D:500:HEM:HBC2	1.64	0.80
2:E:138:VAL:HG12	2:E:143:MET:HG2	1.64	0.79
2:B:116:PHE:HB3	2:B:129:ARG:HD2	1.64	0.79
1:A:385:ALA:O	1:A:390:PRO:CD	2.28	0.78
2:B:205:GLY:HA2	2:B:206:ASN:CG	2.08	0.78
3:C:106:ASN:O	3:C:107:LYS:HG3	1.84	0.78
2:E:120:ASP:HB3	2:E:123:THR:HB	1.66	0.78
2:B:154:ARG:HG2	2:B:154:ARG:HH11	1.49	0.78
3:C:185:THR:O	3:C:185:THR:HG23	1.82	0.78
1:D:313:TRP:HA	1:D:316:MET:HE3	1.66	0.78
2:B:55:ILE:CD1	2:B:179:HIS:NE2	2.47	0.77
1:D:62:GLY:C	4:D:500:HEM:HBC2	2.10	0.77
1:D:140:MET:HE1	1:D:340:ILE:HD13	1.67	0.76
3:C:102:ALA:HB2	3:C:111:PRO:O	1.84	0.76
3:F:48:VAL:O	3:F:48:VAL:CG1	2.32	0.76
2:B:203:PHE:CD2	2:B:204:ALA:CB	2.68	0.76
3:C:89:GLY:N	3:C:161:THR:HG21	2.01	0.76
2:B:203:PHE:CE2	2:B:204:ALA:CB	2.67	0.76
3:C:185:THR:O	3:C:185:THR:CG2	2.33	0.76
2:B:205:GLY:CA	2:B:206:ASN:OD1	2.34	0.75
2:B:115:ASN:N	2:B:115:ASN:ND2	2.30	0.75
3:C:134:HIS:HD2	1:D:329:LYS:HG3	1.48	0.75
2:E:55:ILE:CG2	2:E:56:SER:H	1.99	0.75
2:B:175:PRO:HG3	2:B:241:MET:HE2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:GLY:HA2	1:D:309:THR:HG21	1.70	0.74
2:B:115:ASN:HD22	2:B:115:ASN:H	1.34	0.74
2:B:183:THR:O	2:B:183:THR:HG22	1.86	0.74
1:A:4:ILE:O	1:A:5:PRO:C	2.31	0.73
2:B:116:PHE:CB	2:B:129:ARG:HD2	2.18	0.73
3:F:183:ASP:OD1	3:F:186:THR:N	2.20	0.73
1:A:122:LYS:CE	1:A:350:ASP:OD2	2.36	0.73
2:E:98:ASP:O	2:E:103:GLN:HG2	1.87	0.73
3:C:93:ASP:O	3:C:95:GLY:N	2.21	0.73
1:A:242:LEU:CD2	2:B:280:ILE:HD12	2.19	0.72
2:B:123:THR:CG2	2:B:125:GLU:N	2.42	0.72
2:B:55:ILE:HG22	2:B:56:SER:H	1.55	0.72
1:D:66:VAL:HG21	4:D:500:HEM:CBC	2.19	0.72
1:D:350:ASP:HB2	1:D:408:LEU:HD13	1.72	0.71
1:A:242:LEU:HD21	2:B:280:ILE:CD1	2.20	0.71
3:C:119:MET:HE1	3:C:180:GLU:HA	1.70	0.71
1:D:140:MET:HE1	1:D:340:ILE:CD1	2.20	0.71
2:B:138:VAL:O	2:B:139:SER:HB3	1.89	0.71
2:E:116:PHE:CB	2:E:129:ARG:HD2	2.21	0.71
2:E:116:PHE:HB2	2:E:129:ARG:HD2	1.72	0.71
1:A:366:TRP:CE3	1:A:407:ILE:HD13	2.25	0.71
2:B:86:HIS:HE1	2:B:145:PRO:HD2	1.55	0.71
1:D:12:LYS:HA	1:D:17:ARG:NH1	2.05	0.71
1:A:311:ASP:C	1:A:316:MET:HE2	2.16	0.70
3:F:120:ASP:C	3:F:122:ALA:H	1.99	0.70
3:F:119:MET:CE	3:F:180:GLU:HA	2.21	0.70
1:A:350:ASP:OD1	1:A:350:ASP:C	2.34	0.70
2:E:186:ASP:OD2	2:E:199:HIS:ND1	2.24	0.69
1:A:140:MET:HE1	1:A:340:ILE:HD13	1.72	0.69
2:B:175:PRO:CG	2:B:241:MET:HE2	2.22	0.69
2:B:123:THR:HG22	2:B:125:GLU:H	1.09	0.69
1:D:51:LEU:HD13	4:D:501:HEM:C4B	2.27	0.69
2:B:99:GLU:CA	2:B:103:GLN:HE21	2.04	0.69
2:B:203:PHE:O	2:B:205:GLY:N	2.26	0.69
1:D:8:HIS:H	1:D:8:HIS:HD2	1.38	0.69
2:B:203:PHE:CD1	2:B:208:ILE:HD12	2.28	0.69
1:A:317:LEU:CD2	1:A:321:LEU:CD1	2.70	0.69
3:F:53:SER:O	3:F:54:ILE:CG2	2.41	0.68
1:A:66:VAL:HG21	4:A:500:HEM:CBC	2.24	0.68
2:B:203:PHE:C	2:B:205:GLY:H	2.01	0.68
3:C:95:GLY:CA	3:C:100:ARG:NH2	2.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:117:ARG:O	3:F:176:ILE:HD13	1.93	0.68
1:A:366:TRP:CE3	1:A:407:ILE:CD1	2.77	0.68
3:F:56:VAL:HG21	3:F:69:VAL:HG21	1.76	0.68
3:F:80:ARG:NE	3:F:124:GLU:OE2	2.25	0.68
3:C:103:GLN:NE2	3:C:172:GLN:HG2	2.09	0.67
1:D:136:TYR:CE2	1:D:140:MET:HE2	2.29	0.67
3:C:106:ASN:O	3:C:107:LYS:CG	2.42	0.67
3:F:71:TRP:O	3:F:72:LEU:HB2	1.93	0.67
2:E:138:VAL:CG1	2:E:143:MET:CE	2.73	0.67
3:F:93:ASP:O	3:F:94:LEU:C	2.36	0.67
3:F:143:GLY:HA2	3:F:148:GLY:C	2.19	0.67
1:D:330:PHE:CZ	1:D:334:ILE:HD11	2.30	0.67
1:D:51:LEU:HD13	4:D:501:HEM:C3B	2.30	0.67
1:D:317:LEU:C	1:D:317:LEU:CD2	2.67	0.67
1:A:148:VAL:HA	1:A:155:SER:HB3	1.77	0.67
2:B:196:VAL:O	2:B:196:VAL:HG12	1.95	0.67
2:B:100:GLY:H	2:B:103:GLN:HE21	1.43	0.66
1:A:91:TYR:CE1	2:B:251:ARG:HG3	2.30	0.66
2:E:123:THR:CG2	2:E:124:GLU:H	1.82	0.66
2:B:123:THR:HG21	2:B:125:GLU:H	1.57	0.66
4:A:500:HEM:HBC2	4:A:500:HEM:HHD	1.76	0.66
2:B:89:ARG:O	2:B:134:HIS:CD2	2.48	0.66
3:C:89:GLY:CA	3:C:161:THR:CG2	2.74	0.66
1:A:64:VAL:HG22	3:C:41:GLN:CD	2.21	0.65
3:F:18:PHE:CD1	3:F:18:PHE:C	2.74	0.65
3:C:74:LYS:HD2	3:C:131:VAL:HG21	1.78	0.65
3:C:94:LEU:HD23	3:C:100:ARG:HH12	1.60	0.65
1:A:319:ASN:C	1:A:319:ASN:ND2	2.53	0.65
3:C:103:GLN:HE21	3:C:172:GLN:HG2	1.62	0.65
2:B:203:PHE:CG	2:B:208:ILE:HD12	2.32	0.65
3:C:62:GLU:O	3:C:65:THR:HB	1.97	0.65
1:A:71:PRO:HD2	1:D:71:PRO:HD2	1.79	0.64
3:C:134:HIS:CD2	1:D:329:LYS:HG3	2.32	0.64
2:B:55:ILE:HG22	2:B:56:SER:N	2.11	0.64
3:F:74:LYS:HD2	3:F:131:VAL:HG21	1.78	0.64
1:D:64:VAL:HG22	3:F:41:GLN:NE2	2.12	0.64
1:A:62:GLY:O	4:A:500:HEM:HBC2	1.96	0.64
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.63	0.64
3:C:117:ARG:NH1	3:C:176:ILE:HD12	2.12	0.64
3:C:117:ARG:O	3:C:176:ILE:HD13	1.97	0.64
1:A:223:ASN:HB2	1:A:224:PRO:CD	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:SER:HA	2:B:143:MET:HG2	1.78	0.64
3:C:119:MET:HE1	3:C:180:GLU:CA	2.28	0.64
1:A:108:VAL:C	1:A:112:ILE:HD12	2.23	0.64
1:D:366:TRP:CE3	1:D:407:ILE:CD1	2.81	0.64
2:B:55:ILE:CD1	2:B:179:HIS:CE1	2.81	0.64
1:D:307:ALA:HB1	1:D:394:LEU:HD23	1.80	0.64
1:D:311:ASP:O	1:D:316:MET:HE2	1.98	0.64
2:E:97:ALA:HB2	2:E:109:VAL:HG21	1.79	0.64
1:A:228:GLU:OE2	1:A:355:ARG:NH2	2.30	0.64
2:B:203:PHE:CD2	2:B:204:ALA:HB2	2.32	0.63
2:B:185:TYR:CG	2:B:212:ALA:HB2	2.33	0.63
3:C:131:VAL:HG13	3:C:136:GLY:HA2	1.80	0.63
6:E:500:HEC:CMC	6:E:500:HEC:HBC3	2.28	0.63
3:F:185:THR:O	3:F:185:THR:CG2	2.46	0.63
2:B:123:THR:HG22	2:B:124:GLU:CA	2.26	0.63
1:D:317:LEU:C	1:D:317:LEU:HD22	2.22	0.63
1:A:114:ARG:HD2	1:A:115:GLY:N	2.12	0.63
3:C:75:PRO:HG3	3:C:138:VAL:HG22	1.80	0.63
1:D:138:MET:HE2	1:D:208:LEU:HD11	1.81	0.63
1:D:368:TRP:O	1:D:372:VAL:HG23	1.98	0.63
2:E:138:VAL:HG11	2:E:143:MET:HE3	1.79	0.63
1:D:350:ASP:OD1	1:D:350:ASP:C	2.41	0.62
3:F:71:TRP:CE2	3:F:72:LEU:HD12	2.34	0.62
1:A:66:VAL:CG2	4:A:500:HEM:HBC1	2.28	0.62
1:A:66:VAL:HG21	4:A:500:HEM:HBC1	1.80	0.62
2:B:154:ARG:HG2	2:B:154:ARG:NH1	2.13	0.62
3:C:169:PRO:N	1:D:309:THR:HG22	2.15	0.62
2:B:55:ILE:HD11	2:B:179:HIS:CE1	2.34	0.62
3:C:78:ILE:HG12	3:C:127:VAL:HG22	1.82	0.62
1:D:317:LEU:HD21	1:D:321:LEU:HD11	1.80	0.62
1:A:282:GLU:O	1:A:283:ALA:C	2.41	0.62
1:A:105:PHE:HA	1:A:108:VAL:HG22	1.82	0.61
3:C:143:GLY:O	3:C:148:GLY:HA2	2.00	0.61
2:B:221:TYR:C	2:B:223:ASP:H	2.08	0.61
3:C:183:ASP:OD1	3:C:186:THR:CB	2.48	0.61
3:C:183:ASP:OD1	3:C:186:THR:HB	2.01	0.61
3:F:94:LEU:HD23	3:F:100:ARG:HH12	1.64	0.61
1:A:317:LEU:HD23	1:A:321:LEU:HG	1.82	0.61
3:C:59:SER:HB3	3:C:185:THR:HG1	1.65	0.61
1:D:385:ALA:O	1:D:390:PRO:CG	2.48	0.61
1:A:246:PRO:HB2	2:B:276:LEU:HD21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ASP:CB	1:A:408:LEU:HD13	2.24	0.61
2:E:205:GLY:HA2	2:E:206:ASN:CG	2.20	0.61
2:B:278:GLN:N	2:B:279:PRO:CD	2.63	0.61
2:E:138:VAL:CG1	2:E:143:MET:HE3	2.30	0.61
2:E:216:ASP:OD1	2:E:216:ASP:N	2.33	0.61
1:D:62:GLY:C	4:D:500:HEM:CBC	2.73	0.61
2:E:179:HIS:O	2:E:183:THR:HB	2.01	0.61
3:F:48:VAL:O	3:F:48:VAL:HG13	2.01	0.61
1:A:138:MET:HE2	1:A:208:LEU:HD11	1.82	0.61
3:C:92:VAL:HG13	3:C:96:GLN:OE1	2.00	0.60
1:A:317:LEU:CD2	1:A:317:LEU:C	2.74	0.60
1:D:225:THR:HG22	1:D:427:ASP:OD2	2.01	0.60
1:A:46:ILE:HD12	1:A:47:TRP:CA	2.32	0.60
1:D:282:GLU:O	1:D:283:ALA:C	2.45	0.60
2:B:86:HIS:CE1	2:B:144:GLY:HA3	2.36	0.60
2:E:55:ILE:CD1	2:E:179:HIS:NE2	2.65	0.60
1:A:366:TRP:CD2	1:A:407:ILE:HD13	2.36	0.60
2:B:199:HIS:HD2	2:B:207:TRP:CH2	2.20	0.60
1:D:138:MET:HE3	1:D:204:VAL:CG1	2.31	0.60
1:A:46:ILE:HD11	1:A:47:TRP:CE2	2.37	0.60
1:D:312:VAL:HG22	1:D:394:LEU:HD11	1.83	0.60
1:A:53:PHE:CE2	1:A:260:LEU:HD21	2.37	0.60
1:A:270:MET:N	1:A:271:PRO:CD	2.64	0.60
2:B:203:PHE:HB2	2:B:208:ILE:HD12	1.84	0.60
1:A:12:LYS:O	1:A:17:ARG:NH1	2.35	0.59
2:B:183:THR:O	2:B:183:THR:HG23	2.00	0.59
3:F:119:MET:HE3	3:F:180:GLU:CA	2.32	0.59
3:F:120:ASP:OD1	3:F:123:GLY:N	2.35	0.59
3:C:93:ASP:C	3:C:95:GLY:N	2.61	0.59
2:B:224:GLY:O	2:B:225:THR:C	2.43	0.59
3:C:54:ILE:HG13	3:C:55:GLN:N	2.18	0.59
1:D:138:MET:HE2	1:D:208:LEU:CD1	2.31	0.59
2:B:100:GLY:N	2:B:103:GLN:HE21	1.99	0.59
3:F:160:ASP:OD1	3:F:160:ASP:C	2.44	0.59
1:D:114:ARG:C	1:D:114:ARG:CD	2.74	0.59
1:D:122:LYS:NZ	1:D:354:VAL:O	2.36	0.59
1:A:313:TRP:HD1	1:A:316:MET:HE3	1.68	0.59
2:B:203:PHE:CG	2:B:204:ALA:N	2.43	0.59
3:F:102:ALA:O	3:F:103:GLN:C	2.46	0.59
4:A:500:HEM:O1A	4:A:500:HEM:O1D	2.21	0.58
3:C:93:ASP:O	3:C:94:LEU:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:94:LEU:HD11	3:F:111:PRO:HB2	1.84	0.58
1:D:12:LYS:O	1:D:17:ARG:NH1	2.36	0.58
6:E:500:HEC:HBA1	6:E:500:HEC:HHA	1.85	0.58
3:C:80:ARG:HG3	3:C:125:TRP:CH2	2.38	0.58
3:F:110:ALA:HB1	3:F:116:ASN:ND2	2.18	0.58
1:D:138:MET:HE3	1:D:204:VAL:HG12	1.85	0.58
1:A:308:PHE:CE2	1:A:331:PHE:HE1	2.22	0.58
1:D:133:MET:HG3	1:D:344:ALA:HA	1.85	0.58
3:C:119:MET:HE1	3:C:180:GLU:C	2.29	0.58
1:D:422:GLN:HA	1:D:422:GLN:HE21	1.69	0.57
2:B:111:ALA:O	2:B:115:ASN:ND2	2.37	0.57
1:D:13:THR:HB	1:D:16:GLU:HG3	1.85	0.57
3:F:85:GLU:O	3:F:161:THR:CG2	2.51	0.57
2:B:197:LEU:N	2:B:197:LEU:HD23	2.19	0.57
2:E:186:ASP:OD2	2:E:199:HIS:HB3	2.04	0.57
3:C:18:PHE:CD1	3:C:18:PHE:C	2.81	0.57
2:B:120:ASP:HB3	2:B:123:THR:HB	1.86	0.57
3:F:95:GLY:CA	3:F:100:ARG:NH2	2.61	0.57
3:F:44:PRO:HB2	3:F:49:GLN:HE21	1.69	0.57
3:F:48:VAL:O	3:F:48:VAL:HG12	2.05	0.57
1:A:330:PHE:CE2	1:A:334:ILE:HD11	2.39	0.57
2:B:209:GLN:CB	6:B:500:HEC:O2D	2.53	0.57
3:C:146:ASP:OD2	3:C:167:ARG:NH1	2.37	0.57
1:D:366:TRP:CD2	1:D:407:ILE:HD13	2.40	0.57
1:D:377:LEU:HA	1:D:380:VAL:HG23	1.87	0.57
3:F:71:TRP:CE2	3:F:72:LEU:CD1	2.88	0.57
3:F:146:ASP:C	3:F:147:PHE:CD1	2.82	0.57
2:B:129:ARG:NH1	2:B:134:HIS:O	2.38	0.57
3:C:128:MET:HE1	3:C:150:TRP:CH2	2.39	0.57
2:E:89:ARG:O	2:E:134:HIS:CD2	2.58	0.57
2:E:92:PRO:HA	2:E:134:HIS:HA	1.86	0.57
2:B:89:ARG:O	2:B:134:HIS:HD2	1.85	0.56
1:D:317:LEU:HD21	1:D:321:LEU:CD1	2.35	0.56
1:A:223:ASN:HB2	1:A:224:PRO:HD2	1.87	0.56
2:E:203:PHE:CG	2:E:204:ALA:N	2.73	0.56
3:F:117:ARG:O	3:F:176:ILE:CD1	2.53	0.56
2:B:267:ALA:O	2:B:270:TYR:HB3	2.06	0.56
3:F:119:MET:HE1	3:F:180:GLU:C	2.30	0.56
1:D:312:VAL:HG12	1:D:315:VAL:H	1.71	0.56
3:F:120:ASP:OD1	3:F:120:ASP:C	2.47	0.56
1:A:7:ASP:OD1	1:A:7:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HG22	1:A:5:PRO:O	2.06	0.56
1:D:308:PHE:CD1	1:D:331:PHE:CE1	2.94	0.56
6:E:500:HEC:HBC3	6:E:500:HEC:HMC1	1.86	0.56
1:A:308:PHE:CD2	1:A:331:PHE:CE1	2.94	0.56
3:C:41:GLN:NE2	3:C:42:MET:HG3	2.21	0.56
3:C:93:ASP:C	3:C:95:GLY:H	2.14	0.56
3:C:107:LYS:O	3:C:109:ASP:N	2.39	0.56
1:D:414:ILE:CG2	1:D:414:ILE:O	2.53	0.56
2:E:115:ASN:N	2:E:115:ASN:ND2	2.38	0.55
2:B:208:ILE:HG23	2:B:210:MET:H	1.71	0.55
3:F:27:GLY:O	3:F:28:THR:C	2.49	0.55
3:C:89:GLY:CA	3:C:161:THR:HG21	2.36	0.55
1:D:387:GLY:CA	1:D:390:PRO:HD2	2.31	0.55
2:E:183:THR:HG23	2:E:183:THR:O	2.05	0.55
1:A:270:MET:N	1:A:271:PRO:HD3	2.21	0.55
2:B:256:PHE:CE2	2:B:260:ILE:HD11	2.42	0.55
3:C:80:ARG:NE	3:C:124:GLU:OE2	2.38	0.55
3:C:160:ASP:OD1	3:C:160:ASP:C	2.49	0.55
2:E:241:MET:HE2	2:E:248:MET:HE1	1.89	0.55
1:A:370:LEU:O	1:A:373:ASP:HB3	2.07	0.55
1:D:40:ASN:HD21	1:D:225:THR:HG23	1.70	0.55
2:E:55:ILE:HG23	2:E:56:SER:H	1.72	0.55
2:B:221:TYR:C	2:B:223:ASP:N	2.64	0.54
1:D:276:HIS:CE1	1:D:293:VAL:HB	2.43	0.54
1:A:276:HIS:C	1:A:278:ASP:H	2.15	0.54
2:B:203:PHE:CD1	2:B:208:ILE:CD1	2.89	0.54
3:C:92:VAL:CG1	3:C:96:GLN:OE1	2.55	0.54
3:F:45:SER:OG	3:F:47:ASP:OD1	2.25	0.54
2:E:138:VAL:CG1	2:E:143:MET:HE2	2.37	0.54
1:A:122:LYS:NZ	1:A:354:VAL:O	2.39	0.54
1:D:360:ARG:HB3	1:D:415:GLU:OE2	2.08	0.54
2:B:179:HIS:O	2:B:183:THR:HB	2.07	0.54
2:B:186:ASP:OD2	2:B:199:HIS:ND1	2.40	0.54
1:A:133:MET:SD	4:A:501:HEM:HBC1	2.48	0.54
2:B:179:HIS:HE1	2:B:230:ASP:OD1	1.90	0.54
4:D:501:HEM:HBC2	4:D:501:HEM:CMC	2.35	0.54
3:C:94:LEU:HD23	3:C:100:ARG:HH11	1.70	0.54
4:D:500:HEM:CMB	4:D:500:HEM:HBB2	2.38	0.54
2:E:92:PRO:HB3	2:E:134:HIS:CE1	2.42	0.54
5:A:502:SMA:H33	5:A:502:SMA:H18	1.89	0.53
2:B:152:LYS:HG3	2:B:244:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:THR:O	2:E:183:THR:CG2	2.57	0.53
1:D:126:GLU:O	1:D:129:TRP:HB3	2.07	0.53
2:E:218:GLN:CG	2:E:218:GLN:O	2.56	0.53
3:F:120:ASP:O	3:F:122:ALA:N	2.42	0.53
1:A:62:GLY:C	4:A:500:HEM:CBC	2.81	0.53
1:A:308:PHE:CE2	1:A:331:PHE:CE1	2.96	0.53
1:D:422:GLN:NE2	1:D:422:GLN:CA	2.70	0.53
1:A:138:MET:CE	1:A:208:LEU:HD11	2.39	0.53
2:B:147:LEU:HD23	2:B:150:MET:CE	2.39	0.53
2:E:138:VAL:O	2:E:139:SER:HB3	2.08	0.53
1:A:81:GLU:O	1:A:85:ARG:HG3	2.08	0.53
2:B:255:GLY:O	2:B:259:VAL:HG23	2.08	0.53
3:C:157:SER:OG	3:C:169:PRO:HD2	2.09	0.53
1:A:362:LEU:O	1:A:366:TRP:HD1	1.92	0.53
2:B:95:THR:HA	2:B:98:ASP:OD2	2.09	0.52
2:B:211:ALA:O	2:B:212:ALA:C	2.52	0.52
3:C:41:GLN:HE22	3:C:42:MET:HG3	1.74	0.52
3:C:53:SER:O	3:C:54:ILE:HG22	2.08	0.52
2:E:73:ARG:HD2	2:E:221:TYR:CE2	2.44	0.52
3:F:44:PRO:HB2	3:F:49:GLN:NE2	2.24	0.52
3:F:165:ILE:HD13	3:F:170:ALA:HB3	1.91	0.52
2:E:123:THR:O	2:E:124:GLU:CB	2.43	0.52
1:A:276:HIS:O	1:A:278:ASP:N	2.42	0.52
3:F:95:GLY:HA2	3:F:100:ARG:HH21	1.72	0.52
1:D:66:VAL:HG21	4:D:500:HEM:HBC1	1.88	0.52
1:D:154:MET:HE2	1:D:154:MET:N	2.23	0.52
1:D:363:PHE:O	1:D:364:LYS:C	2.52	0.52
2:E:86:HIS:CE1	2:E:144:GLY:HA3	2.44	0.52
2:E:99:GLU:HA	2:E:103:GLN:NE2	2.24	0.52
1:A:370:LEU:HD22	1:A:403:TYR:CE1	2.45	0.52
1:A:379:TRP:CE3	1:A:380:VAL:HG13	2.45	0.52
1:D:330:PHE:CE1	1:D:334:ILE:HD11	2.44	0.52
1:A:91:TYR:HE1	2:B:251:ARG:HG3	1.72	0.52
3:F:134:HIS:HB3	7:F:500:FES:S1	2.49	0.52
1:A:389:TYR:O	1:A:390:PRO:C	2.46	0.52
1:D:154:MET:HE3	1:D:278:ASP:CB	2.34	0.52
3:F:119:MET:CE	3:F:180:GLU:CA	2.86	0.52
1:A:23:LEU:HD11	1:D:214:TRP:CE3	2.45	0.52
1:D:385:ALA:O	1:D:386:GLU:C	2.53	0.52
1:A:317:LEU:CD2	1:A:321:LEU:HG	2.40	0.51
3:C:42:MET:HE3	1:D:193:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:PHE:CE1	1:D:331:PHE:HE1	2.29	0.51
2:B:92:PRO:HG2	2:B:95:THR:HG23	1.91	0.51
6:B:500:HEC:HHA	6:B:500:HEC:CBA	2.40	0.51
2:E:115:ASN:H	2:E:115:ASN:ND2	1.95	0.51
1:A:138:MET:HE2	1:A:208:LEU:CD1	2.40	0.51
1:A:229:VAL:HG11	1:A:241:THR:HG21	1.92	0.51
2:B:65:LYS:HB3	2:B:249:MET:SD	2.51	0.51
1:D:377:LEU:HA	1:D:380:VAL:CG2	2.40	0.51
2:E:55:ILE:HD12	2:E:179:HIS:CE1	2.46	0.51
1:D:262:VAL:O	1:D:265:ALA:HB3	2.11	0.51
2:E:123:THR:HG21	2:E:125:GLU:CB	2.36	0.51
1:A:364:LYS:O	1:A:368:TRP:HD1	1.93	0.51
1:A:367:PHE:O	1:A:370:LEU:HB3	2.11	0.51
1:D:46:ILE:C	1:D:46:ILE:HD12	2.36	0.51
1:A:362:LEU:O	1:A:366:TRP:CD1	2.63	0.51
2:B:55:ILE:HD12	2:B:179:HIS:CE1	2.46	0.51
2:B:116:PHE:HB2	2:B:129:ARG:HD2	1.92	0.51
2:B:278:GLN:N	2:B:279:PRO:HD2	2.25	0.51
1:D:181:LEU:HD22	1:D:186:VAL:N	2.26	0.51
2:E:73:ARG:HG2	2:E:221:TYR:CD1	2.45	0.51
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.45	0.51
1:D:389:TYR:O	1:D:390:PRO:C	2.49	0.51
2:B:138:VAL:HG12	2:B:143:MET:HG2	1.93	0.50
1:D:8:HIS:CD2	1:D:8:HIS:N	2.72	0.50
1:A:180:LEU:HD22	5:A:502:SMA:H27	1.93	0.50
1:D:114:ARG:HD2	1:D:115:GLY:N	2.27	0.50
1:D:121:TYR:CD2	1:D:346:VAL:HG13	2.46	0.50
2:B:126:ASP:OD1	2:B:126:ASP:N	2.43	0.50
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.47	0.50
1:A:385:ALA:O	1:A:386:GLU:C	2.55	0.50
3:F:104:ASN:ND2	3:F:116:ASN:O	2.43	0.50
