



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:34 AM UTC

PDB ID : 4EGN / pdb_00004egn
Title : The X-ray crystal structure of CYP199A4 in complex with veratric 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 : 2.00 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

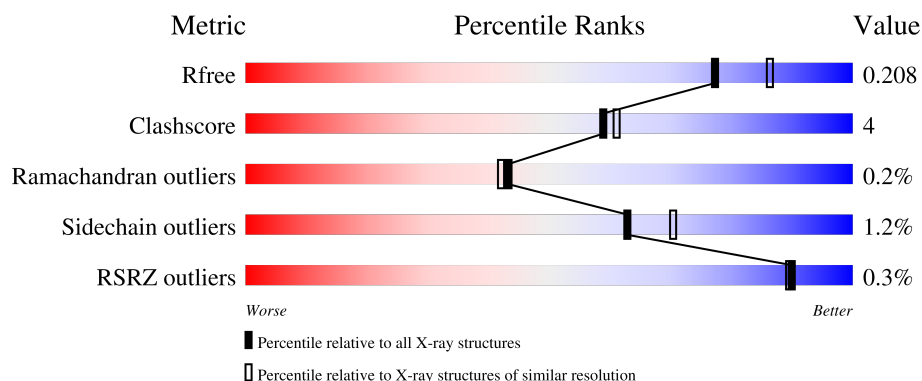
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	 85% 10% . .
1	B	410	 84% 11% .
1	C	410	 81% 14% . .
1	D	410	 84% 10% . .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13711 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	1	0
			3024	1914	534	564	12			
1	B	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			
1	C	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			
1	D	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			

- 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		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



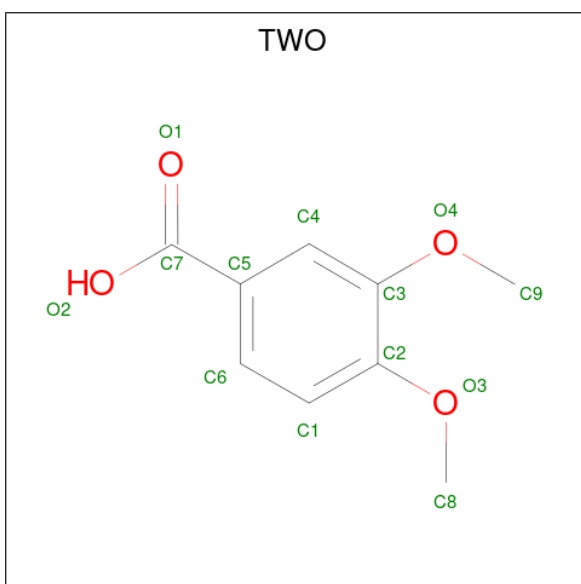
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S		
			5	4	1	0	0
3	B	1	Total	O	S		
			5	4	1	0	0
3	C	1	Total	O	S		
			5	4	1	0	0
3	C	1	Total	O	S		
			5	4	1	0	0
3	C	1	Total	O	S		
			5	4	1	0	0
3	D	1	Total	O	S		
			5	4	1	0	0
3	D	1	Total	O	S		
			5	4	1	0	0
3	D	1	Total	O	S		
			5	4	1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is 3,4-dimethoxybenzoic acid (CCD ID: TWO) (formula: $C_9H_8O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 9 4	0	0
5	B	1	Total C O 13 9 4	0	0
5	C	1	Total C O 13 9 4	0	0
5	D	1	Total C O 13 9 4	0	0

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

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

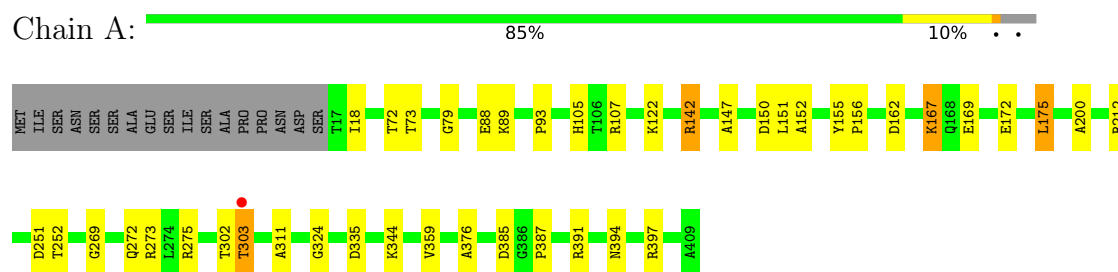
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	358	Total O 358 358	0	0
7	B	349	Total O 349 349	0	0
7	C	345	Total O 345 345	0	0
7	D	265	Total O 265 265	0	0

