



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:21 AM UTC

PDB ID : 4EGO / pdb_00004ego
Title : The X-ray crystal structure of CYP19A4 in complex with indole-6-carboxylic acid
Authors : Zhou, W.; Bell, S.G.; Yang, W.; Zhou, R.M.; Tan, A.B.H.; Wong, L.-L.
Deposited on : 2012-03-31
Resolution : 1.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

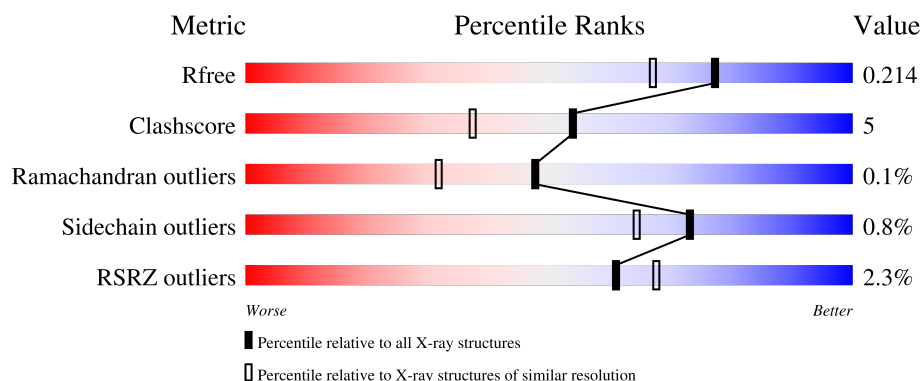
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	410	% 83% 12% .
1	B	410	3% 77% 17% .
1	C	410	% 81% 15% .
1	D	410	3% 77% 17% .

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
3	1F1	A	502	-	X	-	-
3	1F1	A	503	-	X	-	-
3	1F1	B	502	-	X	-	-
3	1F1	B	503	-	X	-	-
3	1F1	C	502	-	X	-	-
3	1F1	C	503	-	X	-	-
3	1F1	D	501	-	X	-	-
5	GOL	A	508	-	X	-	-
5	GOL	B	506	-	X	-	-

2 Entry composition [i](#)

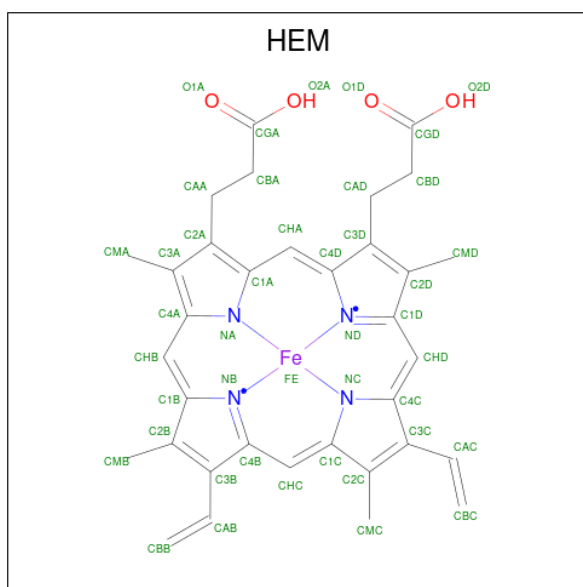
There are 7 unique types of molecules in this entry. The entry contains 13688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	3	0
			3035	1922	535	566	12			
1	B	393	Total	C	N	O	S	0	1	0
			3027	1916	534	566	11			
1	C	393	Total	C	N	O	S	0	0	0
			3021	1912	534	564	11			
1	D	393	Total	C	N	O	S	0	0	0
			3021	1912	534	564	11			

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



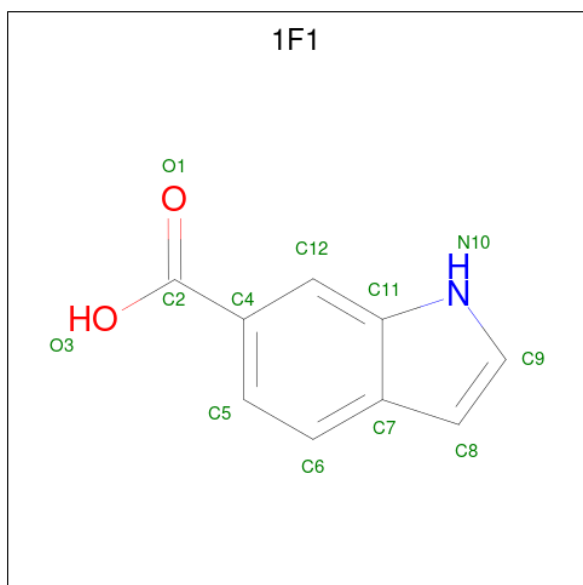
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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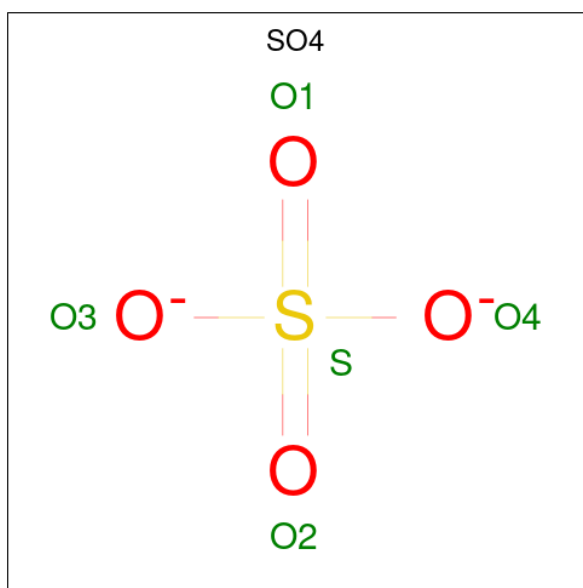
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1H-indole-6-carboxylic acid (CCD ID: 1F1) (formula: C₉H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	D	1	Total	C	N	O	0	0
			12	9	1	2		
3	D	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		
6	D	1	Total	Cl	0	0
			1	1		

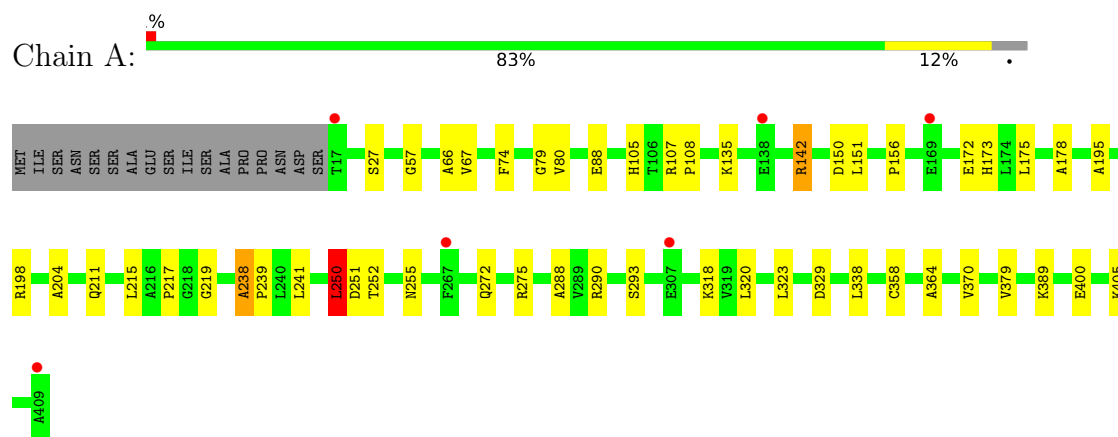
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	347	Total 347	O 347	0	0
7	B	332	Total 332	O 332	0	0
7	C	314	Total 314	O 314	0	0
7	D	225	Total 225	O 225	0	0

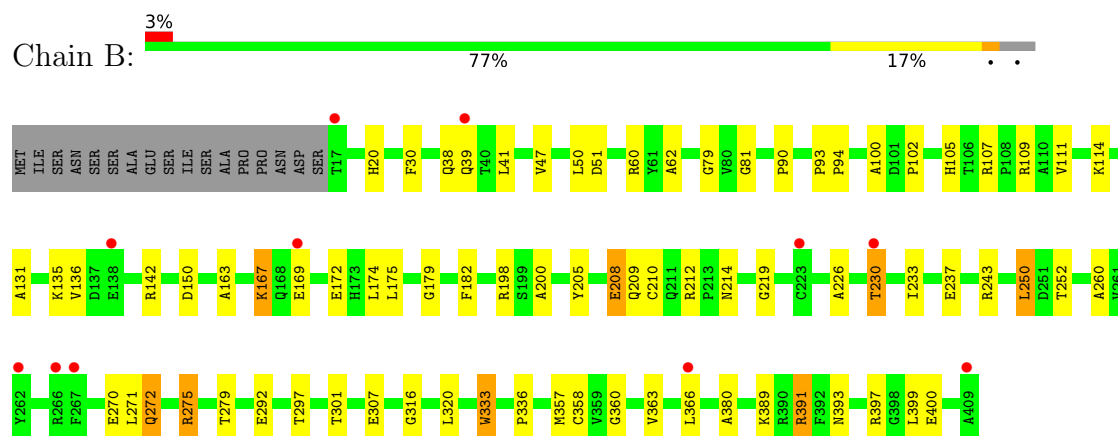
3 Residue-property plots [i](#)

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.

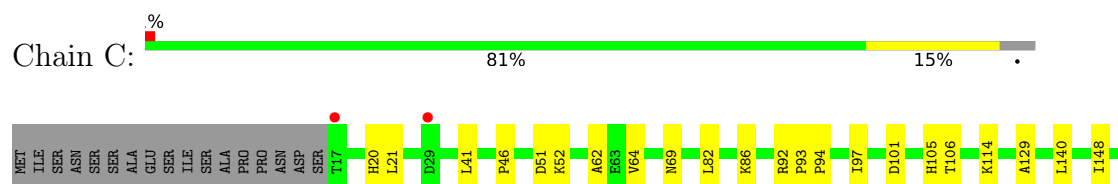
• Molecule 1: Cytochrome P450

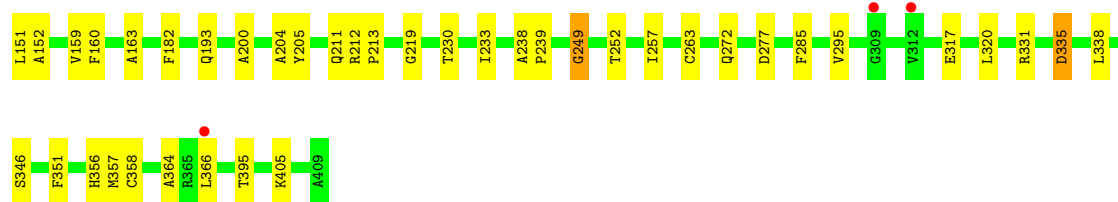


• Molecule 1: Cytochrome P450

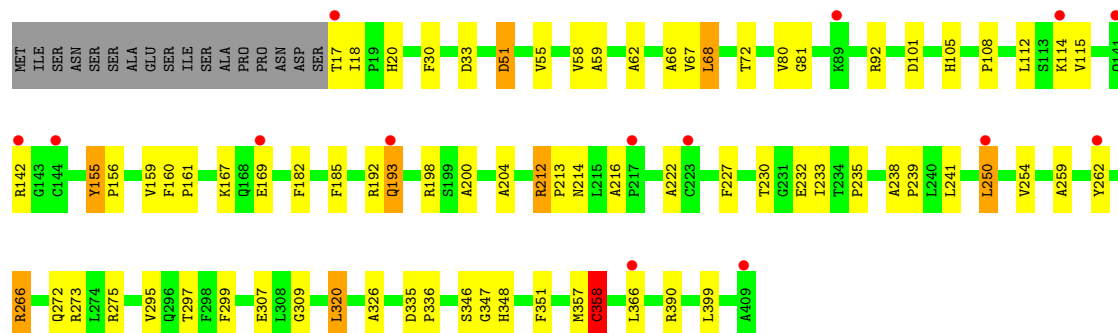
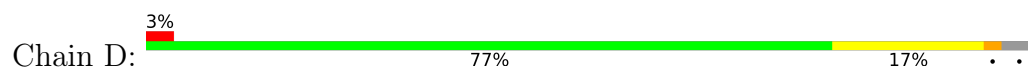