1:D:426:GLU:O	1:D:427:ASP:C	2.53	0.50
2:E:215:SER:O	2:E:218:GLN:CB	2.59	0.50
3:F:47:ASP:OD1	3:F:47:ASP:N	2.36	0.50
1:A:122:LYS:O	1:A:123:ALA:C	2.54	0.50
1:D:13:THR:OG1	1:D:16:GLU:CD	2.55	0.50
1:A:13:THR:OG1	1:A:16:GLU:OE1	2.25	0.50
3:C:51:LEU:H	3:C:51:LEU:CD2	2.25	0.50
2:B:203:PHE:CD2	2:B:204:ALA:HB3	2.47	0.50
2:B:147:LEU:HD23	2:B:150:MET:HE2	1.94	0.49
1:D:313:TRP:HA	1:D:316:MET:CE	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:500:HEM:O1D	4:D:500:HEM:O1A	2.30	0.49
3:F:157:SER:OG	3:F:169:PRO:HD2	2.11	0.49
2:B:245:GLU:OE1	2:B:245:GLU:HA	2.12	0.49
4:A:500:HEM:HBB2	4:A:500:HEM:CMB	2.41	0.49
3:C:106:ASN:C	3:C:107:LYS:HG3	2.36	0.49
3:C:143:GLY:HA2	3:C:148:GLY:O	2.12	0.49
1:D:308:PHE:CE1	1:D:331:PHE:CE1	3.00	0.49
3:F:143:GLY:O	3:F:148:GLY:HA2	2.12	0.49
1:A:307:ALA:HB1	1:A:394:LEU:HD23	1.94	0.49
1:D:188:ASN:O	1:D:189:PRO:C	2.53	0.49
2:B:151:ALA:O	2:B:174:GLY:HA3	2.13	0.49
2:E:116:PHE:HB3	2:E:129:ARG:HD2	1.92	0.49
3:F:91:GLU:O	3:F:92:VAL:C	2.55	0.49
3:F:120:ASP:C	3:F:122:ALA:N	2.66	0.49
1:A:306:ARG:O	1:A:307:ALA:C	2.55	0.49
8:A:2003:HOH:O	3:F:171:PRO:HB3	2.12	0.49
4:A:501:HEM:HBC2	4:A:501:HEM:CMC	2.38	0.49
2:E:55:ILE:CD1	2:E:179:HIS:CE1	2.95	0.49
3:F:61:VAL:CG1	3:F:67:LEU:HB2	2.42	0.49
1:A:343:MET:O	1:A:346:VAL:HG12	2.12	0.49
1:A:387:GLY:CA	1:A:390:PRO:HD2	2.32	0.49
2:E:196:VAL:HG12	2:E:196:VAL:O	2.13	0.49
1:A:317:LEU:CD2	1:A:321:LEU:HD12	2.43	0.49
3:C:103:GLN:NE2	3:C:172:GLN:CG	2.74	0.49
1:A:62:GLY:O	4:A:500:HEM:CBC	2.60	0.48
1:A:154:MET:HE2	1:A:154:MET:CA	2.36	0.48
2:B:123:THR:HG22	2:B:124:GLU:C	2.36	0.48
3:C:179:ALA:HA	3:C:188:LYS:O	2.13	0.48
3:F:110:ALA:HB1	3:F:116:ASN:HD22	1.77	0.48
1:A:313:TRP:HA	1:A:316:MET:HG3	1.94	0.48
3:C:45:SER:OG	3:C:47:ASP:OD1	2.30	0.48
3:C:168:GLY:C	1:D:309:THR:CG2	2.83	0.48
1:A:122:LYS:CE	1:A:350:ASP:CG	2.87	0.48
1:D:138:MET:HG2	1:D:205:ILE:HG13	1.96	0.48
1:A:254:PHE:CE1	2:B:270:TYR:HB2	2.49	0.48
1:A:306:ARG:HB3	3:F:155:HIS:HB3	1.96	0.48
1:A:383:MET:HE2	1:A:389:TYR:CZ	2.49	0.48
1:D:4:ILE:HG13	1:D:231:ARG:NH1	2.27	0.48
2:E:211:ALA:O	2:E:212:ALA:C	2.57	0.48
2:B:217:ASP:HA	2:B:227:ALA:HB3	1.94	0.48
1:A:46:ILE:CD1	1:A:46:ILE:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:GLY:HA2	1:D:309:THR:CG2	2.39	0.48
1:D:414:ILE:O	1:D:414:ILE:HG22	2.08	0.48
2:E:185:TYR:OH	2:E:210:MET:O	2.25	0.48
1:A:91:TYR:CD1	1:A:92:MET:N	2.82	0.48
1:A:228:GLU:OE2	1:A:355:ARG:CZ	2.62	0.48
3:C:119:MET:CE	3:C:180:GLU:CA	2.77	0.48
2:E:129:ARG:NH1	2:E:134:HIS:O	2.45	0.48
1:A:229:VAL:HG11	1:A:241:THR:CG2	2.44	0.48
1:A:378:MET:HB2	1:A:378:MET:HE3	1.69	0.48
3:C:134:HIS:O	1:D:329:LYS:HE3	2.14	0.48
1:D:39:LYS:HG2	1:D:240:ASP:O	2.14	0.48
2:E:92:PRO:HB3	2:E:134:HIS:ND1	2.29	0.48
3:F:139:PRO:HB2	3:F:150:TRP:HB3	1.96	0.48
1:A:23:LEU:O	1:A:25:ILE:N	2.45	0.48
2:B:121:PRO:HG2	2:B:122:GLU:H	1.78	0.48
1:D:185:ALA:O	1:D:186:VAL:C	2.56	0.48
3:C:110:ALA:HB1	3:C:116:ASN:ND2	2.29	0.47
1:D:66:VAL:CG2	4:D:500:HEM:HBC1	2.41	0.47
1:A:62:GLY:C	4:A:500:HEM:HBC2	2.39	0.47
3:C:173:ASN:O	3:C:174:LEU:C	2.56	0.47
2:E:213:PRO:HB2	6:E:500:HEC:HBB2	1.95	0.47
1:A:242:LEU:CD2	2:B:280:ILE:CD1	2.89	0.47
3:C:48:VAL:O	3:C:48:VAL:CG1	2.60	0.47
3:C:51:LEU:H	3:C:51:LEU:HD22	1.79	0.47
1:A:179:TRP:O	1:A:193:ARG:NH1	2.47	0.47
2:B:203:PHE:CB	2:B:208:ILE:HD12	2.43	0.47
3:C:80:ARG:HG3	3:C:125:TRP:CZ3	2.49	0.47
1:D:254:PHE:CE1	2:E:270:TYR:HB2	2.49	0.47
2:E:94:ARG:NH2	3:F:47:ASP:HB3	2.29	0.47
2:E:126:ASP:O	2:E:127:ARG:HB3	2.15	0.47
3:C:43:ASN:ND2	1:D:179:TRP:HD1	2.12	0.47
3:F:120:ASP:OD2	3:F:124:GLU:N	2.47	0.47
1:A:81:GLU:OE1	1:A:85:ARG:NE	2.48	0.47
2:B:138:VAL:HG12	2:B:143:MET:CG	2.45	0.47
2:B:203:PHE:HE2	2:B:204:ALA:HB2	1.65	0.47
3:C:89:GLY:HA3	3:C:161:THR:CG2	2.44	0.47
1:D:41:LEU:HD13	1:D:45:TRP:CD1	2.50	0.47
3:F:54:ILE:HD11	3:F:189:LEU:HD12	1.97	0.47
1:A:32:THR:O	1:A:35:ILE:HG22	2.15	0.47
2:B:115:ASN:ND2	2:B:115:ASN:H	2.06	0.47
3:C:132:CYS:SG	3:C:134:HIS:HB3	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ARG:HD2	1:D:114:ARG:O	2.13	0.47
2:B:271:LEU:O	2:B:272:THR:C	2.57	0.47
3:C:53:SER:O	3:C:54:ILE:CG2	2.62	0.47
1:D:62:GLY:O	1:D:66:VAL:HG23	2.15	0.47
2:E:111:ALA:O	2:E:114:ALA:HB3	2.15	0.47
3:F:91:GLU:O	3:F:92:VAL:O	2.33	0.47
1:A:33:LEU:O	1:A:245:TRP:HB3	2.14	0.47
1:A:229:VAL:HA	1:A:424:ILE:HD12	1.97	0.47
1:A:422:GLN:N	1:A:426:GLU:OE2	2.34	0.47
1:D:122:LYS:CE	1:D:350:ASP:OD2	2.52	0.47
3:F:149:GLY:C	3:F:150:TRP:CE3	2.93	0.47
3:C:102:ALA:O	3:C:117:ARG:NH1	2.44	0.46
2:E:113:ALA:O	2:E:129:ARG:HB2	2.14	0.46
3:F:58:VAL:HG11	3:F:187:ILE:HD12	1.96	0.46
1:A:117:TYR:HB2	1:A:367:PHE:CZ	2.50	0.46
1:A:244:PHE:CE2	1:A:249:VAL:HG23	2.51	0.46
2:E:55:ILE:HD12	2:E:179:HIS:NE2	2.29	0.46
3:F:54:ILE:HD13	3:F:71:TRP:CD1	2.50	0.46
3:F:183:ASP:OD1	3:F:186:THR:CA	2.63	0.46
1:A:162:ILE:HG23	1:A:165:LEU:HD12	1.96	0.46
2:B:119:THR:O	2:B:119:THR:HG22	2.14	0.46
3:C:154:CYS:HB3	5:D:502:SMA:H4	1.96	0.46
1:D:223:ASN:HB2	1:D:224:PRO:HD2	1.96	0.46
2:E:256:PHE:CE2	2:E:260:ILE:HD11	2.51	0.46
3:C:48:VAL:O	3:C:48:VAL:HG13	2.14	0.46
1:A:69:TYR:HE2	1:A:71:PRO:HB3	1.81	0.46
1:A:140:MET:HE1	1:A:340:ILE:CD1	2.44	0.46
2:B:196:VAL:C	2:B:197:LEU:HD23	2.41	0.46
2:B:203:PHE:C	2:B:205:GLY:N	2.65	0.46
1:A:91:TYR:CG	1:A:92:MET:N	2.83	0.46
1:D:372:VAL:O	1:D:373:ASP:C	2.59	0.46
2:B:99:GLU:HA	2:B:103:GLN:CD	2.27	0.46
1:D:153:GLN:HE22	1:D:284:ASN:HB3	1.81	0.46
1:D:295:GLU:OE1	5:D:502:SMA:O8	2.34	0.46
1:D:386:GLU:C	1:D:387:GLY:O	2.58	0.46
2:E:151:ALA:O	2:E:174:GLY:HA3	2.15	0.46
2:B:154:ARG:NH1	2:B:154:ARG:CG	2.78	0.46
3:C:92:VAL:HG21	3:C:164:ARG:NH2	2.31	0.46
1:D:40:ASN:O	1:D:224:PRO:HG2	2.16	0.46
1:A:350:ASP:OD1	1:A:350:ASP:O	2.34	0.45
2:E:215:SER:O	2:E:218:GLN:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:TRP:CE3	1:D:23:LEU:HD11	2.51	0.45
1:A:319:ASN:ND2	1:A:319:ASN:O	2.46	0.45
3:C:74:LYS:HB3	3:C:75:PRO:HD2	1.98	0.45
1:A:64:VAL:HG22	3:C:41:GLN:NE2	2.31	0.45
1:A:422:GLN:HB2	1:A:426:GLU:OE2	2.17	0.45
1:D:225:THR:CG2	1:D:427:ASP:OD2	2.65	0.45
3:F:43:ASN:O	3:F:44:PRO:C	2.58	0.45
1:D:312:VAL:HG12	1:D:315:VAL:HG23	1.98	0.45
3:F:93:ASP:O	3:F:95:GLY:N	2.49	0.45
1:A:401:PHE:O	1:A:402:ALA:C	2.60	0.45
3:C:104:ASN:O	3:C:108:PRO:HA	2.17	0.45
2:E:203:PHE:O	2:E:205:GLY:N	2.37	0.45
1:A:114:ARG:C	1:A:114:ARG:CD	2.74	0.45
2:E:54:ASP:O	2:E:55:ILE:O	2.34	0.45
1:A:180:LEU:O	1:A:193:ARG:HD2	2.17	0.45
2:E:179:HIS:HE1	2:E:230:ASP:OD1	1.99	0.45
3:C:89:GLY:H	3:C:161:THR:HG21	1.79	0.45
1:D:4:ILE:O	1:D:5:PRO:C	2.60	0.45
2:E:127:ARG:HG3	2:E:127:ARG:HH11	1.81	0.45
3:F:75:PRO:HD2	3:F:131:VAL:HG23	1.99	0.45
1:D:313:TRP:HD1	1:D:316:MET:CE	2.30	0.45
2:E:210:MET:O	2:E:211:ALA:C	2.60	0.45
3:C:57:ASP:OD1	3:C:185:THR:HG23	2.17	0.45
3:C:134:HIS:HB3	7:C:500:FES:S1	2.57	0.45
1:D:342:VAL:HG23	1:D:343:MET:N	2.31	0.45
1:D:360:ARG:HB3	1:D:415:GLU:CD	2.41	0.45
1:A:229:VAL:HG13	1:A:241:THR:HG23	1.98	0.44
1:A:257:ALA:O	1:A:261:VAL:HG23	2.18	0.44
1:A:276:HIS:C	1:A:278:ASP:N	2.74	0.44
2:B:102:PRO:O	2:B:103:GLN:C	2.59	0.44
3:C:138:VAL:HG23	1:D:157:TRP:CH2	2.52	0.44
1:D:10:GLU:HG2	1:D:12:LYS:HE2	1.98	0.44
2:E:78:TYR:OH	2:E:86:HIS:O	2.25	0.44
1:A:276:HIS:HA	1:A:277:PRO:HD2	1.80	0.44
2:B:68:GLN:O	2:B:72:GLN:HG3	2.16	0.44
2:E:106:GLU:HA	2:E:106:GLU:OE1	2.18	0.44
1:A:105:PHE:HA	1:A:108:VAL:CG2	2.46	0.44
2:B:86:HIS:CE1	2:B:145:PRO:HD2	2.45	0.44
3:C:165:ILE:HD13	3:C:170:ALA:HB3	1.99	0.44
1:D:180:LEU:O	1:D:193:ARG:HD2	2.18	0.44
1:D:312:VAL:CG2	1:D:394:LEU:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:MET:CE	1:D:208:LEU:HD11	2.47	0.44
1:D:140:MET:HE1	1:D:340:ILE:HD11	1.98	0.44
3:F:154:CYS:O	3:F:155:HIS:CD2	2.71	0.44
3:F:186:THR:CG2	3:F:187:ILE:N	2.80	0.44
1:A:154:MET:CE	1:A:154:MET:HA	2.37	0.44
1:A:363:PHE:O	1:A:364:LYS:C	2.61	0.44
3:C:85:GLU:HB3	3:C:161:THR:OG1	2.17	0.44
2:B:78:TYR:CE2	2:B:83:SER:HB3	2.53	0.44
1:D:23:LEU:O	1:D:25:ILE:N	2.45	0.44
1:D:167:GLY:HA2	1:D:173:GLY:O	2.17	0.44
1:D:312:VAL:CG1	1:D:315:VAL:HG23	2.47	0.44
1:D:319:ASN:C	1:D:319:ASN:ND2	2.59	0.44
2:E:73:ARG:O	2:E:77:VAL:HG23	2.18	0.44
3:F:53:SER:OG	3:F:188:LYS:HE2	2.18	0.44
1:A:361:PRO:HG3	1:A:418:ASP:OD1	2.18	0.44
2:B:149:LEU:O	2:B:150:MET:C	2.61	0.44
1:A:317:LEU:HD23	1:A:317:LEU:C	2.43	0.44
3:C:43:ASN:O	3:C:44:PRO:C	2.61	0.44
2:B:138:VAL:O	2:B:139:SER:CB	2.59	0.43
1:A:360:ARG:O	1:A:364:LYS:HG3	2.17	0.43
1:A:376:VAL:O	1:A:379:TRP:HB3	2.19	0.43
2:B:96:LEU:HD23	2:B:96:LEU:HA	1.78	0.43
2:B:216:ASP:OD1	2:B:216:ASP:N	2.51	0.43
3:C:137:CYS:HB2	3:C:152:CYS:SG	2.58	0.43
1:A:46:ILE:HD11	1:A:47:TRP:CD2	2.53	0.43
3:C:119:MET:HE2	3:C:119:MET:HB3	1.82	0.43
1:D:246:PRO:HB2	2:E:276:LEU:HD21	1.99	0.43
2:E:197:LEU:CB	2:E:207:TRP:HD1	2.31	0.43
1:A:306:ARG:C	1:A:308:PHE:N	2.77	0.43
1:A:317:LEU:C	1:A:317:LEU:HD22	2.43	0.43
2:B:89:ARG:HG3	2:B:146:ASP:CG	2.43	0.43
3:C:111:PRO:HD2	3:C:116:ASN:ND2	2.33	0.43
1:D:13:THR:CB	1:D:16:GLU:HG3	2.47	0.43
1:D:411:LEU:O	1:D:412:GLY:C	2.61	0.43
1:A:13:THR:OG1	1:A:16:GLU:CD	2.62	0.43
4:A:500:HEM:CBC	4:A:500:HEM:HHD	2.46	0.43
2:E:84:ALA:O	2:E:143:MET:HE3	2.19	0.43
1:A:413:ILE:H	1:A:413:ILE:HG13	1.65	0.43
1:D:313:TRP:HD1	1:D:316:MET:HE1	1.83	0.43
1:D:319:ASN:ND2	1:D:319:ASN:O	2.45	0.43
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLY:HA3	1:D:193:ARG:NH2	2.33	0.43
2:E:55:ILE:HD11	2:E:179:HIS:NE2	2.33	0.43
2:E:138:VAL:HG12	2:E:143:MET:CE	2.47	0.43
1:A:229:VAL:CG1	1:A:241:THR:CG2	2.96	0.43
1:D:422:GLN:HE21	1:D:422:GLN:CA	2.32	0.43
2:E:59:PHE:CE1	2:E:241:MET:HG2	2.53	0.43
3:F:102:ALA:HB2	3:F:111:PRO:O	2.19	0.43
3:F:146:ASP:OD2	3:F:167:ARG:NH1	2.51	0.43
3:F:177:PRO:O	3:F:178:VAL:C	2.61	0.43
1:A:46:ILE:HD12	1:A:47:TRP:HA	2.01	0.43
1:A:122:LYS:HE2	1:A:350:ASP:CG	2.44	0.43
1:D:73:VAL:HG12	1:D:151:TRP:CE2	2.53	0.43
1:D:377:LEU:O	1:D:380:VAL:HG23	2.19	0.43
6:E:500:HEC:CMC	6:E:500:HEC:CBC	2.97	0.43
1:D:312:VAL:O	1:D:315:VAL:HB	2.19	0.43
1:A:366:TRP:CE3	1:A:407:ILE:HD11	2.51	0.42
2:B:184:GLY:O	2:B:200:ASN:HA	2.19	0.42
1:D:42:ASN:C	1:D:42:ASN:OD1	2.62	0.42
1:D:357:GLY:O	1:D:358:GLN:C	2.61	0.42
1:D:359:TYR:CD2	1:D:420:MET:HG3	2.54	0.42
1:A:386:GLU:O	1:A:387:GLY:C	2.63	0.42
1:A:12:LYS:O	1:A:13:THR:C	2.62	0.42
1:A:118:TYR:CD1	1:A:224:PRO:HA	2.54	0.42
3:C:132:CYS:C	3:C:134:HIS:H	2.26	0.42
3:F:134:HIS:CE1	3:F:135:LEU:HD12	2.53	0.42
1:A:99:ASN:O	1:A:102:SER:N	2.51	0.42
1:D:72:HIS:HE1	1:D:74:ASP:OD2	2.02	0.42
2:E:138:VAL:HG12	2:E:143:MET:CG	2.40	0.42
2:B:55:ILE:HD12	2:B:179:HIS:NE2	2.34	0.42
2:B:186:ASP:OD1	2:B:188:GLU:HG3	2.19	0.42
2:E:89:ARG:HD3	2:E:90:TYR:CZ	2.54	0.42
3:F:176:ILE:HG23	3:F:177:PRO:HD2	2.02	0.42
1:A:30:TYR:CE2	1:A:34:MET:HE3	2.55	0.42
2:E:245:GLU:OE1	2:E:245:GLU:HA	2.18	0.42
1:A:295:GLU:H	1:A:295:GLU:CD	2.27	0.42
1:A:357:GLY:O	1:A:358:GLN:C	2.62	0.42
1:A:361:PRO:HG3	1:A:418:ASP:CG	2.45	0.42
2:B:98:ASP:C	2:B:103:GLN:HG2	2.43	0.42
2:E:203:PHE:C	2:E:205:GLY:H	2.26	0.42
1:A:121:TYR:CD2	1:A:346:VAL:HG22	2.54	0.42
1:A:368:TRP:O	1:A:372:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:LEU:HD23	2:B:240:LEU:HA	1.73	0.42
2:B:248:MET:O	2:B:249:MET:C	2.61	0.42
1:D:108:VAL:O	1:D:112:ILE:HG13	2.20	0.42
1:D:133:MET:SD	4:D:501:HEM:HBC1	2.60	0.42
1:D:142:THR:HG21	1:D:202:PRO:HG3	2.02	0.42
1:D:386:GLU:O	1:D:387:GLY:C	2.62	0.42
4:D:500:HEM:CMB	4:D:500:HEM:CBB	2.97	0.42
2:E:269:LEU:HD23	2:E:269:LEU:HA	1.81	0.42
1:A:30:TYR:CD1	1:A:30:TYR:C	2.97	0.42
1:A:51:LEU:HD22	1:A:108:VAL:HG13	2.01	0.42
1:D:135:ILE:O	1:D:139:MET:HG3	2.19	0.42
1:A:49:ILE:HD12	1:A:49:ILE:HA	1.79	0.42
3:C:134:HIS:O	1:D:329:LYS:CE	2.68	0.42
3:C:80:ARG:NH2	3:C:124:GLU:OE2	2.51	0.41
2:E:154:ARG:HG2	2:E:154:ARG:HH11	1.85	0.41
2:E:253:GLN:O	2:E:257:VAL:HG23	2.20	0.41
2:B:68:GLN:O	2:B:71:LEU:HB2	2.21	0.41
1:D:317:LEU:CD2	1:D:321:LEU:CD1	2.97	0.41
2:E:258:SER:O	2:E:262:LEU:HG	2.19	0.41
3:F:53:SER:C	3:F:54:ILE:HG23	2.41	0.41
3:F:62:GLU:C	3:F:65:THR:HG1	2.28	0.41
1:A:61:THR:O	1:A:64:VAL:HG12	2.20	0.41
1:A:386:GLU:C	1:A:387:GLY:O	2.58	0.41
3:C:19:LEU:HA	3:C:19:LEU:HD12	1.83	0.41
3:C:160:ASP:HB3	3:C:166:ARG:HH11	1.85	0.41
1:D:127:VAL:O	1:D:128:THR:C	2.63	0.41
1:A:229:VAL:CG1	1:A:241:THR:HG23	2.51	0.41
1:A:360:ARG:HB2	1:A:363:PHE:HB3	2.02	0.41
2:B:200:ASN:N	2:B:206:ASN:O	2.47	0.41
1:D:63:ILE:HA	4:D:500:HEM:CBC	2.50	0.41
1:D:122:LYS:O	1:D:123:ALA:C	2.62	0.41
1:D:377:LEU:O	1:D:378:MET:C	2.64	0.41
1:A:409:PRO:O	1:A:410:LEU:C	2.63	0.41
1:D:13:THR:HB	1:D:16:GLU:H	1.84	0.41
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.85	0.41
1:A:25:ILE:O	1:A:25:ILE:HG13	2.20	0.41
1:D:276:HIS:HA	1:D:277:PRO:HD2	1.64	0.41
3:F:154:CYS:O	3:F:155:HIS:CG	2.73	0.41
1:A:118:TYR:CE1	1:A:224:PRO:HA	2.55	0.41
1:A:330:PHE:CZ	1:A:334:ILE:HD11	2.55	0.41
2:B:134:HIS:C	2:B:135:PHE:O	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:VAL:HA	1:D:155:SER:HB3	2.03	0.41
3:F:135:LEU:HA	3:F:135:LEU:HD23	1.80	0.41
1:A:416:LYS:HA	1:A:417:PRO:HD2	1.70	0.41
3:C:134:HIS:O	1:D:329:LYS:NZ	2.53	0.41
1:D:140:MET:CE	1:D:340:ILE:HD13	2.45	0.41
1:D:253:LEU:O	1:D:256:LEU:HB3	2.21	0.41
2:E:73:ARG:HD2	2:E:221:TYR:CZ	2.55	0.41
1:A:411:LEU:O	1:A:412:GLY:C	2.62	0.41
2:B:210:MET:HB2	6:B:500:HEC:C1D	2.51	0.41
3:C:53:SER:C	3:C:54:ILE:CG2	2.94	0.41
1:D:108:VAL:HG11	1:D:139:MET:SD	2.61	0.41
1:D:288:THR:HA	1:D:289:PRO:HD2	1.92	0.41
2:E:89:ARG:O	2:E:134:HIS:HD2	2.02	0.41
2:E:238:ALA:O	2:E:239:PHE:C	2.64	0.41
1:A:34:MET:O	1:A:35:ILE:C	2.62	0.41
1:D:136:TYR:CE2	1:D:140:MET:CE	3.01	0.41
1:D:201:LEU:HB2	1:D:202:PRO:HD3	2.03	0.41
1:D:416:LYS:HA	1:D:417:PRO:HD2	1.78	0.41
1:A:185:ALA:O	1:A:186:VAL:C	2.63	0.40
1:A:286:LEU:HD21	3:F:70:LYS:HG3	2.03	0.40
1:A:347:PRO:HD2	1:A:348:TRP:CE3	2.56	0.40
4:A:500:HEM:HBB2	4:A:500:HEM:HMB1	2.02	0.40
1:D:123:ALA:HA	1:D:124:PRO:HA	1.83	0.40
1:D:294:PRO:HG2	1:D:302:TYR:CG	2.57	0.40
3:F:102:ALA:O	3:F:104:ASN:N	2.54	0.40
1:A:121:TYR:CE2	1:A:346:VAL:CG2	2.94	0.40
1:A:426:GLU:O	1:A:427:ASP:C	2.63	0.40
2:B:197:LEU:CB	2:B:207:TRP:HD1	2.35	0.40
2:B:249:MET:HE3	2:B:249:MET:HB3	1.95	0.40
1:D:117:TYR:HB2	1:D:367:PHE:CZ	2.56	0.40
1:D:144:PHE:CD1	1:D:144:PHE:C	2.95	0.40
1:D:276:HIS:O	1:D:278:ASP:N	2.54	0.40
2:E:223:ASP:OD1	2:E:223:ASP:C	2.63	0.40
1:A:380:VAL:O	1:A:383:MET:N	2.26	0.40
3:F:92:VAL:HG11	3:F:164:ARG:NH2	2.37	0.40
1:A:6:HIS:HE1	1:A:8:HIS:HB3	1.86	0.40
1:A:306:ARG:O	1:A:308:PHE:N	2.54	0.40
1:D:176:ILE:HG21	1:D:176:ILE:HD13	1.81	0.40
1:A:181:LEU:HD22	1:A:186:VAL:N	2.36	0.40
2:B:175:PRO:CD	2:B:241:MET:HE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/450 (95%)	394 (92%)	26 (6%)	6 (1%)	9	23
1	D	426/450 (95%)	399 (94%)	21 (5%)	6 (1%)	9	23
2	B	200/263 (76%)	173 (86%)	20 (10%)	7 (4%)	3	6
2	E	200/263 (76%)	181 (90%)	14 (7%)	5 (2%)	4	11
3	C	172/190 (90%)	155 (90%)	12 (7%)	5 (3%)	3	9
3	F	172/190 (90%)	145 (84%)	20 (12%)	7 (4%)	2	5
All	All	1596/1806 (88%)	1447 (91%)	113 (7%)	36 (2%)	5	13