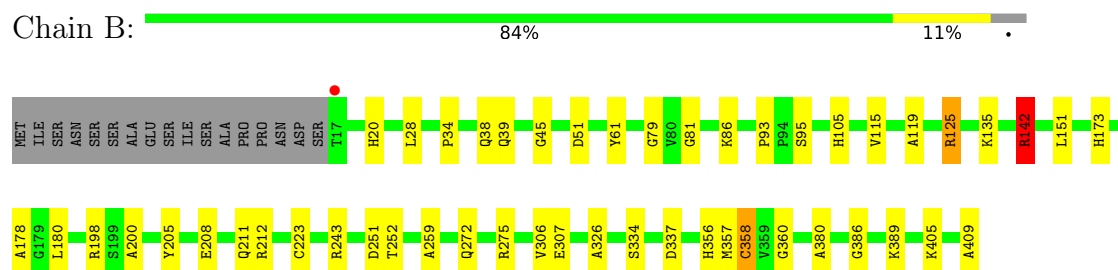
3 Residue-property plots

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

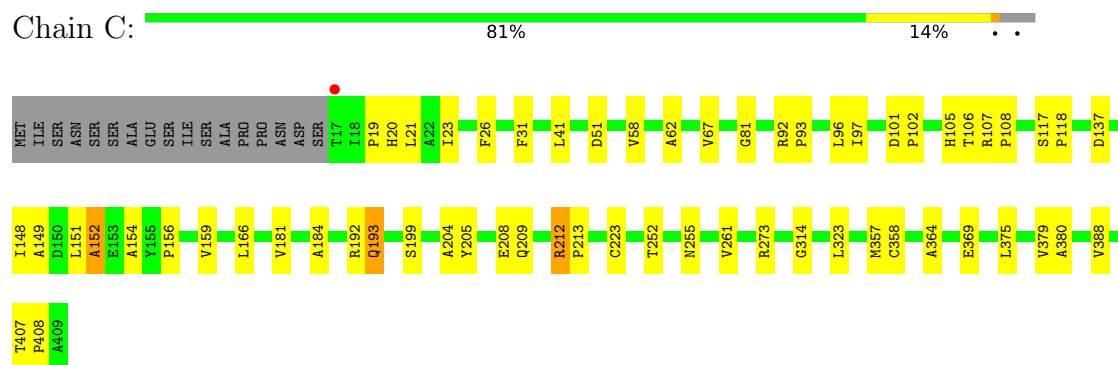
• Molecule 1: Cytochrome P450



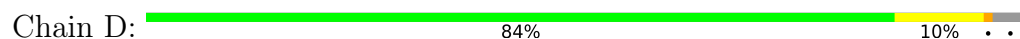
• Molecule 1: Cytochrome P450

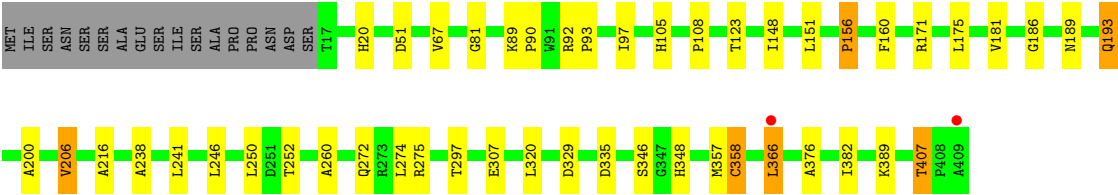


• Molecule 1: Cytochrome P450



• 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	106.53Å 143.44Å 172.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.44 – 2.00 30.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.44-2.00) 98.2 (30.44-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.171 , 0.207 0.174 , 0.208	Depositor DCC
R_{free} test set	8818 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13711	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 40.99 % 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 2.5229e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GOL, SO4, CL, TWO