• Molecule 1: Cytochrome P450





● Molecule 1: Cytochrome P450



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.86Å 143.67Å 172.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.76 39.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	90.0 (39.00-1.76) 89.9 (39.00-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.76Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.182 , 0.214 0.183 , 0.214	Depositor DCC
R_{free} test set	11782 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.59 % 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 7.2997e-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: 1F1, SO4, CL, HEM, GOL

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	1.80	27/3116 (0.9%)	1.37	6/4239 (0.1%)
1	B	1.87	34/3102 (1.1%)	1.50	19/4221 (0.5%)
1	C	1.78	34/3093 (1.1%)	1.38	6/4209 (0.1%)
1	D	1.72	34/3093 (1.1%)	1.41	26/4209 (0.6%)
All	All	1.79	129/12404 (1.0%)	1.41	57/16878 (0.3%)

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	GLY	N-CA	12.03	1.53	1.44
1	D	335	ASP	N-CA	8.95	1.52	1.46
1	C	335	ASP	CA-CB	8.84	1.58	1.52
1	B	226	ALA	N-CA	8.21	1.56	1.46
1	B	79	GLY	N-CA	8.20	1.55	1.45
1	B	111	VAL	CA-CB	7.91	1.63	1.54
1	C	148	ILE	CA-CB	7.88	1.65	1.54
1	D	259	ALA	CA-CB	7.83	1.65	1.53
1	A	67	VAL	CA-C	7.77	1.62	1.52
1	B	131	ALA	CA-CB	7.30	1.64	1.53
1	D	18	ILE	CA-C	7.25	1.59	1.53
1	B	380	ALA	CA-CB	7.21	1.64	1.53
1	B	47	VAL	CA-CB	7.15	1.65	1.54
1	C	193	GLN	CG-CD	7.10	1.69	1.52
1	D	326	ALA	CA-CB	7.05	1.64	1.53
1	C	159	VAL	N-CA	7.04	1.53	1.46
1	A	238	ALA	C-O	-6.99	1.17	1.24
1	B	169	GLU	CG-CD	6.91	1.69	1.52
1	A	288	ALA	CA-CB	6.88	1.64	1.53
1	A	88	GLU	CD-OE2	6.87	1.38	1.25
1	A	204	ALA	CA-CB	6.84	1.64	1.53
1	D	59	ALA	CA-CB	6.77	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	ALA	N-CA	6.74	1.52	1.46
1	B	250	LEU	CG-CD1	-6.69	1.30	1.52
1	A	66	ALA	CA-CB	6.66	1.63	1.53
1	C	200	ALA	CA-CB	6.56	1.62	1.53
1	C	106	THR	CA-CB	6.54	1.63	1.53
1	D	193	GLN	CB-CG	6.51	1.72	1.52
1	C	163	ALA	N-CA	6.50	1.54	1.46
1	B	219	GLY	C-O	6.48	1.31	1.23
1	C	272	GLN	N-CA	6.47	1.54	1.46
1	D	58	VAL	CA-CB	6.46	1.62	1.54
1	C	335	ASP	CA-C	6.45	1.58	1.53
1	B	163	ALA	CA-CB	6.42	1.63	1.53
1	C	395	THR	CA-CB	6.39	1.64	1.54
1	A	219	GLY	N-CA	6.36	1.51	1.44
1	A	195	ALA	CA-CB	6.30	1.63	1.53
1	D	299	PHE	N-CA	-6.29	1.38	1.45
1	C	152	ALA	N-CA	6.27	1.54	1.46
1	C	364	ALA	CA-CB	6.27	1.63	1.53
1	D	67	VAL	C-O	6.23	1.31	1.24
1	C	295	VAL	CA-CB	6.22	1.60	1.53
1	A	379	VAL	CA-CB	6.20	1.62	1.54
1	D	348	HIS	N-CA	6.18	1.54	1.46
1	D	185	PHE	N-CA	6.18	1.54	1.46
1	C	317	GLU	C-O	6.15	1.31	1.23
1	D	193	GLN	CG-CD	6.15	1.67	1.52
1	A	79	GLY	N-CA	6.12	1.52	1.45
1	A	107	ARG	C-O	-6.07	1.18	1.24
1	C	211	GLN	N-CA	6.03	1.53	1.45
1	D	115	VAL	C-O	6.01	1.31	1.24
1	D	295	VAL	CA-CB	6.01	1.60	1.53
1	C	320	LEU	CA-CB	6.00	1.61	1.53
1	C	204	ALA	CA-CB	5.97	1.62	1.53
1	B	233	ILE	C-O	5.95	1.30	1.23
1	A	57	GLY	C-O	5.94	1.30	1.23
1	C	219	GLY	N-CA	5.91	1.52	1.45
1	A	250	LEU	N-CA	5.90	1.53	1.46
1	C	69	ASN	N-CA	5.90	1.53	1.46
1	B	393	ASN	C-O	5.88	1.31	1.23
1	A	255	ASN	N-CA	-5.87	1.38	1.46
1	C	129	ALA	C-O	5.84	1.30	1.24
1	B	62	ALA	N-CA	5.83	1.53	1.46
1	A	329	ASP	N-CA	5.82	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	GLY	C-N	-5.82	1.25	1.33
1	D	320	LEU	CA-CB	5.81	1.61	1.53
1	D	204	ALA	CA-CB	5.78	1.62	1.53
1	A	320	LEU	N-CA	5.76	1.53	1.46
1	C	101	ASP	CA-C	5.72	1.60	1.52
1	D	159	VAL	N-CA	5.71	1.52	1.46
1	C	233	ILE	N-CA	5.70	1.52	1.46
1	D	358	CYS	N-CA	5.68	1.53	1.46
1	B	275	ARG	N-CA	5.65	1.53	1.46
1	D	233	ILE	C-O	5.63	1.30	1.23
1	A	74	PHE	CD2-CE2	5.62	1.55	1.38
1	B	292	GLU	C-O	5.61	1.29	1.23
1	A	217	PRO	N-CA	5.60	1.53	1.47
1	D	101	ASP	CA-C	5.58	1.60	1.52
1	C	64	VAL	CA-CB	5.57	1.61	1.54
1	B	260	ALA	C-O	5.53	1.30	1.24
1	D	200	ALA	CA-CB	5.52	1.60	1.53
1	C	160	PHE	CA-C	5.49	1.59	1.52
1	B	301	THR	CA-C	5.49	1.59	1.52
1	D	309	GLY	N-CA	5.43	1.53	1.45
1	C	285	PHE	CA-C	5.42	1.59	1.52
1	C	62	ALA	CA-CB	5.41	1.61	1.53
1	A	27	SER	CA-CB	5.40	1.61	1.53
1	B	136	VAL	CA-C	5.39	1.59	1.52
1	D	390	ARG	N-CA	5.39	1.52	1.45
1	B	333	TRP	N-CA	5.37	1.52	1.46
1	B	316	GLY	N-CA	5.35	1.52	1.45
1	B	62	ALA	CA-C	5.35	1.59	1.52
1	B	174	LEU	N-CA	5.35	1.52	1.46
1	A	211	GLN	N-CA	5.35	1.52	1.45
1	B	397	ARG	CZ-NH1	5.35	1.40	1.32
1	B	167	LYS	N-CA	5.33	1.52	1.45
1	B	208[A]	GLU	C-O	5.32	1.30	1.24
1	B	208[B]	GLU	C-O	5.32	1.30	1.24
1	B	272	GLN	N-CA	5.28	1.52	1.46
1	D	59	ALA	C-O	5.28	1.30	1.24
1	D	155	TYR	CA-C	5.28	1.58	1.52
1	B	81	GLY	N-CA	5.27	1.49	1.44
1	B	100	ALA	N-CA	5.26	1.52	1.45
1	D	112	LEU	CA-C	-5.25	1.45	1.52
1	D	193	GLN	N-CA	5.25	1.52	1.46
1	A	318	LYS	N-CA	5.23	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	CYS	N-CA	5.22	1.52	1.46
1	D	336	PRO	C-O	5.22	1.30	1.24
1	C	257	ILE	CA-CB	-5.21	1.47	1.54
1	A	255	ASN	CA-C	5.20	1.59	1.52
1	A	172	GLU	CG-CD	5.20	1.65	1.52
1	C	351	PHE	N-CA	5.17	1.52	1.46
1	B	111	VAL	C-O	5.16	1.29	1.24
1	A	290	ARG	CA-CB	5.16	1.61	1.53
1	D	55	VAL	N-CA	5.15	1.51	1.46
1	C	92	ARG	CA-C	5.14	1.57	1.52
1	C	331	ARG	N-CA	5.13	1.53	1.46
1	D	214	ASN	N-CA	5.13	1.52	1.46
1	D	30	PHE	C-O	-5.12	1.18	1.24
1	C	263	CYS	N-CA	5.12	1.52	1.46
1	A	215	LEU	C-O	5.11	1.29	1.24
1	D	347	GLY	N-CA	5.09	1.52	1.45
1	C	277	ASP	C-N	5.09	1.39	1.34
1	B	90	PRO	C-O	5.08	1.29	1.23
1	A	250	LEU	CA-C	5.08	1.57	1.52
1	A	370	VAL	N-CA	5.08	1.52	1.46
1	B	363	VAL	N-CA	5.07	1.52	1.46
1	C	82	LEU	CA-CB	5.05	1.61	1.53
1	D	346	SER	CA-C	5.01	1.59	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ARG	N-CA-C	-9.17	101.66	113.12
1	B	391	ARG	NE-CZ-NH1	-7.17	114.33	121.50
1	D	222	ALA	N-CA-C	-7.16	103.52	111.82
1	D	101	ASP	O-C-N	6.91	127.42	121.20
1	D	92	ARG	CA-C-N	-6.88	113.29	120.38
1	D	92	ARG	C-N-CA	-6.88	113.29	120.38
1	D	66	ALA	N-CA-C	6.84	118.39	111.07
1	D	155	TYR	CA-C-N	-6.81	111.97	119.19
1	D	155	TYR	C-N-CA	-6.81	111.97	119.19
1	A	198	ARG	CB-CG-CD	6.80	126.94	111.30
1	B	237	GLU	N-CA-C	6.67	118.55	111.28
1	B	142	ARG	NE-CZ-NH2	6.58	125.13	119.20
1	D	212	ARG	CA-C-N	-6.52	113.09	119.87
1	D	212	ARG	C-N-CA	-6.52	113.09	119.87
1	D	351	PHE	N-CA-C	-6.49	104.67	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ARG	NE-CZ-NH1	-6.38	115.12	121.50
1	A	142	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	A	172	GLU	CB-CG-CD	6.23	123.18	112.60
1	B	198	ARG	CB-CG-CD	6.08	125.29	111.30
1	B	270	GLU	N-CA-C	5.98	117.88	111.36
1	D	216	ALA	N-CA-C	5.81	117.02	109.64
1	A	80	VAL	N-CA-C	-5.79	107.10	112.43
1	D	68	LEU	N-CA-C	-5.75	105.01	111.28
1	B	102	PRO	N-CA-C	-5.72	103.73	110.70
1	B	397	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	D	80	VAL	CA-C-N	-5.65	116.82	122.69
1	D	80	VAL	C-N-CA	-5.65	116.82	122.69
1	D	200	ALA	CA-C-N	-5.65	113.20	119.19
1	D	200	ALA	C-N-CA	-5.65	113.20	119.19
1	C	97	ILE	CB-CA-C	5.61	116.05	111.05
1	C	205	TYR	N-CA-C	-5.60	105.09	111.14
1	D	266	ARG	CA-CB-CG	-5.48	103.14	114.10
1	D	51	ASP	N-CA-C	5.42	118.99	112.38
1	D	33	ASP	CA-C-N	-5.41	114.68	120.47
1	D	33	ASP	C-N-CA	-5.41	114.68	120.47
1	C	46	PRO	CB-CA-C	-5.40	103.78	112.21
1	B	243	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	B	39	GLN	CB-CG-CD	-5.39	103.44	112.60