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	386	GLU
2	B	124	GLU
2	B	204	ALA
3	C	53	SER
3	C	94	LEU
1	D	13	THR
2	E	55	ILE
2	E	124	GLU
3	F	91	GLU
3	F	92	VAL
1	A	385	ALA
1	D	386	GLU
2	E	203	PHE
2	E	205	GLY
3	F	121	GLU
3	F	142	ASP
1	A	277	PRO
1	A	307	ALA
2	B	188	GLU

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Mol	Chain	Res	Type
2	B	203	PHE
2	B	227	ALA
1	D	277	PRO
2	E	204	ALA
3	F	53	SER
3	F	94	LEU
3	C	92	VAL
1	D	358	GLN
3	F	103	GLN
1	A	426	GLU
3	C	107	LYS
1	D	283	ALA
2	B	225	THR
3	C	54	ILE
2	B	205	GLY
1	D	110	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/376 (93%)	324 (92%)	27 (8%)	12	30
1	D	351/376 (93%)	318 (91%)	33 (9%)	8	21
2	B	166/205 (81%)	145 (87%)	21 (13%)	4	11
2	E	166/205 (81%)	153 (92%)	13 (8%)	11	29
3	C	131/146 (90%)	114 (87%)	17 (13%)	4	10
3	F	131/146 (90%)	113 (86%)	18 (14%)	3	9
All	All	1296/1454 (89%)	1167 (90%)	129 (10%)	7	19