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	1.57	18/3099 (0.6%)	1.26	15/4217 (0.4%)
1	B	1.59	12/3099 (0.4%)	1.29	9/4217 (0.2%)
1	C	1.56	25/3099 (0.8%)	1.22	8/4217 (0.2%)
1	D	1.48	14/3099 (0.5%)	1.27	13/4217 (0.3%)
All	All	1.55	69/12396 (0.6%)	1.26	45/16868 (0.3%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	102	PRO	CA-C	15.66	1.60	1.51
1	A	147	ALA	C-N	-9.00	1.21	1.33
1	D	67	VAL	CA-CB	8.69	1.64	1.54
1	B	79	GLY	N-CA	8.22	1.55	1.45
1	B	306	VAL	CA-CB	8.15	1.65	1.54
1	D	81	GLY	N-CA	8.05	1.50	1.44
1	B	119	ALA	CA-CB	7.83	1.65	1.53
1	C	154	ALA	CA-CB	7.01	1.64	1.53
1	C	380	ALA	CA-CB	7.00	1.64	1.53
1	C	364	ALA	CA-CB	6.87	1.64	1.53
1	A	88	GLU	C-N	-6.77	1.22	1.32
1	A	335	ASP	C-O	6.74	1.27	1.23
1	B	45	GLY	N-CA	6.61	1.53	1.44
1	C	159	VAL	N-CA	6.52	1.52	1.46
1	D	175	LEU	N-CA	6.49	1.52	1.46
1	B	259	ALA	CA-CB	6.24	1.63	1.53
1	B	200	ALA	N-CA	6.20	1.52	1.46
1	B	200	ALA	CA-CB	6.19	1.61	1.53
1	C	193	GLN	CG-CD	6.17	1.67	1.52
1	C	93	PRO	CA-C	5.96	1.57	1.52
1	D	200	ALA	CA-CB	5.93	1.60	1.53
1	D	348	HIS	N-CA	5.93	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	366	LEU	C-O	-5.91	1.17	1.24
1	A	152	ALA	CA-CB	5.90	1.62	1.53
1	B	125	ARG	C-O	-5.89	1.17	1.24
1	C	149	ALA	CA-CB	5.82	1.62	1.53
1	B	211	GLN	C-O	5.73	1.31	1.23
1	C	92	ARG	CA-C	5.73	1.57	1.52
1	C	67	VAL	CA-CB	5.73	1.61	1.54
1	A	303	THR	CB-CG2	-5.67	1.33	1.52
1	A	147	ALA	C-O	5.65	1.31	1.24
1	A	311	ALA	CA-CB	5.61	1.63	1.53
1	A	302	THR	C-O	-5.58	1.17	1.23
1	A	376	ALA	CA-C	5.57	1.60	1.52
1	C	314	GLY	C-O	5.57	1.31	1.23
1	C	204	ALA	CA-CB	5.55	1.62	1.53
1	C	62	ALA	CA-CB	5.53	1.61	1.53
1	D	93	PRO	CA-C	5.46	1.57	1.52
1	C	152	ALA	N-CA	5.45	1.52	1.46
1	C	209	GLN	CA-C	5.43	1.60	1.52
1	C	137	ASP	N-CA	5.39	1.52	1.46
1	A	93	PRO	C-O	-5.37	1.18	1.24
1	A	79	GLY	N-CA	5.36	1.51	1.45
1	D	335	ASP	N-CA	5.36	1.50	1.46
1	D	200	ALA	N-CA	5.34	1.51	1.46
1	C	379	VAL	CA-CB	5.33	1.61	1.54
1	D	238	ALA	CA-CB	5.33	1.60	1.53
1	D	382	ILE	CA-CB	5.33	1.60	1.54
1	A	391	ARG	N-CA	-5.33	1.39	1.46
1	B	95	SER	CA-C	5.31	1.59	1.52
1	C	388	VAL	CA-CB	-5.29	1.47	1.54
1	C	23	ILE	CA-CB	5.28	1.60	1.54
1	A	162	ASP	N-CA	5.26	1.52	1.46
1	C	261	VAL	CA-CB	5.26	1.61	1.54
1	D	260	ALA	CA-CB	5.24	1.61	1.53
1	B	81	GLY	C-O	5.23	1.28	1.23
1	A	359	VAL	CA-CB	5.20	1.62	1.54
1	A	167	LYS	N-CA	5.18	1.52	1.45
1	A	324	GLY	CA-C	5.13	1.57	1.52
1	A	385	ASP	CA-CB	5.13	1.59	1.52
1	B	93	PRO	CA-C	5.10	1.56	1.52
1	D	250	LEU	C-O	-5.10	1.17	1.23
1	D	186	GLY	N-CA	5.07	1.50	1.43
1	A	387	PRO	CA-C	5.06	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	148	ILE	CA-C	5.05	1.59	1.52
1	C	81	GLY	C-O	5.03	1.28	1.23