1	A	364	ALA	N-CA-C	5.34	117.52	111.11
1	B	212	ARG	CA-C-N	-5.34	114.11	119.56
1	B	212	ARG	C-N-CA	-5.34	114.11	119.56
1	C	230	THR	N-CA-C	-5.33	106.45	113.17
1	A	293	SER	N-CA-C	5.28	121.47	109.81
1	D	254	VAL	N-CA-C	-5.27	105.36	110.42
1	D	238	ALA	CA-C-N	-5.26	113.11	118.85
1	D	238	ALA	C-N-CA	-5.26	113.11	118.85
1	C	346	SER	N-CA-C	5.26	117.98	110.24
1	B	30	PHE	N-CA-C	-5.26	105.46	111.14
1	D	62	ALA	N-CA-C	5.22	116.97	111.28
1	B	109	ARG	N-CA-C	-5.18	105.54	111.14
1	C	82	LEU	N-CA-C	5.16	116.99	111.36
1	B	243	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	D	273	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	D	72	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	107	ARG	CA-C-N	-5.04	113.74	119.28
1	B	107	ARG	C-N-CA	-5.04	113.74	119.28
1	B	279	THR	N-CA-C	-5.02	107.10	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3035	0	3015	26	0
1	B	3027	0	2999	41	0
1	C	3021	0	2993	23	0
1	D	3021	0	2993	27	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
3	A	36	0	18	0	0
3	B	24	0	12	3	0
3	C	24	0	12	3	0
3	D	24	0	12	2	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	15	0	0	0	0
4	D	10	0	0	0	0
5	A	12	0	16	0	0
5	B	18	0	24	2	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	347	0	0	3	0
7	B	332	0	0	5	0
7	C	314	0	0	5	0
7	D	225	0	0	5	0
All	All	13688	0	12230	120	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 5.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:HH12	5:B:506:GOL:H32	1.09	1.10
1:D:272:GLN:HE22	1:D:275:ARG:HH11	1.14	0.91
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.21	0.86
1:B:307:GLU:HG2	7:B:670:HOH:O	1.75	0.84
1:B:135:LYS:CE	1:B:150:ASP:O	2.27	0.82
1:B:272:GLN:HE22	1:B:275:ARG:HH11	1.27	0.82
1:B:60:ARG:NH1	5:B:506:GOL:H32	1.93	0.79
1:D:307:GLU:HG2	7:D:717:HOH:O	1.85	0.75
1:D:105:HIS:HD2	7:D:613:HOH:O	1.70	0.73
2:D:502:HEM:HBC2	2:D:502:HEM:HMC1	1.70	0.73
1:D:262:TYR:CE2	1:D:266:ARG:HD3	2.24	0.72
1:B:250:LEU:C	1:B:250:LEU:HD13	2.15	0.71
1:D:105:HIS:HE1	2:D:502:HEM:O1D	1.73	0.71
1:C:105:HIS:HD2	7:C:607:HOH:O	1.74	0.70
1:D:262:TYR:CZ	1:D:266:ARG:HD3	2.27	0.69
1:A:105:HIS:HD2	7:A:626:HOH:O	1.75	0.69
1:B:208[B]:GLU:HG2	7:B:826:HOH:O	1.92	0.68
1:B:135:LYS:HE3	1:B:150:ASP:O	1.95	0.66
1:B:105:HIS:HE1	2:B:501:HEM:O1D	1.79	0.64
1:A:135:LYS:CE	1:A:150:ASP:O	2.46	0.64
1:B:114:LYS:HE3	7:B:804:HOH:O	1.97	0.64
1:A:323:LEU:HD12	1:A:323:LEU:N	2.12	0.63
1:A:135:LYS:HE3	1:A:150:ASP:O	1.97	0.63
1:C:105:HIS:HE1	2:C:501:HEM:O1D	1.81	0.62
1:B:135:LYS:NZ	1:B:150:ASP:O	2.32	0.62
1:B:272:GLN:HE22	1:B:275:ARG:NH1	1.97	0.62
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.83	0.61
1:C:86:LYS:NZ	7:C:767:HOH:O	2.34	0.61
1:D:167:LYS:HE3	1:D:169:GLU:HG2	1.81	0.61
1:A:105:HIS:HE1	2:A:501:HEM:O1D	1.83	0.61
1:A:323:LEU:HD12	1:A:323:LEU:H	1.67	0.60
1:B:167:LYS:NZ	1:B:214:ASN:ND2	2.49	0.60
3:C:503:1F1:H6	7:C:734:HOH:O	2.01	0.60
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.83	0.59
1:C:114:LYS:NZ	7:C:727:HOH:O	2.35	0.59
1:A:405:LYS:HE3	7:A:779:HOH:O	2.01	0.59
1:C:405:LYS:HE3	7:D:749:HOH:O	2.01	0.59
1:D:20:HIS:HD2	1:D:51:ASP:OD1	1.86	0.58
1:B:167:LYS:HZ2	1:B:214:ASN:ND2	2.02	0.57
1:D:17:THR:O	1:D:17:THR:OG1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:GLN:HE22	1:D:275:ARG:NH1	1.95	0.56
1:D:114:LYS:HD3	1:D:227:PHE:CZ	2.43	0.53
1:D:114:LYS:HD3	1:D:227:PHE:HZ	1.73	0.53
1:B:179:GLY:HA3	3:B:503:1F1:C2	2.38	0.53
1:B:230:THR:HG22	1:B:230:THR:O	2.10	0.52
1:B:389:LYS:HE3	1:B:400:GLU:OE2	2.09	0.52
1:C:20:HIS:HD2	1:C:51:ASP:OD1	1.91	0.52
1:A:142:ARG:HD3	1:B:205:TYR:HA	1.92	0.51
1:B:358:CYS:HA	2:B:501:HEM:CHA	2.41	0.51
1:C:21:LEU:HD12	1:C:41:LEU:HD23	1.93	0.51
1:D:250:LEU:HD12	1:D:250:LEU:O	2.12	0.50
1:C:335:ASP:HB3	1:C:338:LEU:HD22	1.94	0.49
1:B:172:GLU:HG2	7:B:747:HOH:O	2.12	0.49
1:B:230:THR:O	1:B:230:THR:CG2	2.60	0.49
1:C:252:THR:HB	2:C:501:HEM:C3B	2.48	0.49
1:A:272:GLN:HE22	1:A:275:ARG:NH1	2.01	0.48
1:A:358:CYS:HA	2:A:501:HEM:CHA	2.44	0.48
3:D:501:1F1:H6	7:D:713:HOH:O	2.14	0.48
1:C:358:CYS:HA	2:C:501:HEM:CHA	2.43	0.48
1:B:20:HIS:HD2	1:B:51:ASP:OD1	1.97	0.47
1:B:297:THR:HB	1:B:320:LEU:HD11	1.97	0.47
1:C:182:PHE:CE2	3:C:502:1F1:H8	2.50	0.47
1:A:175:LEU:HD23	1:A:251[B]:ASP:OD1	2.15	0.47
1:D:399:LEU:HD12	7:D:694:HOH:O	2.16	0.46
1:A:178:ALA:HB3	1:A:251[B]:ASP:CG	2.40	0.46
1:D:235:PRO:O	1:D:239:PRO:HD3	2.16	0.46
1:B:271:LEU:O	1:B:275:ARG:HG3	2.16	0.46
1:A:156:PRO:HB2	1:A:250:LEU:HD11	1.96	0.46
1:B:182:PHE:CZ	3:B:502:1F1:H8	2.51	0.46
1:A:151:LEU:C	1:A:151:LEU:HD23	2.41	0.45
1:C:357:MET:O	1:C:358:CYS:C	2.58	0.45
1:D:108:PRO:HB3	1:D:241:LEU:HD21	1.99	0.45
1:D:230:THR:OG1	1:D:232:GLU:OE1	2.33	0.44
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.99	0.44
1:A:108:PRO:HB3	1:A:241:LEU:HD21	1.98	0.44
1:A:323:LEU:H	1:A:323:LEU:CD1	2.29	0.44
1:A:405:LYS:CE	7:A:779:HOH:O	2.63	0.44
1:D:297:THR:HB	1:D:320:LEU:HD11	1.99	0.44
1:B:167:LYS:NZ	1:B:214:ASN:HD22	2.14	0.44
1:A:252:THR:HB	2:A:501:HEM:C3B	2.52	0.44
1:D:358:CYS:HA	2:D:502:HEM:CHA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HB3	3:B:503:1F1:C8	2.48	0.44
1:B:399:LEU:HD12	7:B:885:HOH:O	2.18	0.43
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.87	0.43
1:A:272:GLN:HE22	1:A:275:ARG:HD3	1.83	0.43
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.90	0.43
1:B:250:LEU:C	1:B:250:LEU:CD1	2.89	0.43
1:C:238:ALA:HB3	1:C:239:PRO:HD3	1.99	0.43
1:D:357:MET:O	1:D:358:CYS:C	2.61	0.43
1:A:272:GLN:NE2	1:A:275:ARG:HD3	2.33	0.43
1:C:51:ASP:O	1:C:52:LYS:C	2.61	0.43
1:C:182:PHE:CZ	3:C:502:1F1:H8	2.54	0.43
1:C:114:LYS:CE	7:C:727:HOH:O	2.66	0.43
1:A:323:LEU:N	1:A:323:LEU:CD1	2.82	0.42
1:B:360:GLY:HA3	2:B:501:HEM:C3C	2.54	0.42
1:B:391:ARG:HH11	1:B:391:ARG:HD2	1.48	0.42
1:D:192:ARG:HH21	1:D:193:GLN:HE22	1.68	0.42
2:C:501:HEM:CMC	2:C:501:HEM:HBC2	2.50	0.42
1:D:68:LEU:HD23	1:D:68:LEU:HA	1.92	0.42
1:C:93:PRO:HA	1:C:94:PRO:HD3	1.81	0.42
1:C:249:GLY:HA2	2:C:501:HEM:C2C	2.54	0.42
1:B:333:TRP:O	1:B:336:PRO:HD3	2.19	0.42
1:C:212:ARG:N	1:C:213:PRO:CD	2.83	0.42
1:D:250:LEU:HD12	1:D:250:LEU:C	2.45	0.41
1:B:38:GLN:HA	1:B:41:LEU:HD12	2.02	0.41
1:D:155:TYR:HB3	1:D:156:PRO:HD3	2.02	0.41
1:B:252:THR:HB	2:B:501:HEM:C3B	2.55	0.41
1:A:142:ARG:HG3	1:B:208[A]:GLU:OE1	2.21	0.41
1:A:238:ALA:HB3	1:A:239:PRO:HD3	2.02	0.41
1:B:50:LEU:HD23	1:B:50:LEU:HA	1.86	0.41
1:B:357:MET:O	1:B:358:CYS:C	2.64	0.41
1:C:356:HIS:O	1:C:357:MET:C	2.64	0.41
1:A:389:LYS:NZ	1:A:400:GLU:OE2	2.53	0.41
1:A:173:HIS:HE2	1:B:150:ASP:CG	2.28	0.40
1:B:167:LYS:HZ1	1:B:214:ASN:HD22	1.69	0.40
1:C:20:HIS:CD2	1:C:51:ASP:OD1	2.73	0.40
1:B:175:LEU:HD23	1:B:250:LEU:HD12	2.02	0.40
1:D:212:ARG:N	1:D:213:PRO:CD	2.84	0.40
1:D:182:PHE:CE2	3:D:503:1F1:H8	2.56	0.40
1:C:151:LEU:C	1:C:151:LEU:HD23	2.46	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	394/410 (96%)	386 (98%)	8 (2%)	0	100	100
1	B	392/410 (96%)	384 (98%)	8 (2%)	0	100	100
1	C	391/410 (95%)	383 (98%)	8 (2%)	0	100	100
1	D	391/410 (95%)	384 (98%)	6 (2%)	1 (0%)	36	21
All	All	1568/1640 (96%)	1537 (98%)	30 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	CYS