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	ILE
1	A	50	VAL
1	A	64	VAL
1	A	108	VAL
1	A	112	ILE
1	A	134	LEU
1	A	174	GLU
1	A	190	THR
1	A	238	LYS
1	A	250	ILE
1	A	253	LEU
1	A	282	GLU
1	A	292	ILE
1	A	305	LEU
1	A	306	ARG
1	A	316	MET
1	A	317	LEU
1	A	319	ASN
1	A	369	LEU
1	A	394	LEU
1	A	408	LEU
1	A	413	ILE
1	A	420	MET
1	A	426	GLU
2	B	89	ARG
2	B	115	ASN
2	B	117	ASP
2	B	119	THR
2	B	123	THR
2	B	141	GLU
2	B	143	MET
2	B	148	SER
2	B	172	ILE
2	B	183	THR
2	B	208	ILE
2	B	217	ASP
2	B	219	VAL
2	B	223	ASP
2	B	231	GLN
2	B	232	MET
2	B	245	GLU

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Mol	Chain	Res	Type
2	B	252	LYS
2	B	254	VAL
2	B	258	SER
2	B	280	ILE
3	C	18	PHE
3	C	48	VAL
3	C	49	GLN
3	C	51	LEU
3	C	56	VAL
3	C	63	THR
3	C	86	ILE
3	C	92	VAL
3	C	98	ILE
3	C	105	SER
3	C	106	ASN
3	C	113	THR
3	C	115	GLU
3	C	131	VAL
3	C	132	CYS
3	C	162	SER
3	C	185	THR
1	D	7	ASP
1	D	8	HIS
1	D	13	THR
1	D	28	LEU
1	D	29	VAL
1	D	39	LYS
1	D	49	ILE
1	D	64	VAL
1	D	114	ARG
1	D	134	LEU
1	D	138	MET
1	D	174	GLU
1	D	190	THR
1	D	238	LYS
1	D	250	ILE
1	D	253	LEU
1	D	258	VAL
1	D	266	ILE
1	D	270	MET
1	D	278	ASP
1	D	292	ILE

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Mol	Chain	Res	Type
1	D	309	THR
1	D	311	ASP
1	D	312	VAL
1	D	317	LEU
1	D	319	ASN
1	D	369	LEU
1	D	376	VAL
1	D	380	VAL
1	D	394	LEU
1	D	416	LYS
1	D	420	MET
1	D	422	GLN
2	E	89	ARG
2	E	115	ASN
2	E	123	THR
2	E	124	GLU
2	E	141	GLU
2	E	143	MET
2	E	148	SER
2	E	183	THR
2	E	208	ILE
2	E	216	ASP
2	E	219	VAL
2	E	231	GLN
2	E	258	SER
3	F	18	PHE
3	F	48	VAL
3	F	51	LEU
3	F	61	VAL
3	F	62	GLU
3	F	63	THR
3	F	65	THR
3	F	69	VAL
3	F	76	VAL
3	F	80	ARG
3	F	94	LEU
3	F	106	ASN
3	F	107	LYS
3	F	115	GLU
3	F	140	ILE
3	F	161	THR
3	F	165	ILE

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Mol	Chain	Res	Type
3	F	185	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	221	ASN
1	A	276	HIS
1	A	291	HIS
1	A	319	ASN
2	B	69	HIS
2	B	103	GLN
2	B	108	GLN
2	B	115	ASN
2	B	134	HIS
2	B	179	HIS
2	B	273	ASN
3	C	40	ASN
3	C	43	ASN
3	C	49	GLN
1	D	8	HIS
1	D	192	ASN
1	D	319	ASN
1	D	422	GLN
2	E	68	GLN
2	E	115	ASN
2	E	134	HIS
3	F	40	ASN
3	F	43	ASN
3	F	49	GLN
3	F	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	500	1	50,50,50	2.09	11 (22%)	67,82,82	1.80	15 (22%)
5	SMA	D	502	-	38,38,38	1.86	7 (18%)	47,52,52	1.90	18 (38%)
7	FES	F	500	3	0,4,4	-	-	-	-	-
4	HEM	D	501	1	50,50,50	1.86	7 (14%)	67,82,82	1.37	9 (13%)
5	SMA	A	502	-	38,38,38	1.89	10 (26%)	47,52,52	2.10	16 (34%)
4	HEM	D	500	1	50,50,50	1.89	10 (20%)	67,82,82	1.67	15 (22%)
6	HEC	B	500	2	46,50,50	1.81	6 (13%)	58,82,82	2.34	15 (25%)
4	HEM	A	501	1	50,50,50	1.78	7 (14%)	67,82,82	1.54	10 (14%)
7	FES	C	500	3	0,4,4	-	-	-	-	-
6	HEC	E	500	2	46,50,50	1.92	7 (15%)	58,82,82	2.33	13 (22%)