1	C	375	LEU	CA-C	5.03	1.59	1.52
1	C	255	ASN	C-O	-5.03	1.17	1.24
1	C	106	THR	CA-CB	5.00	1.61	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	ASP	CA-C-N	-7.77	113.99	119.66
1	C	101	ASP	C-N-CA	-7.77	113.99	119.66
1	B	142	ARG	NE-CZ-NH2	-7.12	112.80	119.20
1	A	107	ARG	CA-C-N	-6.84	111.75	119.28
1	A	107	ARG	C-N-CA	-6.84	111.75	119.28
1	A	18	ILE	CA-C-N	-6.59	112.97	119.76
1	A	18	ILE	C-N-CA	-6.59	112.97	119.76
1	C	96	LEU	CA-C-N	-6.58	116.18	123.16
1	C	96	LEU	C-N-CA	-6.58	116.18	123.16
1	A	212	ARG	CA-C-N	-6.53	113.08	119.87
1	A	212	ARG	C-N-CA	-6.53	113.08	119.87
1	D	200	ALA	CA-C-N	-6.51	112.11	119.28
1	D	200	ALA	C-N-CA	-6.51	112.11	119.28
1	B	212	ARG	CA-C-N	-6.34	113.61	119.82
1	B	212	ARG	C-N-CA	-6.34	113.61	119.82
1	A	303	THR	N-CA-CB	-6.27	101.43	110.65
1	C	212	ARG	CA-C-N	-6.18	113.44	119.87
1	C	212	ARG	C-N-CA	-6.18	113.44	119.87
1	D	335	ASP	O-C-N	6.12	124.34	121.53
1	D	329	ASP	CA-C-N	-6.11	113.52	119.87
1	D	329	ASP	C-N-CA	-6.11	113.52	119.87
1	A	175	LEU	CA-C-N	-6.07	112.76	119.19
1	A	175	LEU	C-N-CA	-6.07	112.76	119.19
1	A	142	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	D	160	PHE	CA-C-N	-5.97	112.42	119.05
1	D	160	PHE	C-N-CA	-5.97	112.42	119.05
1	B	198	ARG	CB-CG-CD	5.88	124.83	111.30
1	D	171	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	D	407	THR	CA-C-N	5.73	125.70	120.03
1	D	407	THR	C-N-CA	5.73	125.70	120.03
1	C	205	TYR	N-CA-C	-5.67	105.02	111.14
1	C	199	SER	N-CA-C	5.62	117.49	111.36
1	B	39	GLN	CB-CG-CD	-5.58	103.11	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	LYS	CB-CA-C	5.49	117.33	109.26
1	A	200	ALA	CA-C-N	-5.49	113.38	119.19
1	A	200	ALA	C-N-CA	-5.49	113.38	119.19
1	B	243	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	B	386	GLY	CA-C-N	5.41	125.58	119.90
1	B	386	GLY	C-N-CA	5.41	125.58	119.90
1	B	243	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	D	123	THR	N-CA-C	5.38	118.06	111.82
1	A	391	ARG	CA-CB-CG	-5.30	103.50	114.10
1	D	216	ALA	N-CA-C	5.24	115.62	109.60
1	A	394	ASN	N-CA-C	5.22	117.71	111.71
1	A	88	GLU	O-C-N	-5.13	116.49	123.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	2998	27	0
1	B	3024	0	2998	26	0
1	C	3024	0	2998	30	0
1	D	3024	0	2998	22	0
2	A	43	0	30	3	0
2	B	43	0	30	6	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	13	0	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	13	0	9	0	0
5	C	13	0	9	3	0
5	D	13	0	9	2	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	358	0	0	5	0
7	B	349	0	0	7	0
7	C	345	0	0	11	0
7	D	265	0	0	7	0
All	All	13711	0	12188	108	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 4.