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	322/334 (96%)	320 (99%)	2 (1%)	78	71
1	B	320/334 (96%)	317 (99%)	3 (1%)	70	60
1	C	319/334 (96%)	318 (100%)	1 (0%)	86	83
1	D	319/334 (96%)	315 (99%)	4 (1%)	61	46
All	All	1280/1336 (96%)	1270 (99%)	10 (1%)	73	64

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	LEU
1	A	338	LEU
1	B	209	GLN
1	B	230	THR
1	B	366	LEU
1	C	366	LEU
1	D	142	ARG
1	D	198	ARG
1	D	250	LEU
1	D	366	LEU

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	105	HIS
1	A	209	GLN
1	A	214	ASN
1	A	272	GLN
1	A	296	GLN
1	B	20	HIS
1	B	105	HIS
1	B	141	GLN
1	B	209	GLN
1	B	214	ASN
1	B	255	ASN
1	B	272	GLN
1	B	296	GLN
1	C	20	HIS
1	C	105	HIS
1	C	214	ASN
1	C	272	GLN
1	C	296	GLN
1	D	20	HIS
1	D	105	HIS
1	D	168	GLN
1	D	193	GLN
1	D	214	ASN
1	D	272	GLN
1	D	283	ASN
1	D	296	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 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$
4	SO4	C	505	-	4,4,4	0.33	0	6,6,6	0.87	0
3	1F1	D	501	-	13,13,13	3.93	7 (53%)	18,18,18	3.68	11 (61%)
4	SO4	A	506	-	4,4,4	0.59	0	6,6,6	0.54	0
3	1F1	A	503	-	13,13,13	3.35	3 (23%)	18,18,18	3.90	12 (66%)
3	1F1	C	503	-	13,13,13	4.40	3 (23%)	18,18,18	3.34	8 (44%)
2	HEM	B	501	1	50,50,50	1.88	14 (28%)	67,82,82	1.98	20 (29%)
4	SO4	D	505	-	4,4,4	0.52	0	6,6,6	1.17	0
2	HEM	C	501	1	50,50,50	1.56	10 (20%)	67,82,82	1.64	14 (20%)
2	HEM	A	501	1	50,50,50	1.84	10 (20%)	67,82,82	2.13	23 (34%)
3	1F1	B	503	-	13,13,13	3.89	7 (53%)	18,18,18	3.42	10 (55%)
3	1F1	A	502	-	13,13,13	3.66	8 (61%)	18,18,18	3.68	12 (66%)
3	1F1	C	502	-	13,13,13	2.92	4 (30%)	18,18,18	3.29	11 (61%)
5	GOL	B	507	-	5,5,5	0.54	0	5,5,5	1.17	0
4	SO4	C	504	-	4,4,4	0.50	0	6,6,6	0.82	0
5	GOL	B	506	-	5,5,5	0.73	0	5,5,5	4.14	4 (80%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	502	1	50,50,50	2.11	18 (36%)	67,82,82	2.23	20 (29%)
4	SO4	B	504	-	4,4,4	0.46	0	6,6,6	0.75	0
3	1F1	B	502	-	13,13,13	3.40	6 (46%)	18,18,18	2.94	12 (66%)
5	GOL	B	505	-	5,5,5	0.69	0	5,5,5	1.30	0
4	SO4	C	506	-	4,4,4	0.47	0	6,6,6	0.52	0
5	GOL	A	508	-	5,5,5	0.42	0	5,5,5	1.81	2 (40%)
5	GOL	A	507	-	5,5,5	0.34	0	5,5,5	1.45	0
3	1F1	D	503	-	13,13,13	2.93	4 (30%)	18,18,18	2.57	9 (50%)
3	1F1	A	504	-	13,13,13	3.16	4 (30%)	18,18,18	2.73	10 (55%)
4	SO4	A	505	-	4,4,4	0.42	0	6,6,6	1.36	1 (16%)
5	GOL	D	506	-	5,5,5	0.34	0	5,5,5	1.33	0
4	SO4	D	504	-	4,4,4	0.51	0	6,6,6	0.51	0
5	GOL	C	507	-	5,5,5	0.53	0	5,5,5	1.12	1 (20%)

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
3	1F1	D	501	-	-	0/4/4/4	0/2/2/2
3	1F1	A	503	-	-	4/4/4/4	0/2/2/2
3	1F1	C	503	-	-	4/4/4/4	0/2/2/2
2	HEM	B	501	1	-	0/14/54/54	-
2	HEM	C	501	1	-	1/14/54/54	-
2	HEM	A	501	1	-	2/14/54/54	-
3	1F1	B	503	-	-	4/4/4/4	0/2/2/2
3	1F1	A	502	-	-	0/4/4/4	0/2/2/2
3	1F1	C	502	-	-	0/4/4/4	0/2/2/2
5	GOL	B	507	-	-	2/4/4/4	-
5	GOL	B	506	-	-	2/4/4/4	-
2	HEM	D	502	1	-	3/14/54/54	-
3	1F1	B	502	-	-	0/4/4/4	0/2/2/2
5	GOL	B	505	-	-	0/4/4/4	-
5	GOL	A	508	-	-	4/4/4/4	-
5	GOL	A	507	-	-	2/4/4/4	-
3	1F1	D	503	-	-	0/4/4/4	0/2/2/2
3	1F1	A	504	-	-	0/4/4/4	0/2/2/2
5	GOL	D	506	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	507	-	-	1/4/4/4	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	1F1	C9-C8	12.45	1.59	1.36
3	B	503	1F1	C9-C8	10.38	1.55	1.36
3	D	501	1F1	C9-C8	10.30	1.55	1.36
3	A	503	1F1	C9-C8	10.08	1.55	1.36
3	A	504	1F1	C9-C8	9.61	1.54	1.36
3	C	503	1F1	C9-N10	8.71	1.53	1.38
3	A	502	1F1	C9-C8	8.32	1.51	1.36
3	C	502	1F1	C9-C8	8.25	1.51	1.36
3	B	502	1F1	C9-C8	7.97	1.51	1.36
3	D	503	1F1	C9-C8	7.60	1.50	1.36
3	B	503	1F1	C9-N10	6.19	1.49	1.38
3	D	501	1F1	C9-N10	6.16	1.49	1.38
3	A	502	1F1	C5-C4	5.97	1.48	1.39
2	D	502	HEM	C3D-C2D	5.59	1.48	1.36
2	A	501	HEM	C3D-C2D	5.19	1.48	1.36
2	B	501	HEM	FE-NA	5.03	2.11	1.95
3	A	502	1F1	C7-C11	-4.94	1.33	1.41
3	A	503	1F1	C9-N10	4.89	1.46	1.38
3	B	502	1F1	C11-N10	-4.85	1.30	1.37
2	D	502	HEM	FE-NA	4.83	2.11	1.95
2	A	501	HEM	CMC-C2C	4.73	1.60	1.50
2	B	501	HEM	C3D-C2D	4.55	1.46	1.36
3	D	503	1F1	C9-N10	4.48	1.46	1.38
3	B	502	1F1	C9-N10	4.43	1.46	1.38
3	A	504	1F1	C9-N10	4.42	1.46	1.38
3	B	503	1F1	O1-C2	4.39	1.35	1.22
2	D	502	HEM	FE-NB	4.33	2.08	1.94
2	C	501	HEM	FE-NB	4.31	2.08	1.94
2	D	502	HEM	FE-NC	4.24	2.09	1.95
2	A	501	HEM	CAB-C3B	3.97	1.58	1.47
3	D	503	1F1	C5-C4	3.72	1.45	1.39
2	D	502	HEM	CAC-C3C	3.71	1.57	1.47
2	A	501	HEM	C4A-C3A	3.65	1.51	1.43
3	C	502	1F1	C9-N10	3.61	1.44	1.38
3	B	502	1F1	C5-C4	3.59	1.44	1.39
3	D	501	1F1	C12-C4	3.58	1.44	1.39
2	C	501	HEM	C3D-C2D	3.57	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	1F1	C12-C11	-3.54	1.34	1.39
3	C	502	1F1	C5-C4	3.48	1.44	1.39
2	D	502	HEM	CAB-C3B	3.43	1.56	1.47
2	D	502	HEM	C1A-C2A	3.41	1.51	1.44
3	D	501	1F1	C7-C8	3.32	1.53	1.43
3	A	502	1F1	C12-C11	-3.27	1.34	1.39
2	D	502	HEM	FE-ND	3.26	2.04	1.94
3	D	501	1F1	C4-C2	3.22	1.56	1.49
3	D	501	1F1	C12-C11	3.18	1.44	1.39
3	C	502	1F1	C11-N10	-3.16	1.32	1.37
2	D	502	HEM	CMA-C3A	3.15	1.57	1.50
2	B	501	HEM	C1C-C2C	3.09	1.51	1.45
2	B	501	HEM	C1D-ND	3.09	1.44	1.38
2	B	501	HEM	CMC-C2C	3.05	1.57	1.50
3	A	502	1F1	C12-C4	2.99	1.44	1.39
2	A	501	HEM	CMD-C2D	2.97	1.56	1.50
2	B	501	HEM	C4C-NC	-2.93	1.34	1.39
3	C	503	1F1	C7-C8	2.89	1.52	1.43
2	A	501	HEM	CHB-C1B	2.87	1.44	1.38
3	A	502	1F1	C6-C7	-2.83	1.36	1.41
2	C	501	HEM	CAB-C3B	2.80	1.54	1.47
2	B	501	HEM	CAB-C3B	2.78	1.54	1.47
2	C	501	HEM	CMB-C2B	2.76	1.56	1.50
3	B	503	1F1	C12-C4	2.75	1.43	1.39
2	B	501	HEM	CAC-C3C	2.73	1.54	1.47
2	B	501	HEM	C4A-NA	-2.68	1.34	1.39
3	B	502	1F1	C7-C8	2.65	1.51	1.43
3	D	503	1F1	C12-C4	2.61	1.43	1.39
2	D	502	HEM	CMD-C2D	2.60	1.56	1.50
2	C	501	HEM	O1D-CGD	2.53	1.30	1.22
2	B	501	HEM	CAD-C3D	2.52	1.57	1.51
2	A	501	HEM	FE-NA	2.46	2.03	1.95
2	D	502	HEM	CAA-C2A	2.44	1.57	1.51
2	A	501	HEM	C4D-C3D	2.43	1.49	1.45
2	B	501	HEM	CBD-CAD	2.42	1.60	1.51
3	A	504	1F1	C5-C4	2.36	1.43	1.39
2	C	501	HEM	CBD-CAD	2.35	1.60	1.51
3	B	503	1F1	C7-C8	2.34	1.50	1.43
2	A	501	HEM	FE-NC	2.34	2.02	1.95
2	B	501	HEM	FE-NB	2.32	2.02	1.94
3	D	501	1F1	C5-C4	2.31	1.42	1.39
2	D	502	HEM	CMC-C2C	2.31	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	FE-NC	2.29	2.02	1.95
2	D	502	HEM	C1C-NC	-2.29	1.35	1.39
3	A	503	1F1	C5-C4	2.28	1.42	1.39
3	B	503	1F1	C5-C4	2.25	1.42	1.39
2	C	501	HEM	CMA-C3A	2.22	1.55	1.50
2	B	501	HEM	CAA-C2A	2.21	1.57	1.51
2	D	502	HEM	CMB-C2B	2.20	1.55	1.50
3	A	502	1F1	C11-N10	-2.20	1.34	1.37
2	D	502	HEM	CHC-C4B	2.20	1.44	1.39
3	A	504	1F1	C7-C8	2.20	1.50	1.43
2	D	502	HEM	O1D-CGD	2.20	1.29	1.22
3	B	503	1F1	C4-C2	2.19	1.54	1.49
2	C	501	HEM	CAC-C3C	2.17	1.53	1.47
2	B	501	HEM	O1D-CGD	2.09	1.28	1.22
2	D	502	HEM	CBD-CAD	2.08	1.59	1.51
3	A	502	1F1	C9-N10	2.07	1.41	1.38
2	D	502	HEM	C4B-NB	-2.06	1.34	1.38
2	C	501	HEM	C3C-C4C	-2.05	1.42	1.46
2	A	501	HEM	O2A-CGA	-2.01	1.24	1.30