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
4	HEM	A	500	1	-	5/14/54/54	-
5	SMA	D	502	-	-	3/34/34/34	0/2/2/2
7	FES	F	500	3	-	-	0/1/1/1
4	HEM	D	501	1	-	4/14/54/54	-
5	SMA	A	502	-	-	1/34/34/34	0/2/2/2
4	HEM	D	500	1	-	4/14/54/54	-
6	HEC	B	500	2	-	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	501	1	-	3/14/54/54	-
7	FES	C	500	3	-	-	0/1/1/1
6	HEC	E	500	2	-	8/14/54/54	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	HEM	C3D-C2D	8.17	1.54	1.36
4	D	500	HEM	C3D-C2D	7.76	1.53	1.36
5	D	502	SMA	C20-C19	7.30	1.38	1.33
4	D	501	HEM	C3D-C2D	7.15	1.52	1.36
4	D	501	HEM	FE-ND	7.13	2.16	1.94
6	E	500	HEC	CAC-C3C	6.49	1.56	1.35
4	A	501	HEM	C3D-C2D	6.23	1.50	1.36
6	B	500	HEC	CAC-C3C	6.03	1.54	1.35
4	A	501	HEM	FE-ND	5.98	2.13	1.94
6	B	500	HEC	CAB-C3B	5.89	1.54	1.35
6	E	500	HEC	CAB-C3B	5.64	1.53	1.35
6	E	500	HEC	C3D-C2D	5.58	1.53	1.38
5	A	502	SMA	C20-C19	5.28	1.37	1.33
6	B	500	HEC	C3D-C2D	5.21	1.52	1.38
4	A	500	HEM	FE-NC	5.09	2.12	1.95
4	A	500	HEM	FE-ND	5.09	2.10	1.94
4	D	500	HEM	FE-NC	3.90	2.08	1.95
4	A	500	HEM	FE-NB	3.85	2.06	1.94
4	D	500	HEM	FE-NB	3.71	2.06	1.94
5	A	502	SMA	C3-C2	3.66	1.41	1.34
4	D	500	HEM	FE-NA	3.65	2.07	1.95
5	D	502	SMA	C14-C15	-3.28	1.39	1.50
5	A	502	SMA	C14-C15	-3.22	1.39	1.50
4	D	500	HEM	CMB-C2B	3.21	1.57	1.50
5	D	502	SMA	C3-C4	-3.20	1.40	1.47
5	D	502	SMA	C18-C19	-3.18	1.39	1.46
4	A	501	HEM	CAB-C3B	3.18	1.55	1.47
4	A	500	HEM	CMC-C2C	3.15	1.57	1.50
5	A	502	SMA	O1-C8A	-3.11	1.33	1.38
5	A	502	SMA	C3-C4	-3.11	1.40	1.47
4	A	501	HEM	CAC-C3C	3.10	1.55	1.47
4	D	501	HEM	CMA-C3A	3.04	1.57	1.50
5	D	502	SMA	C4A-C4	-3.01	1.38	1.46
4	A	500	HEM	CMB-C2B	3.01	1.56	1.50
5	A	502	SMA	C4A-C4	-3.00	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	500	HEM	CMC-C2C	2.99	1.56	1.50
4	A	501	HEM	CMA-C3A	2.90	1.56	1.50
5	A	502	SMA	O5-C5	2.86	1.41	1.37
4	D	500	HEM	FE-ND	2.81	2.03	1.94
4	D	501	HEM	CAC-C3C	2.81	1.54	1.47
5	D	502	SMA	C3-C2	2.71	1.39	1.34
4	D	500	HEM	CAC-C3C	2.71	1.54	1.47
4	D	501	HEM	CAB-C3B	2.68	1.54	1.47
4	A	500	HEM	CMA-C3A	2.63	1.56	1.50
4	D	500	HEM	CMA-C3A	2.63	1.56	1.50
5	A	502	SMA	C18-C19	-2.62	1.40	1.46
4	A	500	HEM	CAC-C3C	2.59	1.54	1.47
4	A	500	HEM	FE-NA	2.55	2.03	1.95
4	D	501	HEM	FE-NB	2.51	2.02	1.94
5	A	502	SMA	C9-C2	2.49	1.56	1.49
4	A	501	HEM	FE-NB	2.42	2.02	1.94
6	E	500	HEC	C3B-C2B	-2.40	1.33	1.41
6	E	500	HEC	CMC-C2C	2.39	1.55	1.50
4	A	501	HEM	C4D-ND	-2.37	1.36	1.40
6	B	500	HEC	C3B-C2B	-2.36	1.33	1.41
4	A	500	HEM	CAB-C3B	2.32	1.53	1.47
4	A	500	HEM	CMD-C2D	2.31	1.55	1.50
5	A	502	SMA	O7-C7M	2.25	1.49	1.42
6	B	500	HEC	C2A-C3A	-2.25	1.31	1.36
5	D	502	SMA	C9-C2	2.21	1.55	1.49
6	E	500	HEC	C2A-C3A	-2.15	1.32	1.36
4	D	501	HEM	FE-NA	2.11	2.02	1.95
6	E	500	HEC	CHB-C1B	-2.09	1.34	1.39
6	B	500	HEC	C3C-C2C	-2.03	1.34	1.41
4	D	500	HEM	C3B-C2B	-2.02	1.33	1.37

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	500	HEC	CBB-CAB-C3B	-10.46	106.53	127.43
6	B	500	HEC	CBB-CAB-C3B	-9.31	108.82	127.43
6	B	500	HEC	CBC-CAC-C3C	-8.63	110.18	127.43
6	E	500	HEC	CBC-CAC-C3C	-7.91	111.62	127.43
4	A	500	HEM	C4D-ND-C1D	6.02	112.33	105.21
4	D	500	HEM	C4D-ND-C1D	5.37	111.57	105.21
5	A	502	SMA	O5-C5-C4A	5.33	123.39	115.84
4	D	501	HEM	C4D-ND-C1D	4.61	110.66	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	HEM	CAD-CBD-CGD	-4.52	101.68	113.67
4	A	501	HEM	CAD-C3D-C4D	4.49	132.53	124.70
6	E	500	HEC	CAA-C2A-C3A	-4.25	119.90	127.87
4	A	501	HEM	C4D-ND-C1D	4.15	110.12	105.21
5	A	502	SMA	C26-C19-C18	4.14	124.41	118.09
6	E	500	HEC	CAA-C2A-C1A	4.01	133.01	124.85
4	D	500	HEM	C4B-C3B-C2B	3.97	110.93	107.28
4	D	501	HEM	CAD-CBD-CGD	-3.92	103.27	113.67
6	B	500	HEC	CAA-C2A-C3A	-3.89	120.58	127.87
5	A	502	SMA	O1-C2-C3	-3.88	118.40	121.81
5	D	502	SMA	O5-C5-C4A	3.87	121.32	115.84
4	A	500	HEM	C4C-C3C-C2C	3.85	110.16	106.81
6	B	500	HEC	CHB-C4A-NA	3.83	128.62	124.45
6	B	500	HEC	CAA-C2A-C1A	3.78	132.54	124.85
4	A	500	HEM	CHC-C4B-NB	3.78	128.49	124.42
6	B	500	HEC	C4D-ND-C1D	3.72	111.89	105.82
5	A	502	SMA	C13-C14-C15	-3.72	104.07	112.11
6	E	500	HEC	C4D-ND-C1D	3.72	111.89	105.82
4	A	501	HEM	CMD-C2D-C1D	3.71	130.82	125.03
4	D	500	HEM	CHC-C4B-NB	3.67	128.38	124.42
4	A	501	HEM	CAD-C3D-C2D	-3.63	121.07	127.87
5	D	502	SMA	C22-C11-C10	3.62	115.94	110.34
5	D	502	SMA	O7-C7-C8	3.61	118.30	114.53
5	A	502	SMA	C23-O12-C12	-3.53	105.41	114.47
5	A	502	SMA	C22-C11-C10	3.42	115.63	110.34
4	D	500	HEM	C3B-C4B-NB	-3.42	107.01	109.47
6	E	500	HEC	CHB-C4A-NA	3.32	128.07	124.45
5	A	502	SMA	O7-C7-C8	3.24	117.92	114.53
5	A	502	SMA	C22-C11-C12	-3.24	105.85	111.14
4	A	500	HEM	CMC-C2C-C1C	3.23	130.41	124.73
4	A	500	HEM	CHA-C1A-NA	3.16	129.59	123.86
4	A	501	HEM	C1D-C2D-C3D	-3.14	103.68	106.98
6	B	500	HEC	CAA-CBA-CGA	-3.12	105.40	113.67
5	D	502	SMA	C26-C19-C18	3.11	122.84	118.09
6	E	500	HEC	O1A-CGA-CBA	-3.06	113.38	123.09
4	D	501	HEM	CMD-C2D-C1D	3.04	129.79	125.03
4	A	500	HEM	C4B-C3B-C2B	3.03	110.07	107.28
5	D	502	SMA	C13-C14-C15	-2.99	105.66	112.11
5	A	502	SMA	C6-C5-C4A	-2.96	116.63	121.79
4	D	500	HEM	C4C-C3C-C2C	2.95	109.37	106.81
4	D	501	HEM	CAD-C3D-C4D	2.93	129.80	124.70
4	D	500	HEM	CHA-C4D-ND	2.89	127.94	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	HEM	CBA-CAA-C2A	-2.88	104.56	112.53
4	A	500	HEM	C3B-C4B-NB	-2.87	107.41	109.47
5	D	502	SMA	O12-C12-C13	-2.81	103.82	107.97
4	A	500	HEM	C1B-NB-C4B	2.81	108.54	105.21
6	E	500	HEC	CAD-CBD-CGD	-2.75	106.37	113.67
4	D	500	HEM	CMC-C2C-C1C	2.73	129.53	124.73
4	A	500	HEM	CMA-C3A-C4A	2.72	129.56	125.42
5	A	502	SMA	C26-C19-C20	-2.69	116.20	123.63
6	B	500	HEC	CHA-C4D-ND	2.69	128.73	123.86
6	E	500	HEC	O2A-CGA-CBA	2.66	122.39	114.00
4	D	500	HEM	CBA-CAA-C2A	-2.64	105.23	112.53
4	A	500	HEM	CMD-C2D-C1D	2.63	129.14	125.03
5	A	502	SMA	C25-O14-C14	-2.59	107.05	112.99
6	B	500	HEC	CBD-CAD-C3D	-2.58	105.41	112.53
5	D	502	SMA	O14-C14-C15	2.55	118.47	111.05
6	E	500	HEC	CBD-CAD-C3D	-2.53	105.55	112.53
5	D	502	SMA	C14-C15-C16	-2.51	120.80	125.88
6	B	500	HEC	O1A-CGA-CBA	-2.49	115.18	123.09
5	A	502	SMA	O12-C12-C13	2.49	111.64	107.97
5	D	502	SMA	C23-O12-C12	-2.46	108.15	114.47
4	D	501	HEM	C1D-C2D-C3D	-2.45	104.40	106.98
5	D	502	SMA	C3M-C3-C2	-2.45	119.63	123.28
4	D	500	HEM	CHD-C1D-ND	2.44	127.05	124.42
4	A	500	HEM	C2D-C1D-ND	-2.41	107.12	109.90
6	B	500	HEC	CMC-C2C-C1C	-2.40	121.76	125.42
5	A	502	SMA	C11-C12-C13	2.40	120.69	114.29
5	D	502	SMA	O5-C5-C6	-2.40	119.95	124.08
5	A	502	SMA	O5-C5-C6	-2.39	119.97	124.08
4	A	500	HEM	C2A-C1A-NA	-2.38	107.51	110.15
5	D	502	SMA	C26-C19-C20	-2.38	117.07	123.63
4	D	500	HEM	CBB-CAB-C3B	-2.37	115.69	127.53
4	D	501	HEM	O1D-CGD-CBD	-2.36	115.59	123.09
4	A	501	HEM	O2D-CGD-CBD	2.36	121.46	114.00
6	B	500	HEC	CAD-CBD-CGD	-2.35	107.44	113.67
6	E	500	HEC	CHA-C1A-C2A	2.35	128.57	124.86
5	D	502	SMA	C9-C10-C11	-2.33	110.10	114.46
4	D	500	HEM	CBD-CAD-C3D	-2.33	106.10	112.53
6	E	500	HEC	CHA-C4D-ND	2.32	128.07	123.86
6	B	500	HEC	CHC-C1C-NC	2.32	128.07	123.86
5	D	502	SMA	O1-C2-C3	-2.31	119.78	121.81
4	A	501	HEM	CHC-C4B-NB	2.28	126.88	124.42
4	D	500	HEM	CAA-CBA-CGA	-2.28	107.62	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	500	HEM	CMB-C2B-C1B	2.23	128.52	125.03
5	D	502	SMA	C21-C20-C19	-2.23	115.78	127.72
6	B	500	HEC	O1D-CGD-CBD	-2.21	116.08	123.09
4	A	500	HEM	CMC-C2C-C3C	-2.21	123.08	128.43
5	D	502	SMA	O1-C2-C9	2.20	114.78	110.12
4	D	500	HEM	C1B-NB-C4B	2.19	107.80	105.21
6	B	500	HEC	CHD-C1D-ND	2.17	127.80	123.86
4	D	501	HEM	CHD-C4C-NC	2.16	126.81	124.45
5	A	502	SMA	C21-C20-C19	-2.14	116.26	127.72
6	E	500	HEC	CAA-CBA-CGA	-2.14	108.00	113.67
4	A	501	HEM	CHD-C4C-NC	2.13	126.77	124.45
4	D	500	HEM	C2A-C1A-NA	-2.12	107.80	110.15
4	A	501	HEM	CHA-C1A-NA	2.10	127.67	123.86
5	D	502	SMA	C11-C12-C13	2.09	119.86	114.29
5	A	502	SMA	C7-C6-C5	2.08	123.00	118.98
5	D	502	SMA	C16-C17-C18	-2.05	119.81	124.65
4	D	501	HEM	C1B-NB-C4B	2.04	107.62	105.21
4	D	501	HEM	CHA-C1A-NA	2.02	127.52	123.86
4	A	500	HEM	CBC-CAC-C3C	-2.01	117.47	127.53