All (108) 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:C:273:ARG:HB3	7:C:847:HOH:O	1.40	1.22
1:D:206:VAL:HG13	7:D:793:HOH:O	1.38	1.21
1:B:405:LYS:HD3	7:B:879:HOH:O	1.41	1.18
1:A:73:THR:O	1:A:303:THR:HG22	1.48	1.13
1:B:208:GLU:HG2	7:B:678:HOH:O	1.50	1.11
1:C:97:ILE:HB	7:C:911:HOH:O	1.52	1.08
1:A:72:THR:O	1:A:303:THR:HG21	1.53	1.08
1:C:108:PRO:HB2	7:C:911:HOH:O	1.52	1.08
1:C:369:GLU:HA	7:C:873:HOH:O	1.76	0.84
1:D:246:LEU:CD1	7:D:793:HOH:O	2.26	0.82
1:D:246:LEU:HD12	7:D:793:HOH:O	1.81	0.80
1:A:73:THR:HA	1:A:303:THR:CG2	2.13	0.78
1:D:105:HIS:HD2	7:D:605:HOH:O	1.67	0.76
1:D:156:PRO:HG3	7:D:803:HOH:O	1.86	0.76
1:B:272:GLN:HE22	1:B:275:ARG:HH11	1.36	0.73
1:A:344:LYS:HE3	7:A:862:HOH:O	1.89	0.72
1:A:105:HIS:HD2	7:A:606:HOH:O	1.72	0.71
1:B:105:HIS:HD2	7:B:602:HOH:O	1.74	0.71
1:A:73:THR:C	1:A:303:THR:HG22	2.15	0.70
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.73	0.70
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.72	0.70
1:D:407:THR:HG23	7:D:782:HOH:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.41	0.69
1:C:105:HIS:HD2	7:C:613:HOH:O	1.75	0.68
1:D:20:HIS:HD2	1:D:51:ASP:OD1	1.76	0.67
1:D:181:VAL:HG11	5:D:506:TWO:H4	1.76	0.66
1:C:105:HIS:HE1	2:C:501:HEM:O1D	1.80	0.65
1:D:105:HIS:HE1	2:D:501:HEM:O1D	1.80	0.65
1:C:208:GLU:HG2	7:C:638:HOH:O	1.96	0.65
1:B:105:HIS:HE1	2:B:501:HEM:O1D	1.79	0.64
1:B:307:GLU:HG2	7:B:948:HOH:O	1.97	0.63
1:C:20:HIS:HD2	1:C:51:ASP:OD1	1.83	0.61
1:B:125:ARG:NH1	7:B:886:HOH:O	2.34	0.60
1:C:19:PRO:HG2	7:C:892:HOH:O	2.01	0.60
1:D:108:PRO:HB3	1:D:241:LEU:HD21	1.84	0.59
1:A:73:THR:CA	1:A:303:THR:CG2	2.81	0.59
1:A:105:HIS:HE1	2:A:501:HEM:O1D	1.86	0.58
1:C:192:ARG:HH21	1:C:193:GLN:HE22	1.50	0.57
1:C:357:MET:HE1	7:C:901:HOH:O	2.05	0.57
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.86	0.57
1:D:189:ASN:O	1:D:193:GLN:HG2	2.07	0.55
1:D:181:VAL:CG1	5:D:506:TWO:H4	2.38	0.54
1:A:73:THR:C	1:A:303:THR:CG2	2.81	0.54
1:D:272:GLN:HE22	1:D:275:ARG:HH11	1.55	0.53
1:B:20:HIS:HD2	1:B:51:ASP:OD1	1.92	0.53
1:B:389:LYS:HE2	7:B:836:HOH:O	2.07	0.53
1:A:73:THR:HA	1:A:303:THR:HG21	1.92	0.52
1:A:172:GLU:HG2	7:A:951:HOH:O	2.07	0.52
1:A:252:THR:HB	2:A:501:HEM:C3B	2.44	0.52
1:A:142:ARG:HD3	1:B:205:TYR:HA	1.91	0.52
1:C:212:ARG:HB3	1:C:213:PRO:HD3	1.92	0.52
1:A:89:LYS:HE3	7:A:732:HOH:O	2.09	0.52
1:B:337:ASP:HB2	7:B:643:HOH:O	2.10	0.51
1:D:20:HIS:CD2	1:D:51:ASP:OD1	2.62	0.51
1:A:272:GLN:HE22	1:A:275:ARG:NH1	2.07	0.51
1:C:252:THR:HB	2:C:501:HEM:C3B	2.45	0.51
1:D:246:LEU:HD13	7:D:793:HOH:O	2.01	0.51
1:A:167:LYS:HE3	1:A:169:GLU:HB3	1.92	0.50