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	1F1	C11-C7-C8	10.15	113.00	106.59
3	B	503	1F1	C11-C7-C8	8.04	111.67	106.59
3	C	503	1F1	C11-C7-C8	7.75	111.49	106.59
5	B	506	GOL	C3-C2-C1	-7.69	83.61	111.80
3	A	502	1F1	C6-C7-C11	7.48	127.30	119.23
3	A	503	1F1	C5-C6-C7	-7.24	111.98	121.74
2	D	502	HEM	C1B-NB-C4B	7.07	113.58	105.21
2	A	501	HEM	C3B-C4B-NB	7.03	114.52	109.47
3	A	503	1F1	C6-C7-C11	6.68	126.44	119.23
3	C	502	1F1	C11-C7-C8	6.55	110.73	106.59
3	C	503	1F1	C7-C11-N10	6.02	112.36	107.53
3	A	504	1F1	C11-C7-C8	5.97	110.36	106.59
2	D	502	HEM	C3B-C4B-NB	-5.89	105.24	109.47
3	C	502	1F1	C5-C6-C7	-5.82	113.89	121.74
3	C	503	1F1	C8-C9-N10	-5.76	103.59	110.25
2	D	502	HEM	CHC-C4B-NB	5.71	130.57	124.42
3	D	503	1F1	C8-C9-N10	-5.64	103.74	110.25
3	A	502	1F1	C11-C7-C8	5.42	110.02	106.59
3	A	502	1F1	C8-C9-N10	-5.42	103.98	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	1F1	C7-C11-N10	5.39	111.85	107.53
3	D	501	1F1	C7-C8-C9	-5.39	100.48	107.05
3	A	503	1F1	C11-C7-C8	5.20	109.88	106.59
2	B	501	HEM	CHC-C4B-NB	-5.12	118.91	124.42
3	A	503	1F1	C7-C11-N10	5.09	111.61	107.53
3	A	503	1F1	C5-C4-C12	5.06	125.10	119.25
3	A	502	1F1	C11-N10-C9	5.05	112.60	108.91
3	B	503	1F1	C6-C7-C11	5.05	124.68	119.23
3	B	503	1F1	C5-C6-C7	-5.02	114.97	121.74
2	B	501	HEM	CHC-C1C-NC	4.95	129.84	124.45
2	D	502	HEM	CHD-C1D-ND	4.91	129.71	124.42
3	B	503	1F1	C7-C8-C9	-4.79	101.22	107.05
2	A	501	HEM	C1B-NB-C4B	-4.74	99.59	105.21
3	C	503	1F1	C7-C8-C9	-4.66	101.37	107.05
3	B	503	1F1	C8-C9-N10	-4.65	104.88	110.25
3	C	502	1F1	C11-N10-C9	4.62	112.29	108.91
3	A	503	1F1	C8-C9-N10	-4.61	104.92	110.25
2	D	502	HEM	C4D-ND-C1D	4.52	110.56	105.21
2	A	501	HEM	CHD-C4C-NC	4.50	129.36	124.45
3	A	504	1F1	C7-C8-C9	-4.49	101.57	107.05
3	B	502	1F1	C7-C8-C9	-4.47	101.61	107.05
3	D	503	1F1	C6-C7-C11	4.46	124.04	119.23
2	C	501	HEM	O2D-CGD-O1D	-4.43	111.95	123.33
3	A	502	1F1	C6-C7-C8	-4.41	122.46	134.97
2	D	502	HEM	C2B-C1B-NB	-4.40	104.79	109.84
3	D	501	1F1	O3-C2-C4	4.38	126.08	114.84
2	A	501	HEM	CHB-C4A-NA	4.38	131.80	123.86
2	C	501	HEM	CBD-CAD-C3D	-4.36	100.48	112.53
3	C	502	1F1	C8-C9-N10	-4.34	105.24	110.25
2	A	501	HEM	C2D-C1D-ND	4.31	114.89	109.90
2	B	501	HEM	CHD-C4C-NC	4.22	129.04	124.45
2	C	501	HEM	O2D-CGD-CBD	4.22	127.32	114.00
2	B	501	HEM	C2D-C1D-ND	4.21	114.77	109.90
3	A	503	1F1	C4-C12-C11	-4.18	111.67	119.43
3	A	503	1F1	C12-C11-N10	-4.13	125.24	131.62
3	B	502	1F1	C12-C11-N10	-4.10	125.28	131.62
3	D	501	1F1	C11-N10-C9	4.03	111.86	108.91
3	A	503	1F1	C6-C7-C8	-4.00	123.61	134.97
3	B	503	1F1	C6-C7-C8	-3.99	123.65	134.97
3	B	502	1F1	C11-C7-C8	3.96	109.09	106.59
3	A	502	1F1	C5-C6-C7	-3.95	116.40	121.74
3	A	504	1F1	C7-C11-N10	3.92	110.67	107.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	HEM	CMA-C3A-C4A	-3.92	119.45	125.42
3	B	502	1F1	C5-C6-C7	-3.89	116.49	121.74
3	D	501	1F1	C12-C4-C2	3.84	126.84	119.96
2	B	501	HEM	C3B-C4B-NB	3.81	112.20	109.47
3	D	503	1F1	C11-N10-C9	3.68	111.60	108.91
3	C	502	1F1	C7-C8-C9	-3.67	102.57	107.05
5	B	506	GOL	O2-C2-C3	3.65	124.27	109.18
2	B	501	HEM	C4C-NC-C1C	3.63	111.74	105.82
2	A	501	HEM	C3A-C4A-NA	-3.62	104.34	110.14
3	C	502	1F1	C6-C7-C11	3.58	123.09	119.23
3	B	502	1F1	C8-C9-N10	-3.53	106.17	110.25
3	A	502	1F1	C7-C11-N10	3.51	110.35	107.53
2	D	502	HEM	C4A-C3A-C2A	3.48	110.81	106.82
3	A	502	1F1	O3-C2-C4	3.46	123.73	114.84
3	D	501	1F1	O3-C2-O1	-3.46	115.91	123.35
3	C	502	1F1	C12-C11-N10	-3.45	126.29	131.62
3	A	503	1F1	C7-C8-C9	-3.44	102.85	107.05
3	D	503	1F1	C7-C11-N10	3.40	110.26	107.53
2	C	501	HEM	CAD-CBD-CGD	-3.39	104.67	113.67
3	D	501	1F1	C8-C9-N10	-3.39	106.33	110.25
3	A	502	1F1	C7-C8-C9	-3.34	102.97	107.05
2	A	501	HEM	C4C-NC-C1C	3.33	111.24	105.82
3	A	502	1F1	C6-C5-C4	-3.30	117.27	120.80
3	A	502	1F1	O3-C2-O1	-3.26	116.34	123.35
2	B	501	HEM	C4C-CHD-C1D	-3.22	119.19	126.02
2	D	502	HEM	CBD-CAD-C3D	-3.21	103.67	112.53
3	D	501	1F1	C6-C5-C4	3.18	124.20	120.80
3	C	502	1F1	C4-C12-C11	-3.17	113.54	119.43
3	C	503	1F1	C12-C11-N10	-3.17	126.73	131.62
2	B	501	HEM	CBD-CAD-C3D	-3.14	103.84	112.53
3	C	503	1F1	C6-C7-C8	-3.12	126.11	134.97
3	C	503	1F1	C5-C6-C7	-3.12	117.53	121.74
3	C	502	1F1	C6-C7-C8	-3.12	126.12	134.97
3	A	504	1F1	C5-C6-C7	-3.11	117.54	121.74
3	B	503	1F1	C7-C11-N10	3.11	110.03	107.53
3	B	502	1F1	C11-N10-C9	3.07	111.16	108.91
3	B	502	1F1	C6-C7-C11	3.03	122.50	119.23
2	A	501	HEM	C2B-C1B-NB	3.02	113.31	109.84
2	C	501	HEM	CMD-C2D-C1D	3.01	129.74	125.03
2	B	501	HEM	CMD-C2D-C1D	2.96	129.66	125.03
2	D	502	HEM	O2D-CGD-CBD	2.95	123.32	114.00
3	C	503	1F1	C6-C7-C11	2.94	122.40	119.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBD-CAD-C3D	-2.94	104.41	112.53
3	A	504	1F1	C6-C7-C11	2.93	122.39	119.23
2	D	502	HEM	O1A-CGA-CBA	-2.92	113.83	123.09
2	A	501	HEM	CMC-C2C-C1C	-2.91	119.61	124.73
2	A	501	HEM	CHC-C1C-NC	2.89	127.60	124.45
5	B	506	GOL	O1-C1-C2	-2.86	97.48	110.38
2	A	501	HEM	O2D-CGD-CBD	2.86	123.03	114.00
2	C	501	HEM	CAD-C3D-C4D	2.83	129.62	124.70
3	A	504	1F1	C8-C9-N10	-2.80	107.02	110.25
3	D	501	1F1	C6-C7-C8	-2.77	127.10	134.97
3	B	502	1F1	O3-C2-O1	-2.76	117.41	123.35
3	C	502	1F1	C5-C4-C12	2.75	122.43	119.25
3	A	504	1F1	C6-C7-C8	-2.74	127.19	134.97
2	A	501	HEM	C4A-C3A-C2A	2.74	109.95	106.82
3	B	503	1F1	C12-C11-N10	-2.74	127.39	131.62
2	B	501	HEM	C4D-ND-C1D	-2.74	101.97	105.21
3	B	503	1F1	C4-C12-C11	-2.70	114.42	119.43
3	D	503	1F1	C12-C11-C7	-2.69	119.92	122.59
3	D	503	1F1	C6-C7-C8	-2.66	127.43	134.97
2	C	501	HEM	CHD-C1D-ND	2.65	127.28	124.42
3	D	501	1F1	C5-C6-C7	-2.65	118.16	121.74
2	A	501	HEM	CAD-CBD-CGD	-2.65	106.63	113.67
2	D	502	HEM	CMB-C2B-C1B	2.65	129.18	125.03
2	C	501	HEM	CHB-C4A-NA	2.60	128.58	123.86
3	D	503	1F1	C6-C5-C4	-2.58	118.04	120.80
2	D	502	HEM	CHB-C1B-NB	2.58	127.56	124.37
2	B	501	HEM	C2C-C1C-NC	-2.58	104.87	109.64
2	B	501	HEM	C4C-C3C-C2C	2.58	109.05	106.81
3	A	504	1F1	O3-C2-C4	2.57	121.44	114.84
3	D	503	1F1	C5-C6-C7	-2.56	118.29	121.74
4	A	505	SO4	O2-S-O1	2.56	127.06	109.06
2	A	501	HEM	C3D-C4D-ND	2.55	112.97	110.17
2	B	501	HEM	C1D-C2D-C3D	-2.53	104.32	106.98
2	C	501	HEM	C4C-C3C-C2C	2.52	109.00	106.81
2	A	501	HEM	C1D-C2D-C3D	-2.52	104.33	106.98
3	A	504	1F1	C5-C4-C12	2.50	122.14	119.25
2	A	501	HEM	C4A-NA-C1A	2.48	109.86	105.82
2	B	501	HEM	CAD-C3D-C4D	2.47	128.99	124.70
3	A	503	1F1	C11-N10-C9	2.44	110.70	108.91
2	C	501	HEM	O2A-CGA-CBA	2.43	121.69	114.00
2	D	502	HEM	C2D-C1D-ND	-2.43	107.10	109.90
2	B	501	HEM	CAA-CBA-CGA	-2.42	107.25	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	1F1	C11-C7-C8	2.41	108.12	106.59
2	A	501	HEM	CHC-C4B-NB	-2.38	121.86	124.42
2	B	501	HEM	CAC-C3C-C4C	-2.38	119.15	124.82
3	A	502	1F1	C12-C11-N10	-2.35	127.99	131.62
2	B	501	HEM	O1D-CGD-CBD	-2.34	115.68	123.09
2	D	502	HEM	C1A-C2A-C3A	-2.34	103.25	106.87
2	A	501	HEM	C2C-C1C-NC	-2.32	105.34	109.64
3	B	502	1F1	C6-C7-C8	-2.32	128.38	134.97
2	B	501	HEM	CMC-C2C-C1C	2.29	128.77	124.73
2	C	501	HEM	CHD-C4C-NC	2.29	126.95	124.45
3	B	503	1F1	C5-C4-C12	2.29	121.90	119.25
2	C	501	HEM	O2A-CGA-O1A	-2.29	117.45	123.33
2	B	501	HEM	CMA-C3A-C2A	2.28	130.45	125.62
2	C	501	HEM	C4A-C3A-C2A	2.28	109.42	106.82
2	D	502	HEM	CAD-C3D-C4D	2.26	128.63	124.70
5	A	508	GOL	O3-C3-C2	-2.24	100.30	110.38
3	A	503	1F1	C12-C4-C2	-2.23	115.97	119.96
3	D	501	1F1	C5-C4-C2	-2.23	115.97	120.37
2	A	501	HEM	CMD-C2D-C1D	2.19	128.46	125.03
2	C	501	HEM	C3B-C2B-C1B	2.16	108.04	106.41
2	A	501	HEM	O1D-CGD-CBD	-2.16	116.23	123.09
3	B	502	1F1	O3-C2-C4	2.15	120.35	114.84
3	A	504	1F1	C12-C11-N10	-2.14	128.31	131.62
2	A	501	HEM	C4A-CHB-C1B	-2.12	121.25	126.25
2	B	501	HEM	CHD-C1D-C2D	-2.12	121.68	125.03
5	A	508	GOL	C3-C2-C1	-2.08	104.18	111.80
3	C	502	1F1	C12-C11-C7	2.07	124.65	122.59
2	A	501	HEM	CHD-C1D-C2D	-2.07	121.76	125.03
2	D	502	HEM	O2A-CGA-O1A	2.06	128.64	123.33
3	B	502	1F1	C5-C4-C12	2.06	121.63	119.25
2	D	502	HEM	CAD-CBD-CGD	-2.06	108.21	113.67
5	B	506	GOL	O2-C2-C1	-2.04	100.73	109.18
5	C	507	GOL	O1-C1-C2	-2.04	101.19	110.38
2	D	502	HEM	C4B-C3B-C2B	2.04	109.15	107.28
2	D	502	HEM	CMB-C2B-C3B	-2.02	123.53	128.43