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	500	HEC	C1A-C2A-CAA-CBA
6	B	500	HEC	C3A-C2A-CAA-CBA
6	B	500	HEC	C2C-C3C-CAC-CBC
6	B	500	HEC	C4C-C3C-CAC-CBC
6	E	500	HEC	C3A-C2A-CAA-CBA
6	E	500	HEC	C2C-C3C-CAC-CBC
6	E	500	HEC	C4C-C3C-CAC-CBC
6	E	500	HEC	C1A-C2A-CAA-CBA
4	D	500	HEM	C3D-CAD-CBD-CGD
5	D	502	SMA	O1-C2-C9-C10
6	B	500	HEC	C4B-C3B-CAB-CBB
6	B	500	HEC	C2B-C3B-CAB-CBB
6	E	500	HEC	C2B-C3B-CAB-CBB
6	E	500	HEC	CAD-CBD-CGD-O1D
4	A	500	HEM	C3D-CAD-CBD-CGD
6	B	500	HEC	CAD-CBD-CGD-O1D
4	D	501	HEM	CAA-CBA-CGA-O1A
4	A	501	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
4	D	501	HEM	CAA-CBA-CGA-O2A
4	A	500	HEM	CAA-CBA-CGA-O1A
4	A	501	HEM	CAA-CBA-CGA-O2A
6	B	500	HEC	CAD-CBD-CGD-O2D
6	E	500	HEC	CAD-CBD-CGD-O2D
4	A	500	HEM	CAA-CBA-CGA-O2A
4	D	500	HEM	CAA-CBA-CGA-O2A
4	D	500	HEM	CAA-CBA-CGA-O1A
4	A	500	HEM	CAD-CBD-CGD-O2D
5	A	502	SMA	C3-C2-C9-C10
5	D	502	SMA	C3-C2-C9-C10
4	D	501	HEM	CAD-CBD-CGD-O2D
4	D	501	HEM	CAD-CBD-CGD-O1D
6	E	500	HEC	C4B-C3B-CAB-CBB
4	D	500	HEM	CAD-CBD-CGD-O2D
4	A	500	HEM	CAD-CBD-CGD-O1D
4	A	501	HEM	C2A-CAA-CBA-CGA
6	B	500	HEC	CAA-CBA-CGA-O2A
5	D	502	SMA	C11-C10-C9-C2

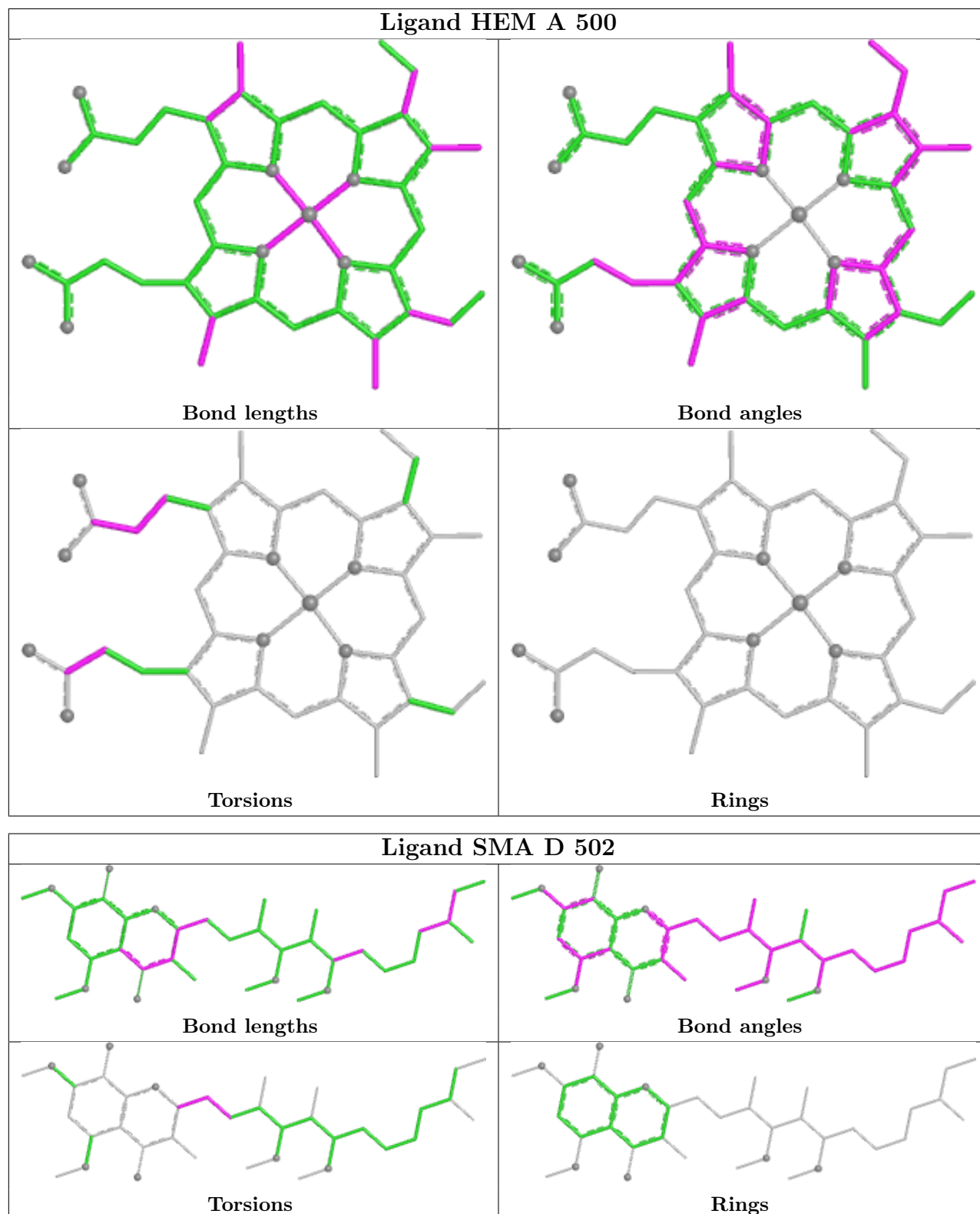
There are no ring outliers.

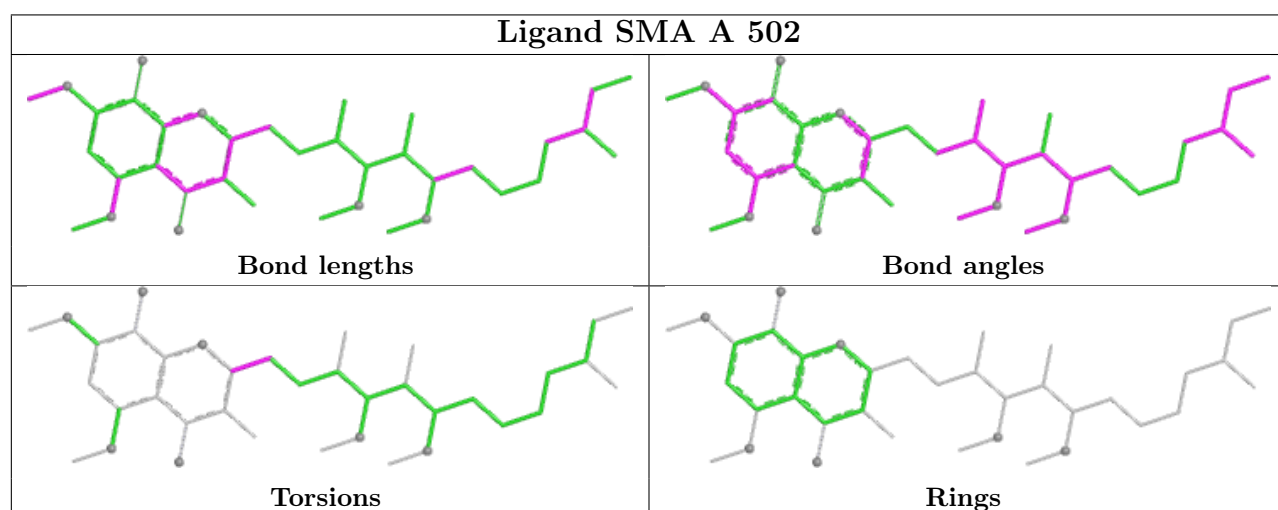
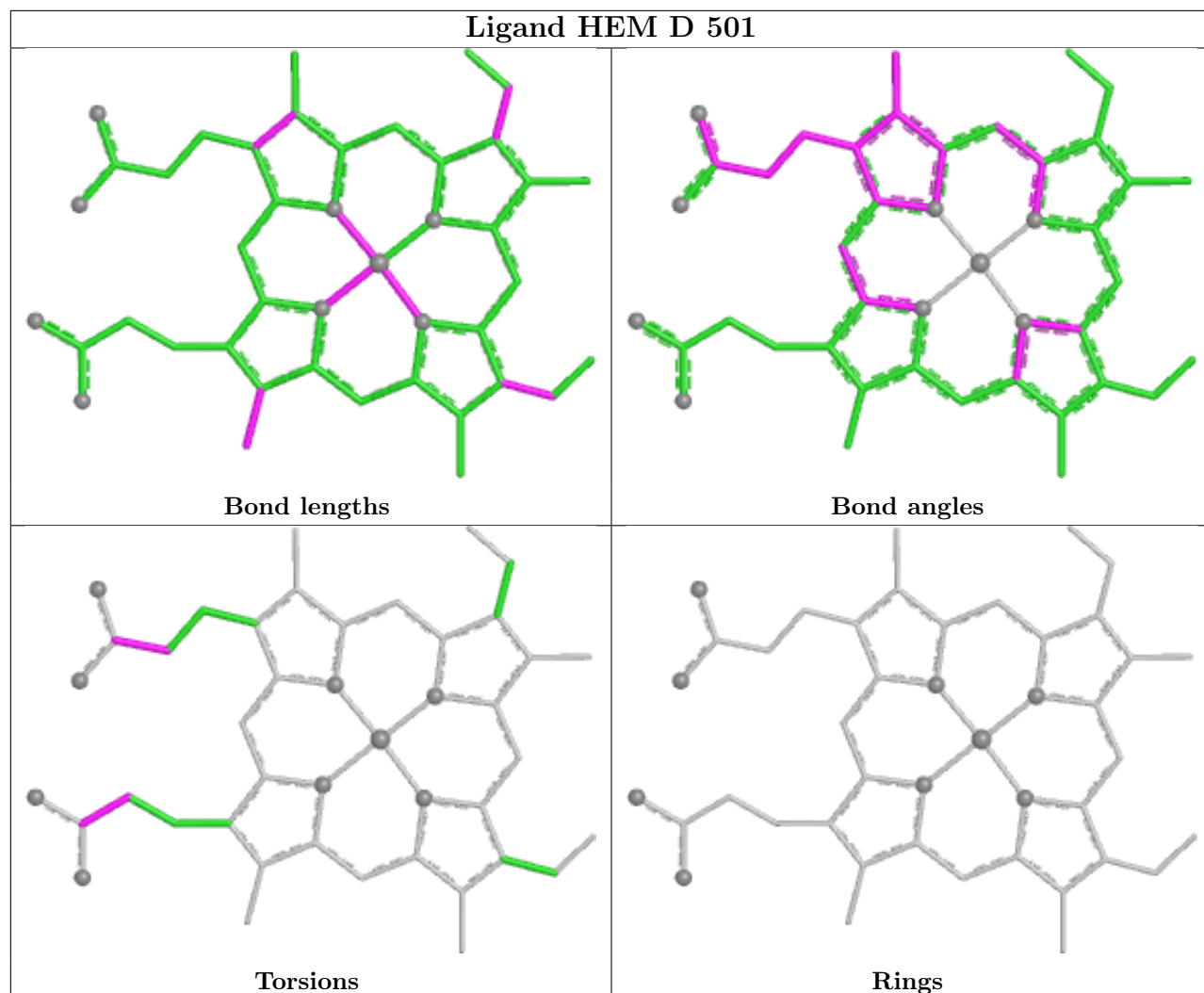
10 monomers are involved in 50 short contacts:

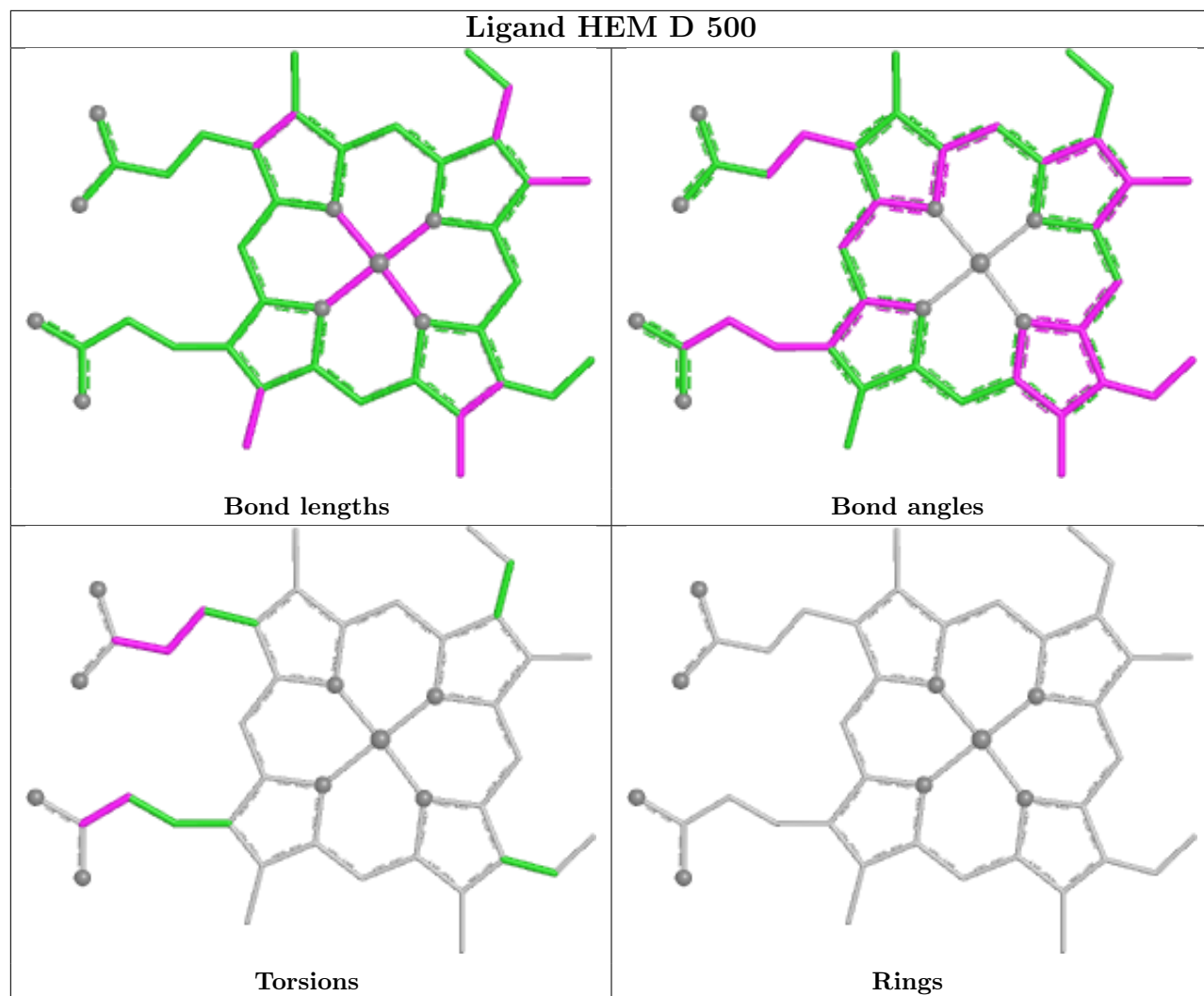
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	HEM	15	0
5	D	502	SMA	2	0
7	F	500	FES	1	0
4	D	501	HEM	5	0
5	A	502	SMA	2	0
4	D	500	HEM	13	0
6	B	500	HEC	3	0
4	A	501	HEM	3	0
7	C	500	FES	1	0
6	E	500	HEC	5	0