1:C:181:VAL:CG1	5:C:506:TWO:H4	2.42	0.50
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.92	0.50
1:C:58:VAL:HG13	7:C:893:HOH:O	2.12	0.49
1:C:21:LEU:HD12	1:C:41:LEU:HD23	1.93	0.49
1:D:274:LEU:HG	1:D:376:ALA:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLY:HA3	2:B:501:HEM:C3C	2.48	0.48
1:B:252:THR:HB	2:B:501:HEM:C3B	2.47	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.43	0.48
1:A:175:LEU:HD23	1:A:251:ASP:OD1	2.13	0.48
1:C:223[A]:CYS:SG	7:C:918:HOH:O	2.28	0.48
1:D:151:LEU:C	1:D:151:LEU:HD23	2.38	0.48
1:A:151:LEU:C	1:A:151:LEU:HD23	2.39	0.47
1:C:20:HIS:CD2	1:C:51:ASP:OD1	2.66	0.46
1:C:152:ALA:O	1:C:156:PRO:HD2	2.16	0.46
1:C:184:ALA:HA	1:C:192:ARG:HG3	1.97	0.46
1:D:252:THR:HB	2:D:501:HEM:C3B	2.51	0.46
1:C:181:VAL:HG12	5:C:506:TWO:H4	1.98	0.45
1:D:97:ILE:HG12	2:D:501:HEM:CGD	2.46	0.45
1:C:107:ARG:HB3	1:C:108:PRO:HD3	1.98	0.44
1:C:407:THR:HG23	1:C:408:PRO:HD2	1.99	0.44
1:D:357:MET:O	1:D:358:CYS:C	2.61	0.44
1:A:73:THR:CA	1:A:303:THR:HG21	2.47	0.44
1:B:356:HIS:O	1:B:357:MET:C	2.59	0.43
1:C:357:MET:O	1:C:358:CYS:C	2.60	0.43
1:D:90:PRO:HB2	1:D:92:ARG:O	2.17	0.43
1:C:21:LEU:HG	7:C:892:HOH:O	2.18	0.43
1:C:97:ILE:HD13	1:C:97:ILE:HG21	1.69	0.43
1:A:169:GLU:CD	1:B:142:ARG:HH22	2.26	0.43
1:C:151:LEU:C	1:C:151:LEU:HD23	2.44	0.43
1:A:269:GLY:O	1:A:273:ARG:HG3	2.19	0.42
1:B:151:LEU:HD23	1:B:151:LEU:C	2.44	0.42
1:A:155:TYR:HB3	1:A:156:PRO:HD3	2.00	0.42
1:B:34:PRO:O	1:B:38:GLN:HG3	2.20	0.42
1:B:135:LYS:HA	1:B:135:LYS:HD3	1.93	0.42
1:B:20:HIS:CD2	1:B:51:ASP:OD1	2.71	0.41
1:B:380:ALA:HB2	1:B:409:ALA:HA	2.02	0.41
1:B:115:VAL:HG22	1:B:223[A]:CYS:SG	2.60	0.41
1:A:272:GLN:NE2	1:A:275:ARG:HD3	2.36	0.41
1:A:397:ARG:NH1	7:A:950:HOH:O	2.25	0.41
1:B:178:ALA:HB3	1:B:251:ASP:CG	2.45	0.41
1:C:26:PHE:HA	1:C:31:PHE:CZ	2.56	0.41
1:B:272:GLN:HE22	1:B:275:ARG:NH1	2.11	0.41
1:B:61:TYR:HA	1:B:326:ALA:HB1	2.02	0.41
1:C:117:SER:HB2	1:C:118:PRO:HD2	2.03	0.41
1:A:150:ASP:CG	1:B:173:HIS:HE2	2.29	0.40
1:A:303:THR:HG22	1:A:303:THR:H	1.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:HEM:C4D	5:C:506:TWO:H9	2.56	0.40
1:D:297:THR:HB	1:D:320:LEU:HD11	2.03	0.40
1:C:192:ARG:NH2	1:C:193:GLN:HE22	2.18	0.40
1:B:358:CYS:HA	2:B:501:HEM:CHA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/410 (96%)	386 (98%)	6 (2%)	0	100	100
1	B	392/410 (96%)	384 (98%)	7 (2%)	1 (0%)	36	35
1	C	392/410 (96%)	386 (98%)	6 (2%)	0	100	100
1	D	392/410 (96%)	382 (97%)	8 (2%)	2 (0%)	24	21
All	All	1568/1640 (96%)	1538 (98%)	27 (2%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	CYS
1	D	358	CYS
1	D	148	ILE