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	GOL	O1-C1-C2-C3
5	B	507	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	D	506	GOL	O1-C1-C2-O2
5	D	506	GOL	O1-C1-C2-C3
3	B	503	1F1	O1-C2-C4-C12
3	A	503	1F1	O3-C2-C4-C12
3	A	503	1F1	O3-C2-C4-C5
3	A	503	1F1	O1-C2-C4-C12
3	B	503	1F1	O1-C2-C4-C5
3	A	503	1F1	O1-C2-C4-C5
3	B	503	1F1	O3-C2-C4-C12
5	A	508	GOL	O1-C1-C2-O2
5	B	507	GOL	O1-C1-C2-O2
3	C	503	1F1	O3-C2-C4-C12
5	A	507	GOL	O1-C1-C2-C3
5	A	508	GOL	C1-C2-C3-O3
5	B	506	GOL	C1-C2-C3-O3
5	C	507	GOL	O1-C1-C2-C3
5	A	507	GOL	O1-C1-C2-O2
3	B	503	1F1	O3-C2-C4-C5
3	C	503	1F1	O1-C2-C4-C12
3	C	503	1F1	O3-C2-C4-C5
3	C	503	1F1	O1-C2-C4-C5
5	A	508	GOL	O2-C2-C3-O3
5	B	506	GOL	O2-C2-C3-O3
2	A	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	D	502	HEM	CAA-CBA-CGA-O1A
2	D	502	HEM	CAD-CBD-CGD-O2D
2	D	502	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

11 monomers are involved in 27 short contacts:

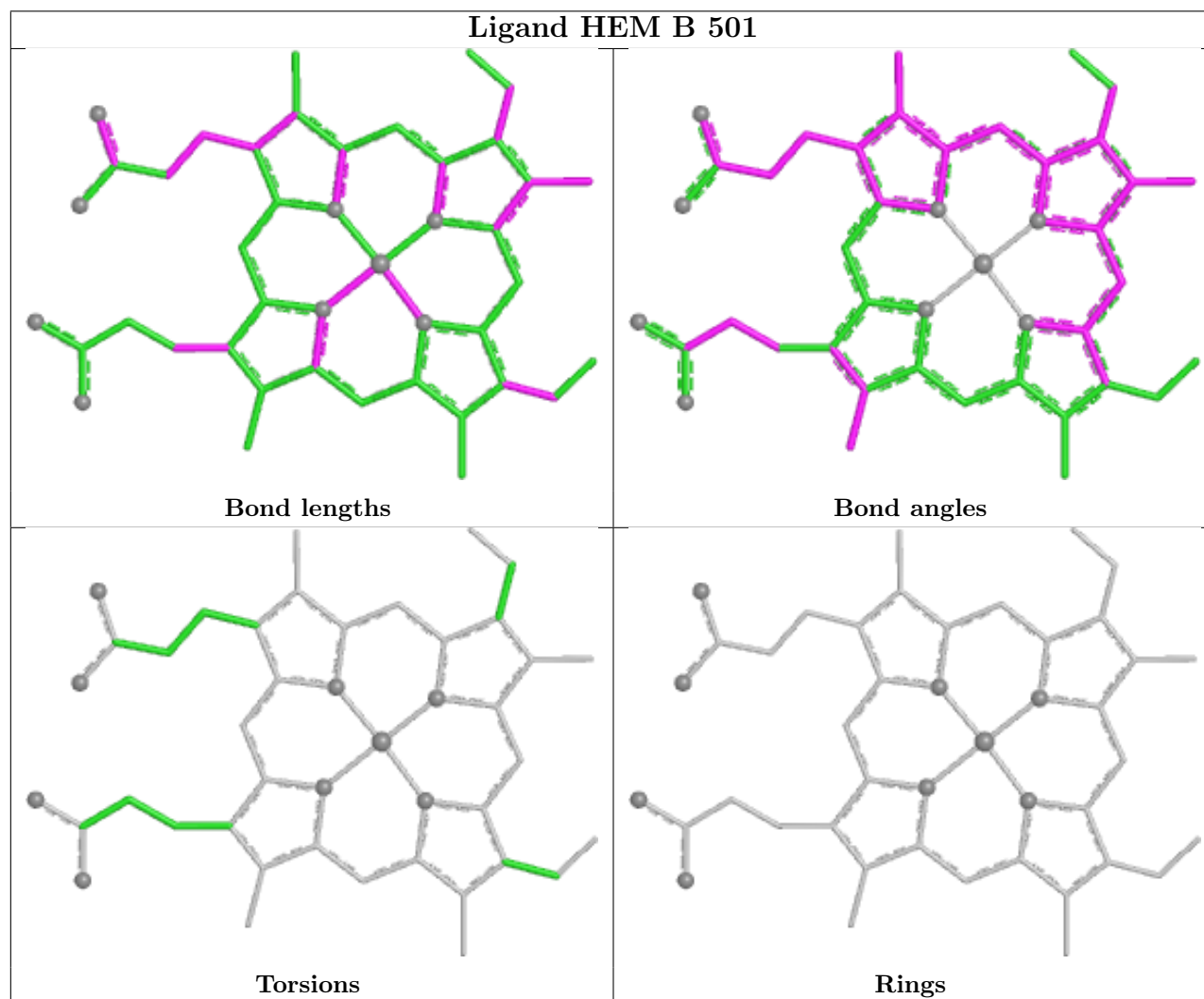
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	1F1	1	0
3	C	503	1F1	1	0
2	B	501	HEM	5	0
2	C	501	HEM	5	0
2	A	501	HEM	4	0
3	B	503	1F1	2	0
3	C	502	1F1	2	0
5	B	506	GOL	2	0