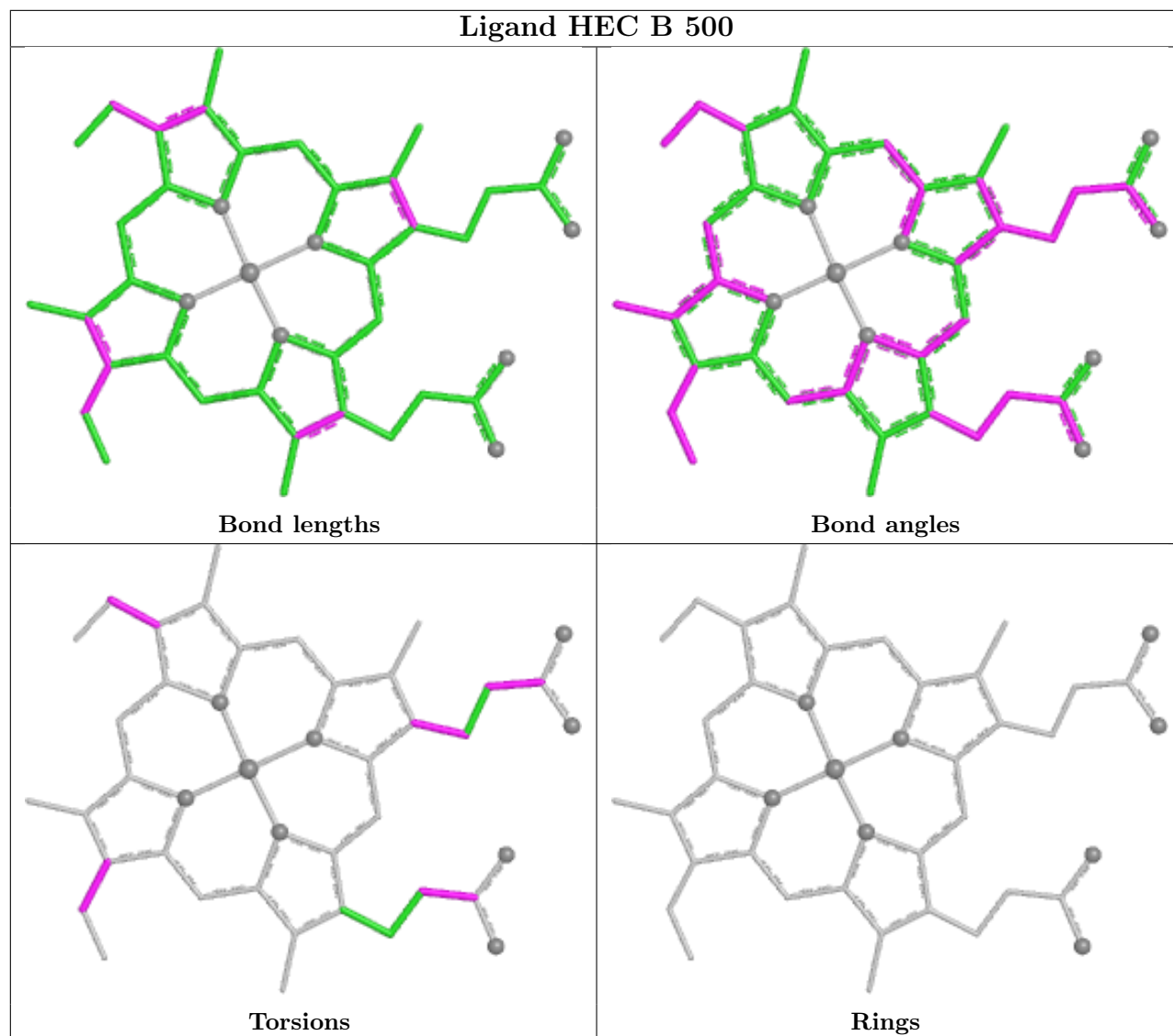
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

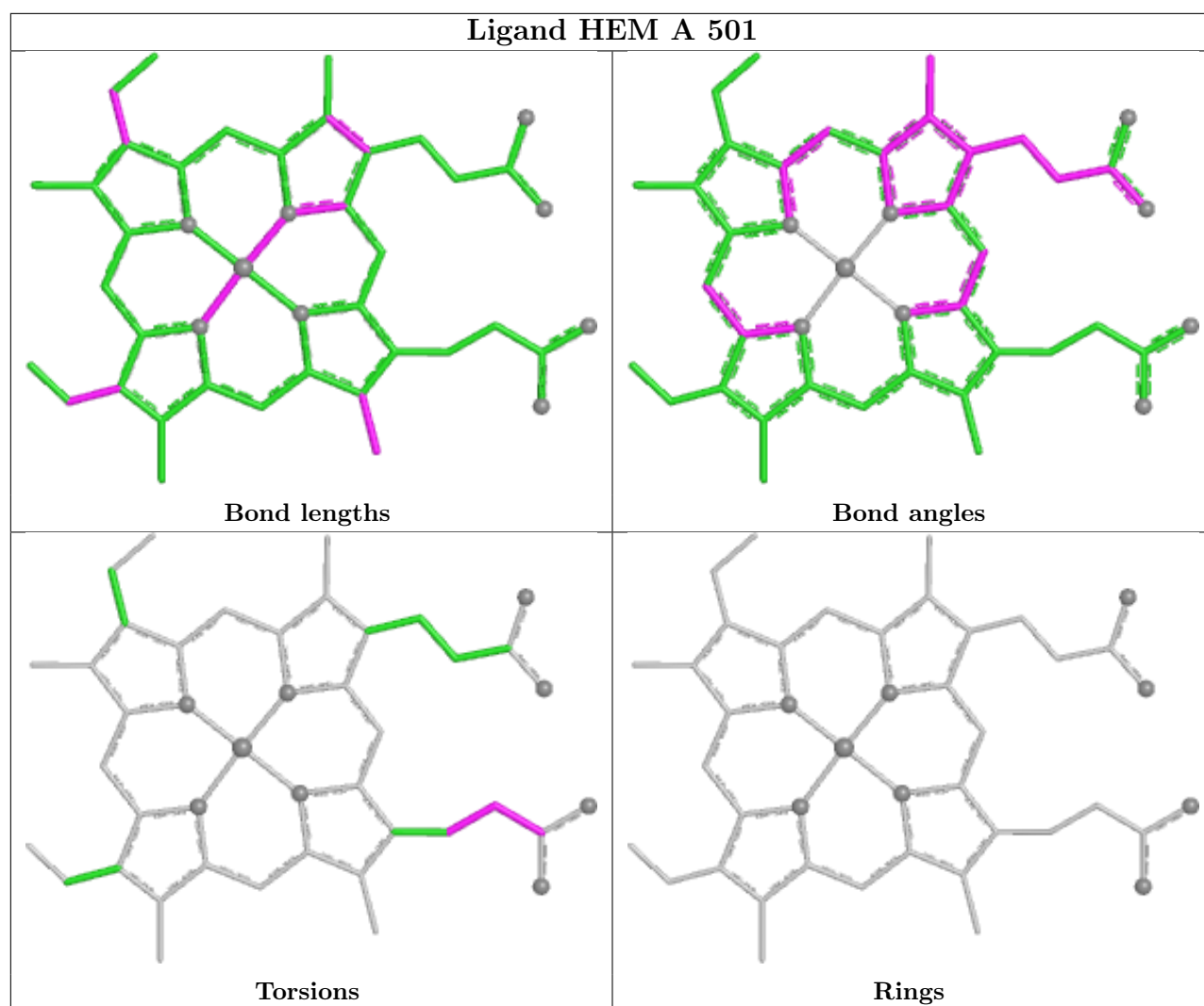
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

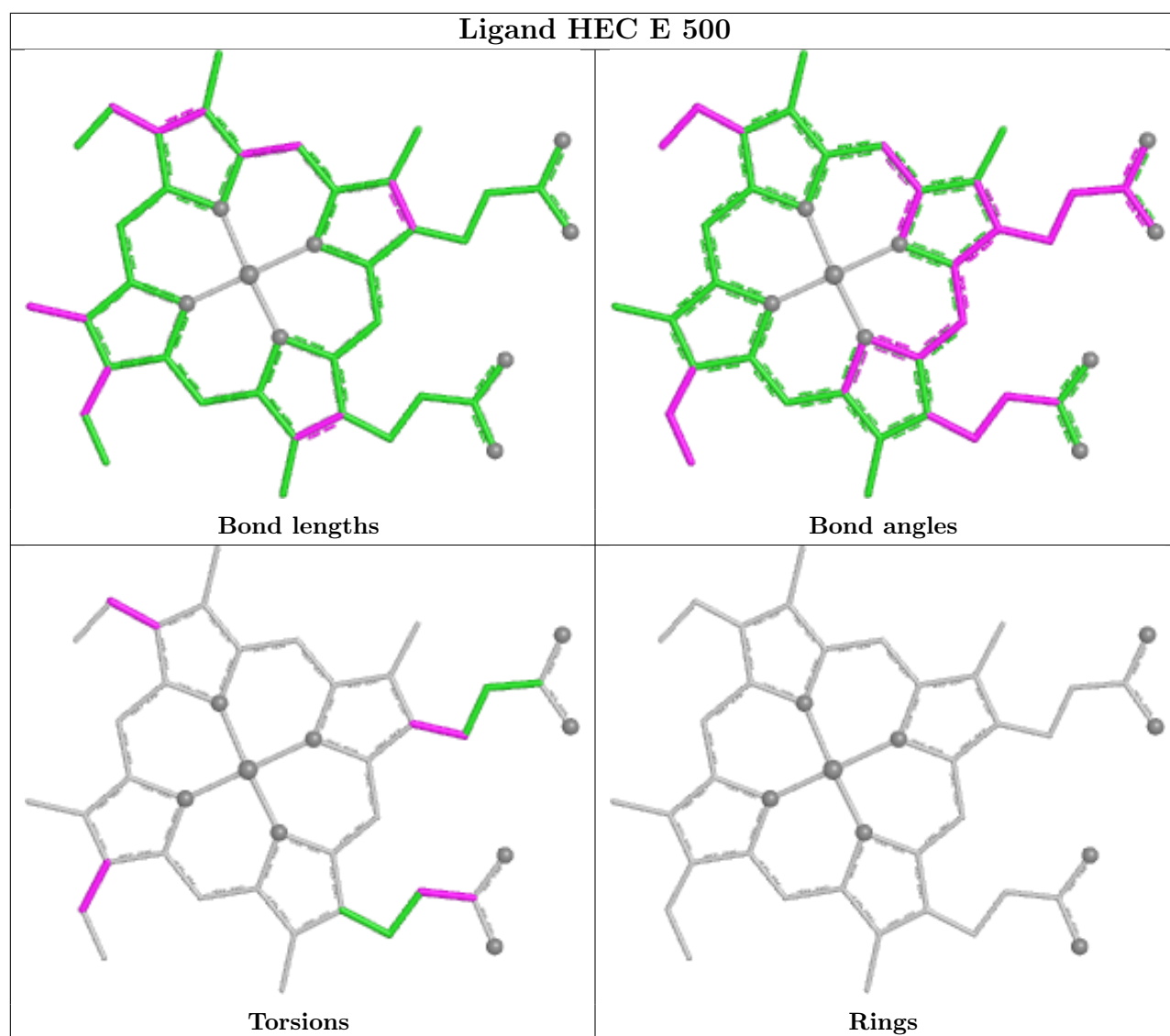












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/450 (95%)	0.04	6 (1%) 73 72	9, 21, 41, 61	0
1	D	428/450 (95%)	-0.15	6 (1%) 73 72	9, 22, 44, 61	0
2	B	206/263 (78%)	0.43	12 (5%) 29 25	18, 33, 54, 69	0
2	E	206/263 (78%)	0.27	8 (3%) 43 39	18, 35, 55, 71	0
3	C	174/190 (91%)	0.43	11 (6%) 26 23	12, 31, 46, 54	0
3	F	174/190 (91%)	0.57	16 (9%) 14 12	13, 38, 59, 62	0
All	All	1616/1806 (89%)	0.17	59 (3%) 45 41	9, 27, 52, 71	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	54	ASP	5.7
3	F	184	ASP	4.7
3	F	50	ALA	4.3
3	F	121	GLU	4.1
1	D	430	ALA	3.9
3	F	122	ALA	3.8
1	D	311	ASP	3.8
3	F	190	GLY	3.7
3	C	184	ASP	3.5
2	E	122	GLU	3.5
2	E	55	ILE	3.3
3	F	96	GLN	3.3
1	A	311	ASP	3.3
2	B	190	LYS	3.1
3	C	91	GLU	3.0
1	A	430	ALA	3.0
2	B	205	GLY	2.9
2	B	222	GLU	2.8
2	E	172	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	8	HIS	2.8
2	B	172	ILE	2.8
2	B	55	ILE	2.7
2	B	204	ALA	2.7
2	B	122	GLU	2.7
3	C	120	ASP	2.7
3	F	92	VAL	2.6
2	E	121	PRO	2.6
3	F	83	GLU	2.5
1	D	320	TRP	2.5
3	F	125	TRP	2.5
3	F	180	GLU	2.5
1	A	387	GLY	2.4
1	A	388	ILE	2.4
3	C	88	ALA	2.4
3	C	94	LEU	2.4
2	E	204	ALA	2.4
3	C	54	ILE	2.3
3	C	190	GLY	2.3
3	F	62	GLU	2.3
3	F	142	ASP	2.3
1	D	387	GLY	2.2
1	D	385	ALA	2.2
3	C	18	PHE	2.2
2	B	207	TRP	2.1
1	A	426	GLU	2.1
2	B	117	ASP	2.1
3	C	114	ASP	2.1
2	B	256	PHE	2.1
3	C	125	TRP	2.1
3	C	21	TYR	2.1
2	E	196	VAL	2.1
2	B	54	ASP	2.1
3	F	51	LEU	2.1
3	F	64	GLY	2.1
1	A	382	ALA	2.0
3	F	179	ALA	2.0
2	E	190	LYS	2.0
3	F	181	PHE	2.0
2	B	144	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

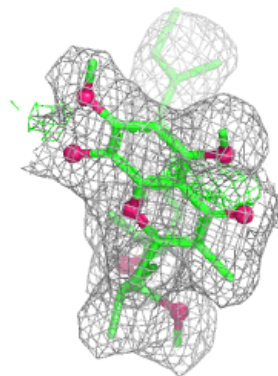
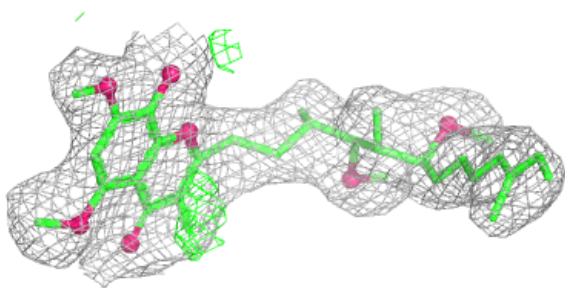
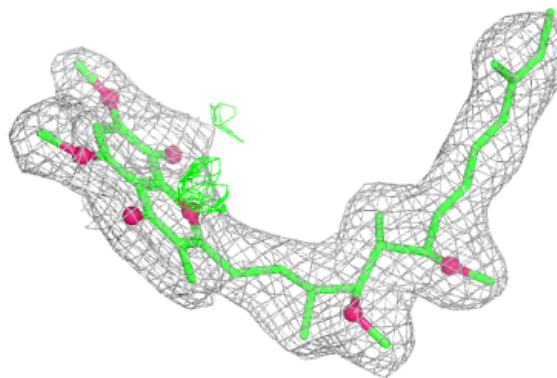
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SMA	A	502	37/37	0.95	0.09	12,17,33,36	0
6	HEC	B	500	43/43	0.96	0.10	19,26,37,42	0
6	HEC	E	500	43/43	0.96	0.09	24,29,34,36	0
5	SMA	D	502	37/37	0.97	0.07	6,14,37,41	0
4	HEM	D	500	43/43	0.97	0.08	12,16,23,25	0
4	HEM	A	500	43/43	0.97	0.08	9,14,22,25	0
4	HEM	A	501	43/43	0.98	0.07	9,14,16,18	0
4	HEM	D	501	43/43	0.98	0.07	7,17,26,27	0
7	FES	C	500	4/4	0.99	0.04	22,26,26,28	0
7	FES	F	500	4/4	0.99	0.04	16,20,22,23	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.