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/334 (96%)	319 (100%)	1 (0%)	86	91
1	B	320/334 (96%)	315 (98%)	5 (2%)	55	62
1	C	320/334 (96%)	318 (99%)	2 (1%)	78	85
1	D	320/334 (96%)	313 (98%)	7 (2%)	45	50
All	All	1280/1336 (96%)	1265 (99%)	15 (1%)	63	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	B	28	LEU
1	B	86	LYS
1	B	142	ARG
1	B	180	LEU
1	B	334	SER
1	C	166	LEU
1	C	323	LEU
1	D	156	PRO
1	D	193	GLN
1	D	206	VAL
1	D	307	GLU
1	D	346	SER
1	D	366	LEU
1	D	389	LYS

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	283	ASN
1	B	20	HIS
1	B	105	HIS
1	B	141	GLN
1	B	209	GLN
1	B	214	ASN
1	B	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	296	GLN
1	C	20	HIS
1	C	105	HIS
1	C	193	GLN
1	C	209	GLN
1	C	214	ASN
1	C	283	ASN
1	C	296	GLN
1	D	20	HIS
1	D	105	HIS
1	D	141	GLN
1	D	168	GLN
1	D	203	GLN
1	D	272	GLN
1	D	296	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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
5	TWO	A	504	-	13,13,13	1.13	1 (7%)	17,17,17	1.63	2 (11%)
5	TWO	C	506	-	13,13,13	0.96	0	17,17,17	2.28	9 (52%)
4	GOL	A	503	-	5,5,5	0.40	0	5,5,5	0.94	0
5	TWO	D	506	-	13,13,13	1.40	3 (23%)	17,17,17	1.30	2 (11%)
2	HEM	A	501	1	50,50,50	1.81	12 (24%)	67,82,82	1.68	14 (20%)
4	GOL	D	505	-	5,5,5	0.45	0	5,5,5	1.05	0
4	GOL	B	504	-	5,5,5	0.52	0	5,5,5	0.70	0
2	HEM	D	501	1	50,50,50	2.33	15 (30%)	67,82,82	1.73	15 (22%)
3	SO4	C	502	-	4,4,4	0.33	0	6,6,6	0.56	0
3	SO4	B	502	-	4,4,4	0.54	0	6,6,6	0.97	0
4	GOL	B	503	-	5,5,5	0.78	0	5,5,5	2.04	2 (40%)
3	SO4	C	504	-	4,4,4	0.43	0	6,6,6	0.68	0
2	HEM	B	501	1	50,50,50	2.11	15 (30%)	67,82,82	1.78	14 (20%)
3	SO4	C	503	-	4,4,4	0.43	0	6,6,6	1.03	0
4	GOL	C	505	-	5,5,5	0.90	0	5,5,5	1.14	1 (20%)
3	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.52	0
5	TWO	B	505	-	13,13,13	1.14	1 (7%)	17,17,17	2.22	9 (52%)
3	SO4	D	503	-	4,4,4	0.29	0	6,6,6	0.82	0
3	SO4	A	502	-	4,4,4	0.67	0	6,6,6	0.94	0
3	SO4	D	502	-	4,4,4	0.54	0	6,6,6	0.81	0
2	HEM	C	501	1	50,50,50	1.75	10 (20%)	67,82,82	1.37	11 (16%)