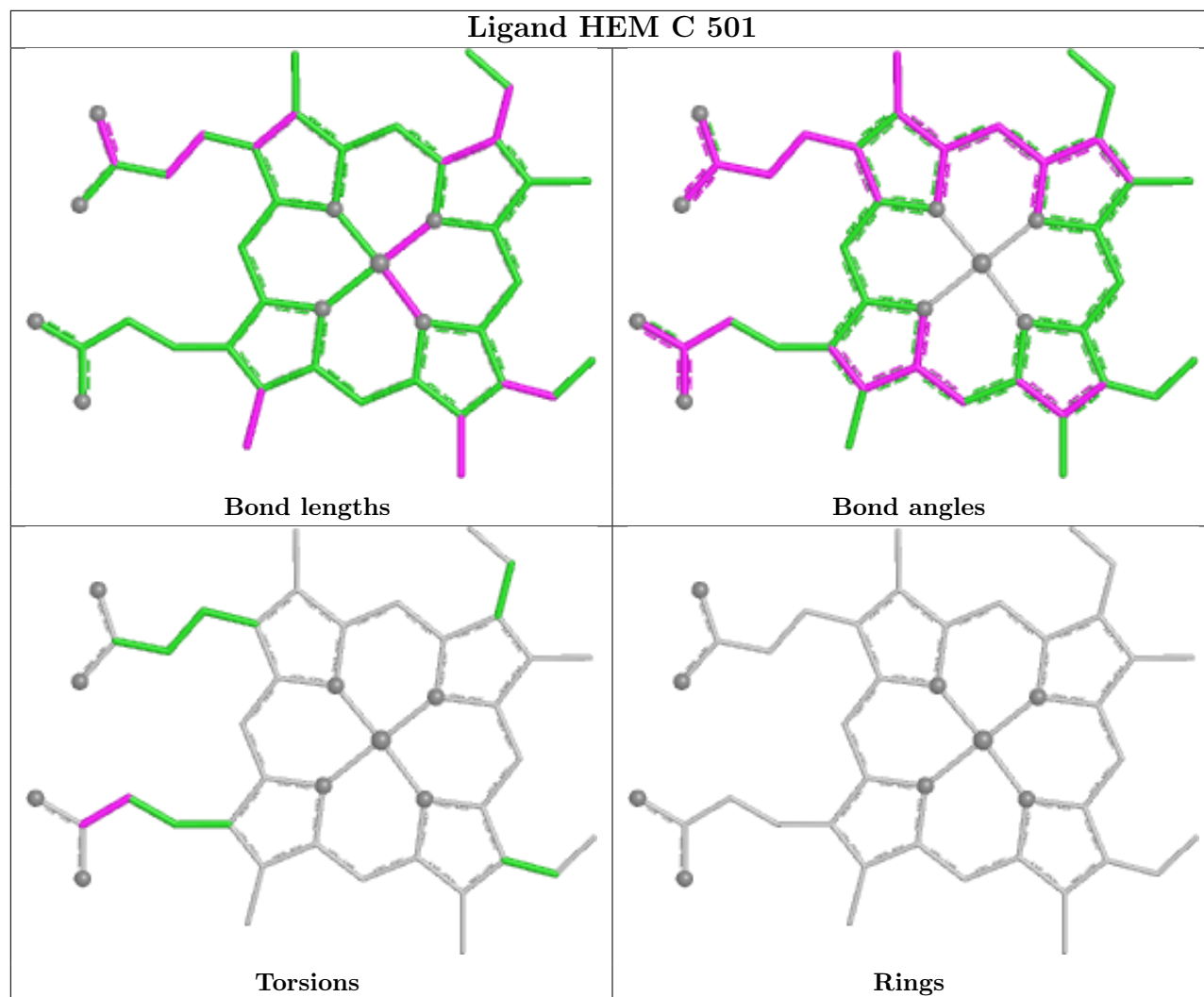
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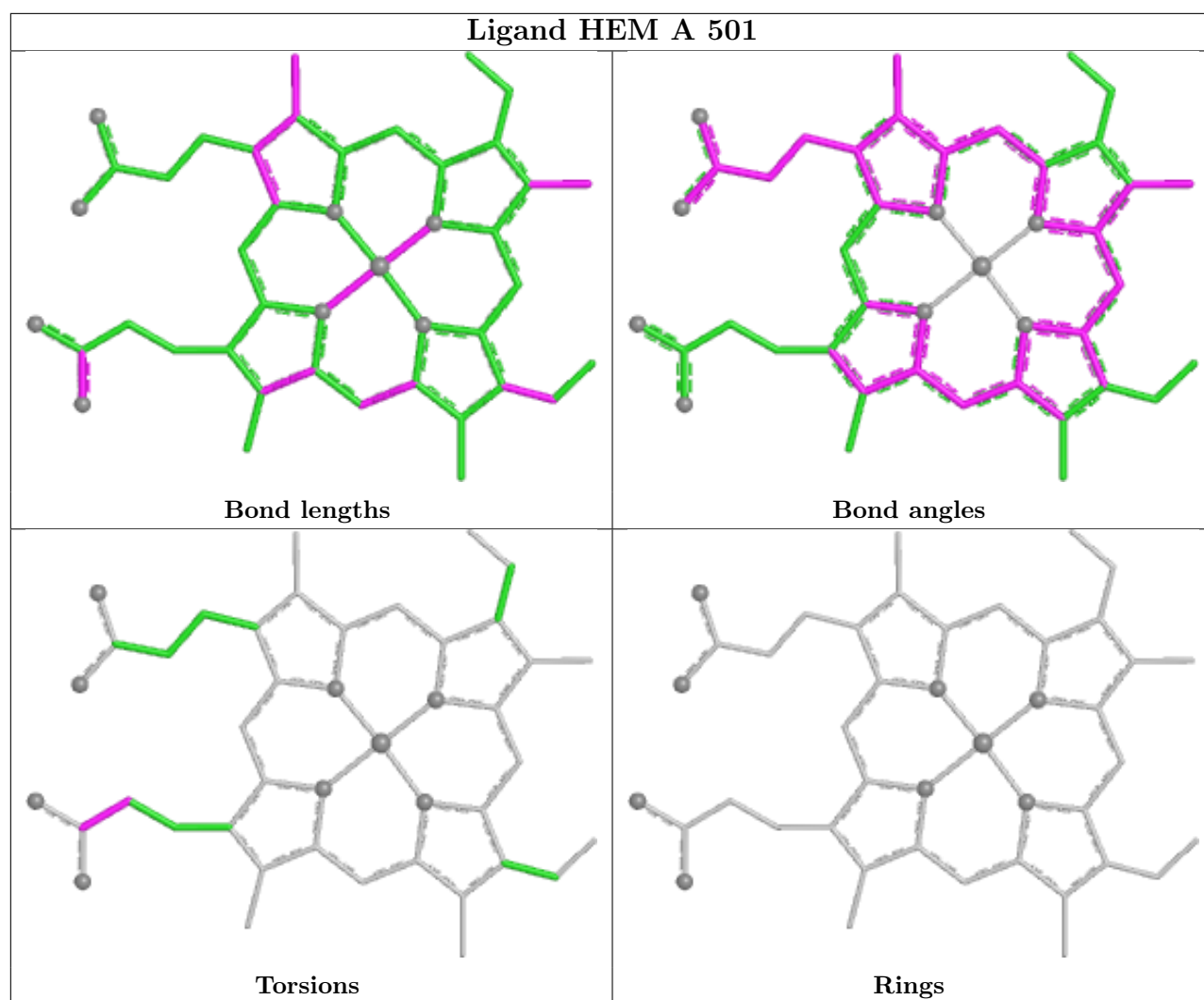
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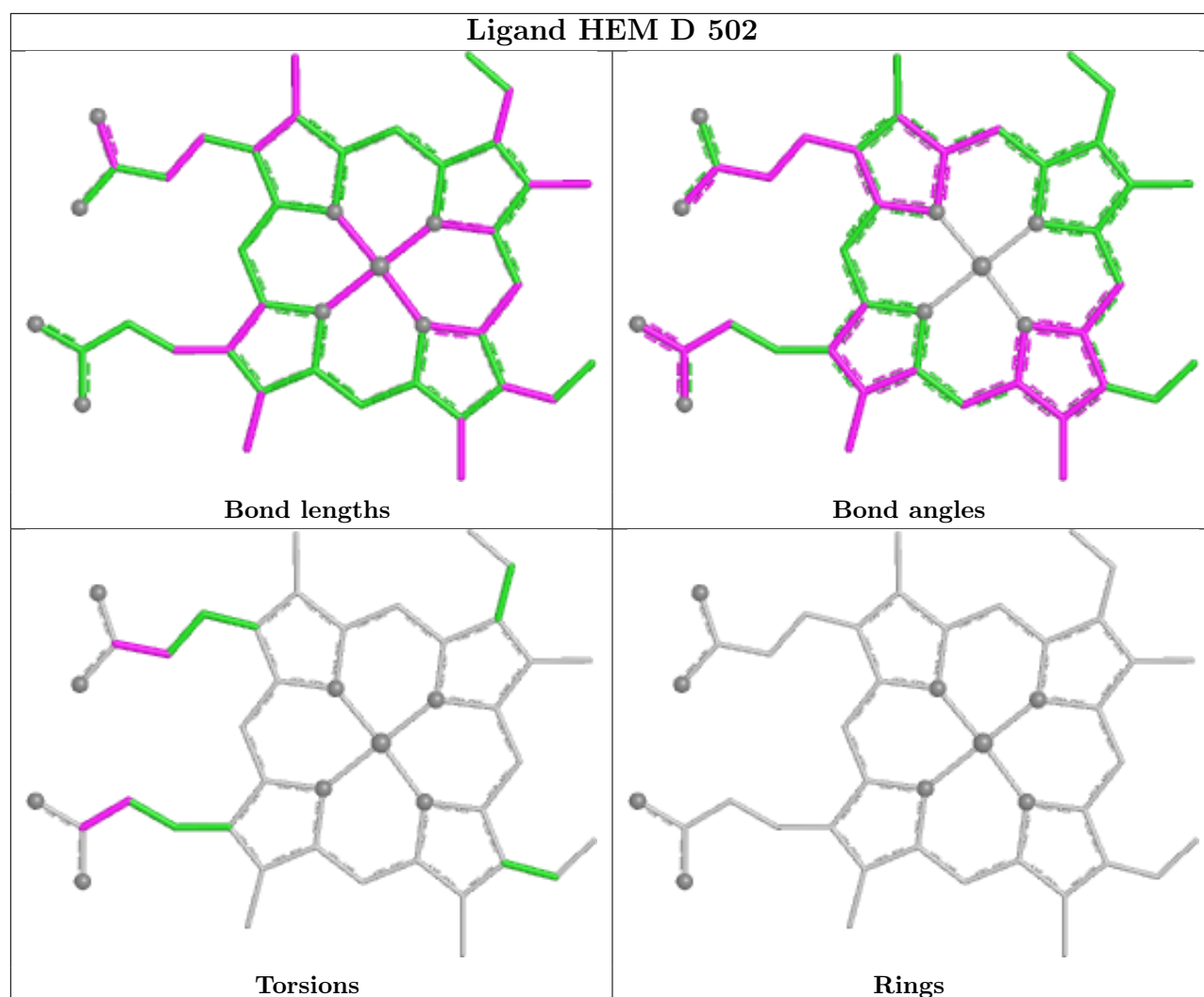
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	HEM	3	0
3	B	502	1F1	1	0
3	D	503	1F1	1	0

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	393/410 (95%)	-0.28	6 (1%) 72 78	11, 18, 30, 38	3 (0%)
1	B	393/410 (95%)	-0.09	11 (2%) 55 61	11, 19, 31, 42	1 (0%)
1	C	393/410 (95%)	-0.04	5 (1%) 75 81	14, 21, 33, 41	0
1	D	393/410 (95%)	0.33	14 (3%) 46 52	15, 25, 39, 54	0
All	All	1572/1640 (95%)	-0.02	36 (2%) 61 67	11, 21, 35, 54	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	THR	4.1
1	D	17	THR	3.6
1	B	223	CYS	3.4
1	B	169	GLU	3.1
1	B	366	LEU	2.8
1	D	250	LEU	2.8
1	A	169	GLU	2.8
1	D	169	GLU	2.8
1	C	17	THR	2.7
1	D	89	LYS	2.6
1	B	409	ALA	2.6
1	C	309	GLY	2.5
1	C	29	ASP	2.4
1	D	366	LEU	2.4
1	B	266	ARG	2.3
1	A	17	THR	2.3
1	A	307	GLU	2.3
1	D	217	PRO	2.3
1	B	39	GLN	2.3
1	D	409	ALA	2.3
1	A	267	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	262	TYR	2.2
1	C	366	LEU	2.2
1	D	193	GLN	2.2
1	D	262	TYR	2.2
1	A	409	ALA	2.1
1	D	223	CYS	2.1
1	D	114	LYS	2.1
1	D	142	ARG	2.1
1	B	230	THR	2.1
1	B	267	PHE	2.1
1	A	138	GLU	2.0
1	B	138	GLU	2.0
1	D	144	CYS	2.0
1	D	141	GLN	2.0
1	C	312	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	1F1	C	503	12/12	0.70	0.24	74,77,78,79	0
3	1F1	B	503	12/12	0.71	0.25	38,43,52,57	0
3	1F1	D	501	12/12	0.76	0.17	48,50,53,56	0
5	GOL	B	506	6/6	0.78	0.22	32,35,38,40	0
4	SO4	C	506	5/5	0.79	0.34	30,30,30,30	0
3	1F1	A	503	12/12	0.79	0.19	40,45,58,59	0
4	SO4	D	505	5/5	0.85	0.14	46,52,54,58	0
5	GOL	A	508	6/6	0.86	0.17	38,52,54,58	0