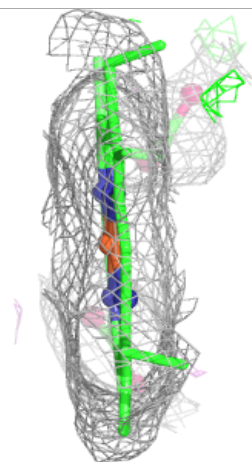
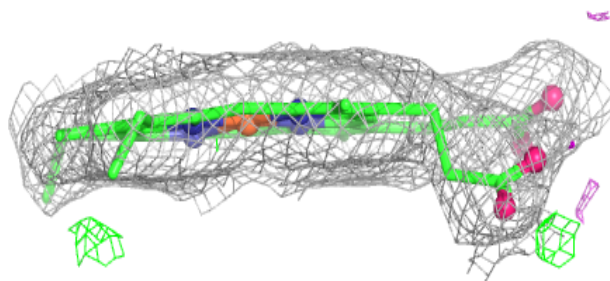
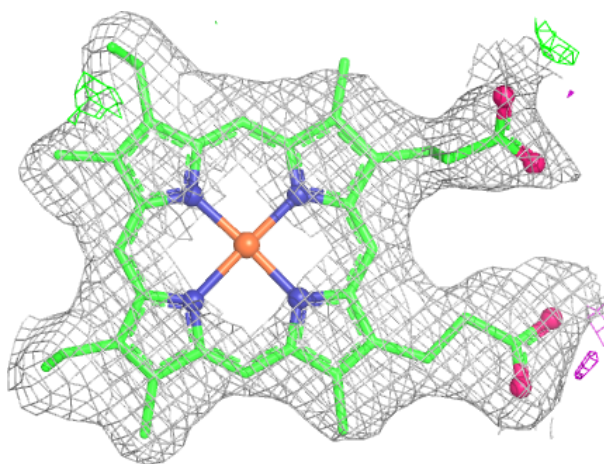
Electron density around SMA A 502:

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



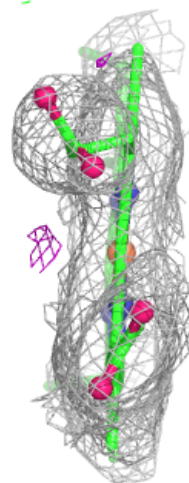
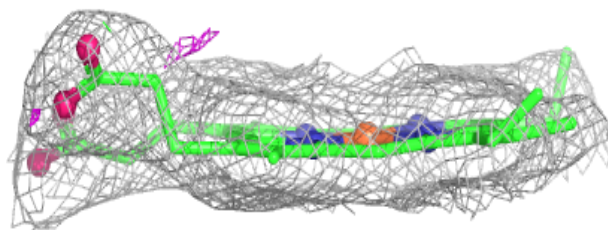
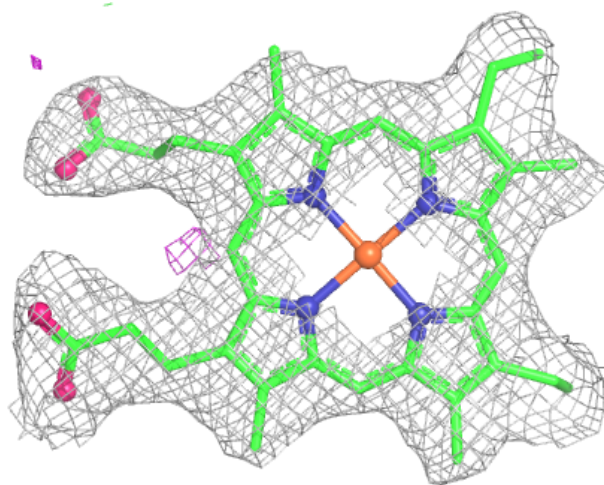
Electron density around HEC B 500:

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



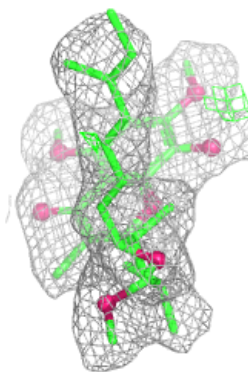
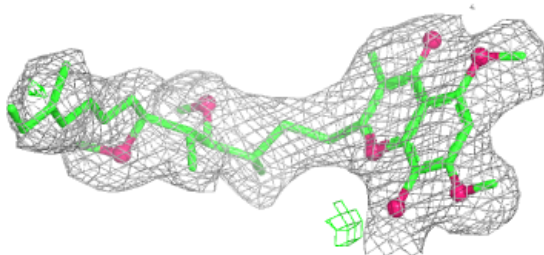
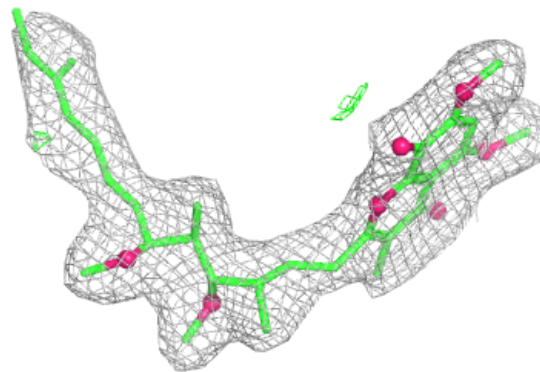
Electron density around HEC E 500:

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



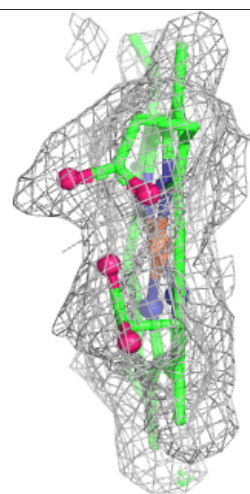
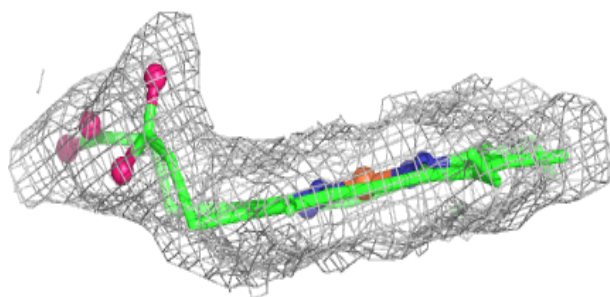
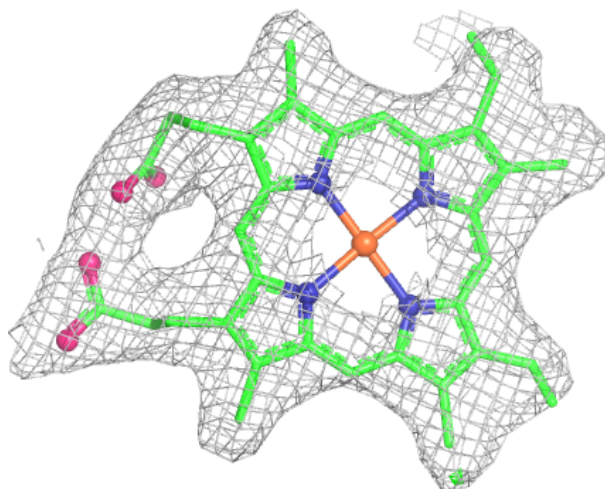
Electron density around SMA D 502:

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



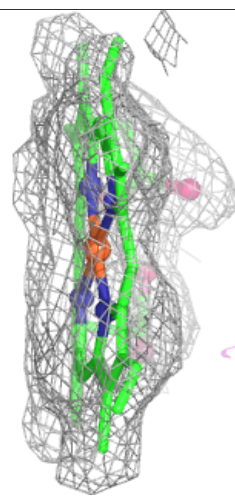
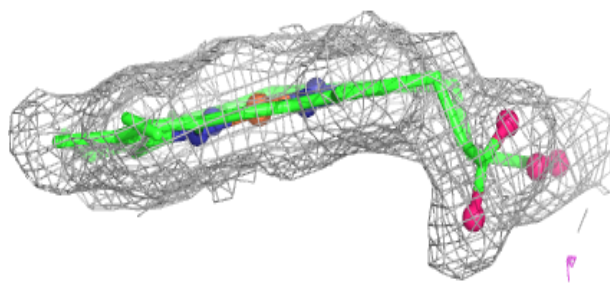
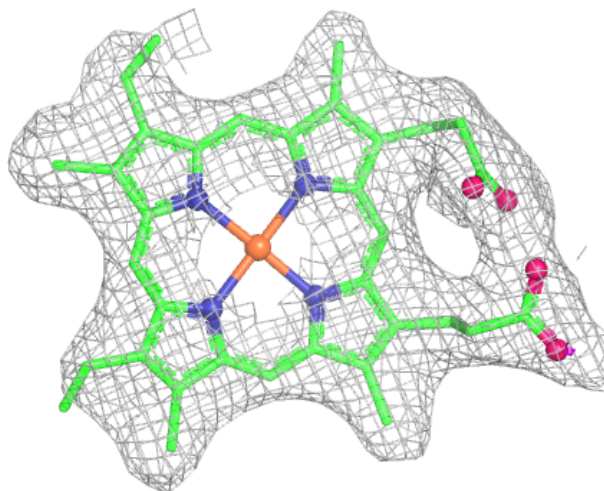
Electron density around HEM D 500:

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



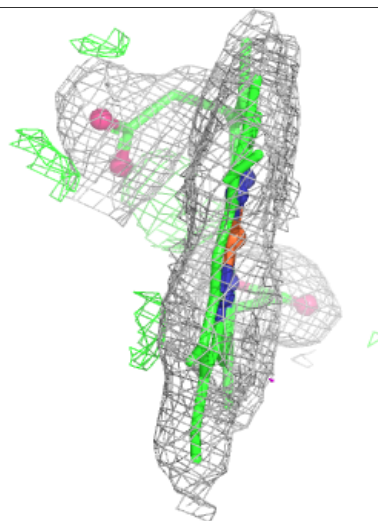
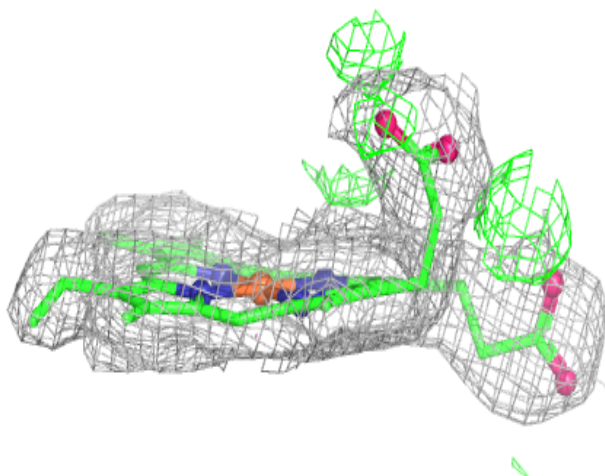
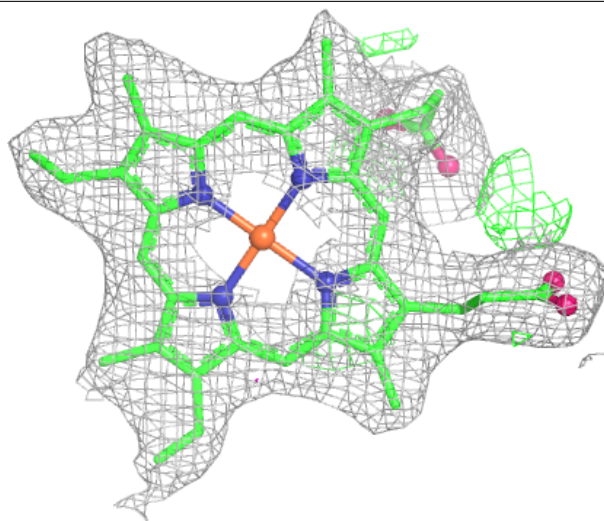
Electron density around HEM A 500:

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and green (positive)



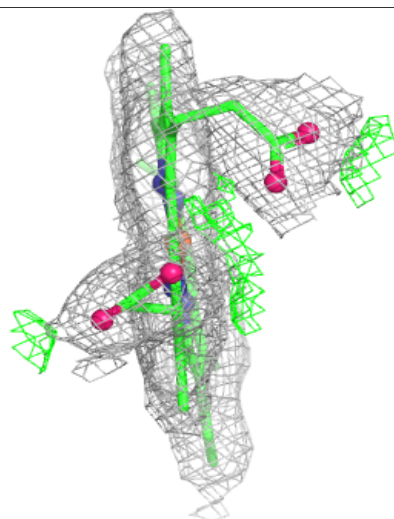
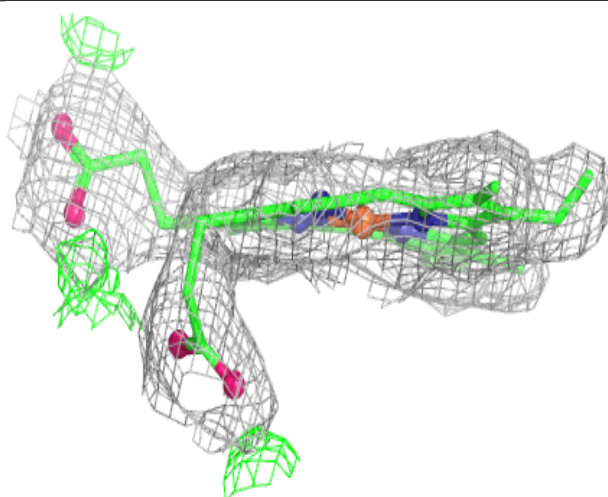
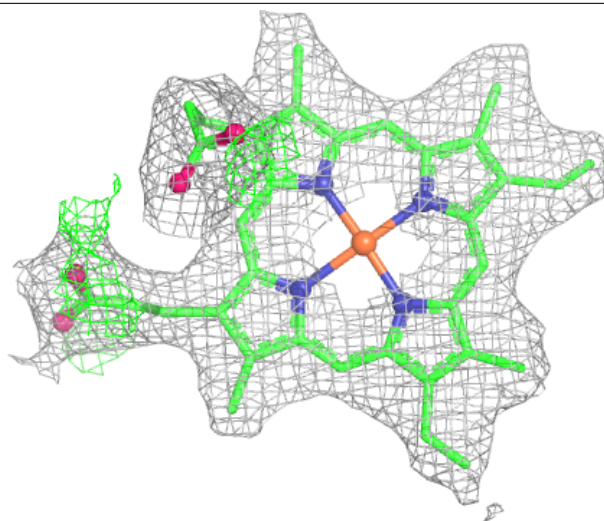
Electron density around HEM A 501:

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



Electron density around HEM D 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.