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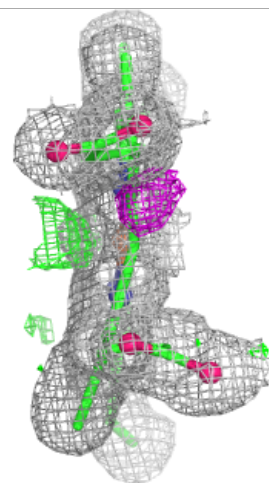
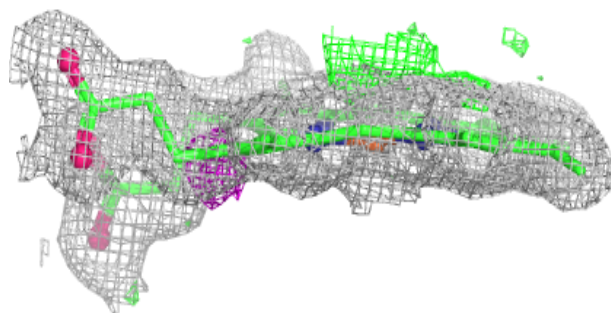
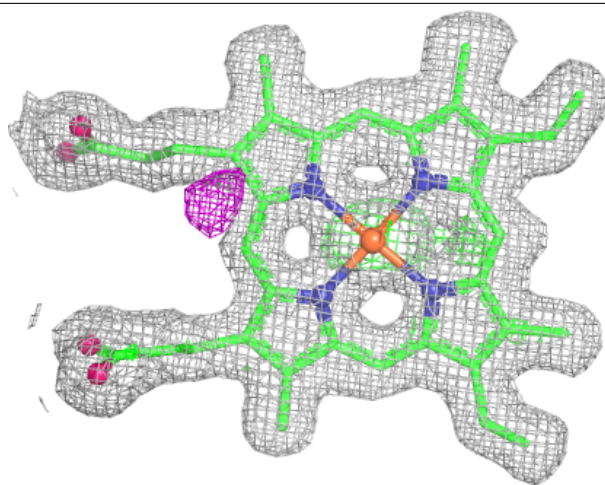
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	506	5/5	0.86	0.29	30,30,30,30	0
5	GOL	B	507	6/6	0.88	0.14	31,45,52,55	0
3	1F1	A	504	12/12	0.93	0.10	23,31,46,49	0
5	GOL	B	505	6/6	0.94	0.09	18,21,24,34	0
5	GOL	C	507	6/6	0.94	0.09	22,25,29,35	0
5	GOL	D	506	6/6	0.94	0.11	21,33,36,37	0
4	SO4	A	505	5/5	0.95	0.10	24,32,37,38	0
3	1F1	D	503	12/12	0.95	0.07	16,21,22,24	0
5	GOL	A	507	6/6	0.95	0.08	20,23,28,32	0
4	SO4	C	505	5/5	0.96	0.08	36,39,45,47	0
4	SO4	D	504	5/5	0.96	0.13	33,37,40,43	0
6	CL	D	507	1/1	0.96	0.10	32,32,32,32	0
3	1F1	C	502	12/12	0.97	0.06	15,17,19,20	0
3	1F1	B	502	12/12	0.98	0.04	11,13,15,15	0
2	HEM	D	502	43/43	0.98	0.06	12,18,22,24	0
6	CL	B	508	1/1	0.98	0.04	18,18,18,18	0
4	SO4	C	504	5/5	0.98	0.08	24,24,26,27	0
4	SO4	B	504	5/5	0.99	0.06	22,23,27,27	0
2	HEM	A	501	43/43	0.99	0.05	10,13,15,17	0
3	1F1	A	502	12/12	0.99	0.03	10,14,15,17	0
6	CL	A	509	1/1	0.99	0.03	17,17,17,17	0
2	HEM	B	501	43/43	0.99	0.04	10,13,15,19	0
6	CL	C	508	1/1	0.99	0.04	27,27,27,27	0
2	HEM	C	501	43/43	0.99	0.04	12,16,18,21	0

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

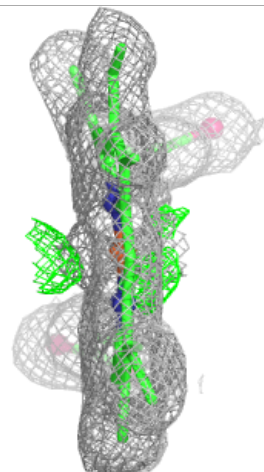
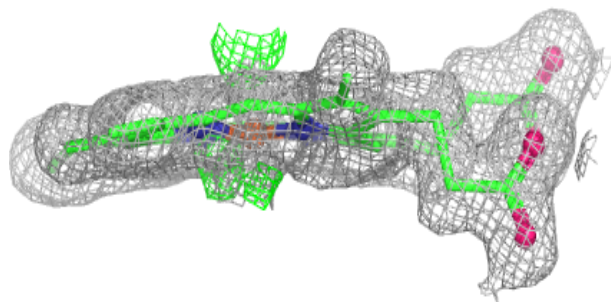
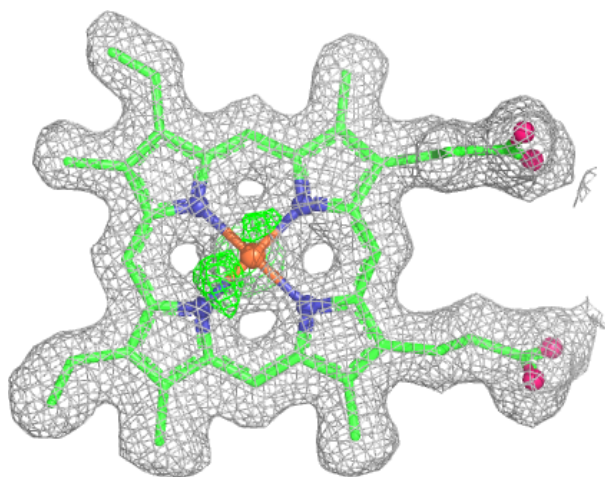
Electron density around HEM D 502:

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



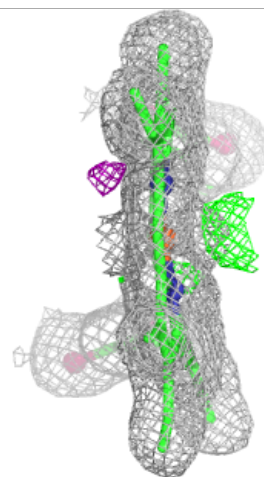
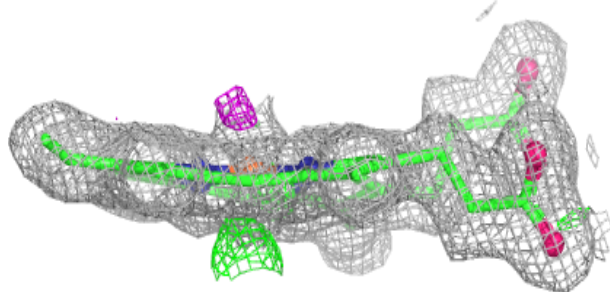
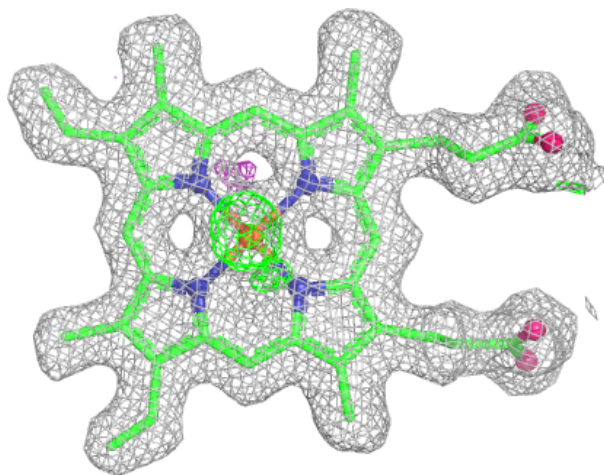
Electron density around HEM A 501:

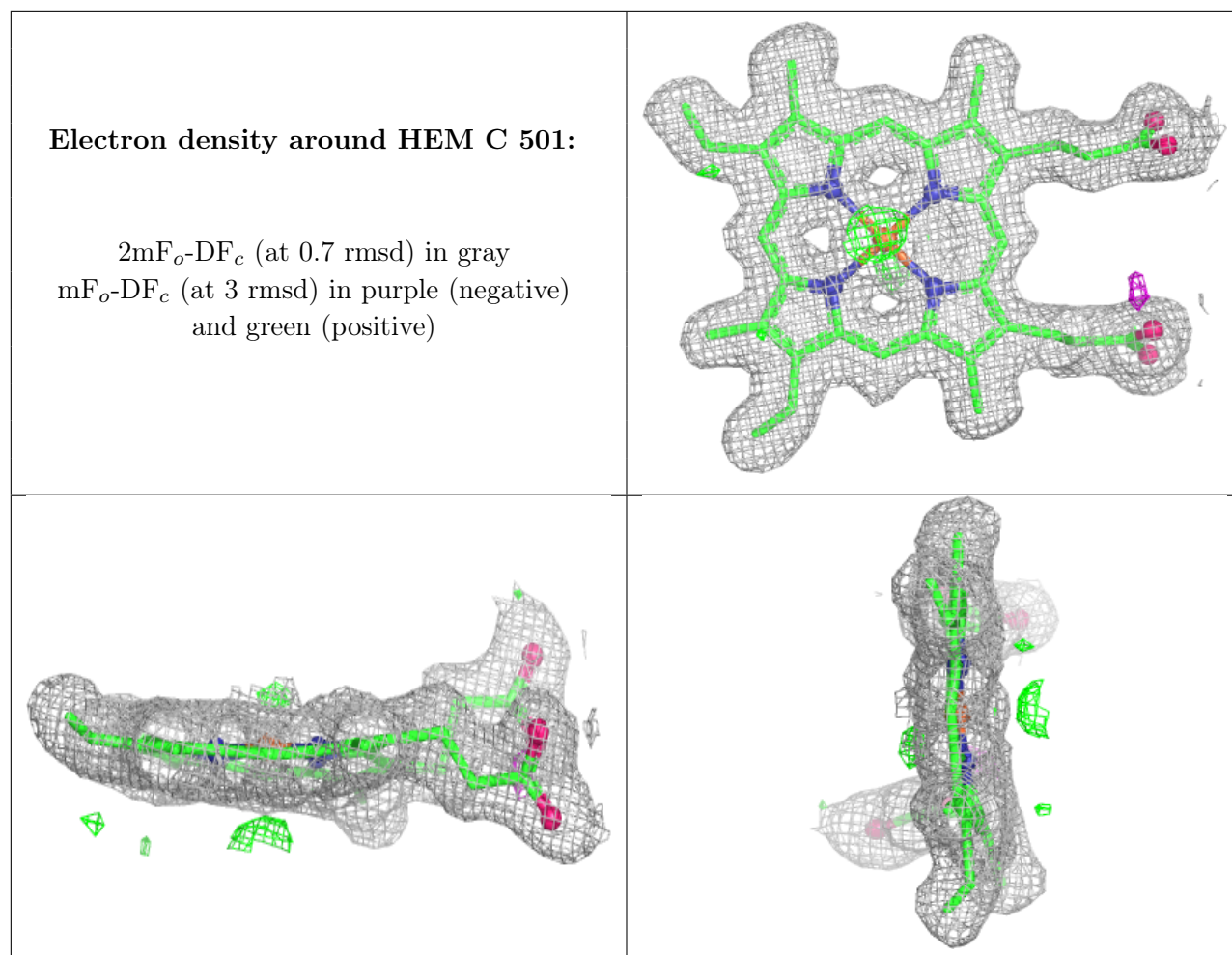
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.