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	GOL	B	504	-	-	1/4/4/4	-
5	TWO	A	504	-	-	2/8/8/8	0/1/1/1
2	HEM	D	501	1	-	2/14/54/54	-
2	HEM	B	501	1	-	2/14/54/54	-
5	TWO	B	505	-	-	2/8/8/8	0/1/1/1
5	TWO	C	506	-	-	0/8/8/8	0/1/1/1
4	GOL	C	505	-	-	0/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
5	TWO	D	506	-	-	2/8/8/8	0/1/1/1
2	HEM	A	501	1	-	2/14/54/54	-
4	GOL	B	503	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	505	-	-	2/4/4/4	-
2	HEM	C	501	1	-	1/14/54/54	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3D-C2D	6.50	1.50	1.36
2	D	501	HEM	FE-ND	6.15	2.13	1.94
2	D	501	HEM	FE-NA	5.77	2.14	1.95
2	B	501	HEM	FE-NA	5.70	2.14	1.95
2	D	501	HEM	FE-NC	5.47	2.13	1.95
2	C	501	HEM	C3D-C2D	5.28	1.48	1.36
2	B	501	HEM	C3D-C2D	5.19	1.48	1.36
2	A	501	HEM	FE-NC	4.81	2.11	1.95
2	A	501	HEM	C3D-C2D	4.78	1.47	1.36
2	B	501	HEM	FE-NB	4.48	2.08	1.94
2	B	501	HEM	FE-NC	4.44	2.09	1.95
2	C	501	HEM	FE-NB	4.12	2.07	1.94
2	D	501	HEM	FE-NB	4.12	2.07	1.94
2	A	501	HEM	FE-NA	3.88	2.07	1.95
2	A	501	HEM	FE-NB	3.53	2.05	1.94
2	C	501	HEM	FE-NC	3.47	2.06	1.95
2	D	501	HEM	CMC-C2C	3.46	1.57	1.50
2	B	501	HEM	FE-ND	3.37	2.05	1.94
2	C	501	HEM	CMA-C3A	3.36	1.57	1.50
2	A	501	HEM	CAB-C3B	3.29	1.56	1.47
2	B	501	HEM	C1A-NA	-3.28	1.33	1.39
2	C	501	HEM	CAC-C3C	3.27	1.56	1.47
2	D	501	HEM	CAB-C3B	3.25	1.56	1.47
2	C	501	HEM	CAB-C3B	3.17	1.55	1.47
2	B	501	HEM	CAD-C3D	3.07	1.59	1.51
2	D	501	HEM	CAA-C2A	3.01	1.59	1.51
2	A	501	HEM	CMD-C2D	2.99	1.56	1.50
2	B	501	HEM	C2A-C3A	-2.99	1.31	1.38
2	D	501	HEM	CMD-C2D	2.92	1.56	1.50
2	A	501	HEM	FE-ND	2.89	2.03	1.94
2	C	501	HEM	FE-NA	2.85	2.04	1.95
2	B	501	HEM	CMD-C2D	2.84	1.56	1.50
2	A	501	HEM	CMC-C2C	2.79	1.56	1.50
2	B	501	HEM	CAC-C3C	2.79	1.54	1.47
5	B	505	TWO	O1-C7	2.71	1.30	1.22
2	D	501	HEM	CAD-C3D	2.70	1.58	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	506	TWO	C2-C3	-2.69	1.35	1.40
2	B	501	HEM	CAB-C3B	2.66	1.54	1.47
2	A	501	HEM	CHB-C1B	2.60	1.43	1.38
2	C	501	HEM	CMC-C2C	2.55	1.56	1.50
5	D	506	TWO	O1-C7	2.51	1.30	1.22
2	D	501	HEM	C1B-NB	-2.48	1.35	1.40
2	B	501	HEM	CBD-CGD	2.38	1.56	1.50
2	B	501	HEM	CMB-C2B	2.33	1.55	1.50
2	D	501	HEM	CMA-C3A	2.30	1.55	1.50
5	A	504	TWO	C4-C5	2.24	1.42	1.39
5	D	506	TWO	C4-C3	2.17	1.42	1.38
2	D	501	HEM	C1D-C2D	2.16	1.48	1.44
2	B	501	HEM	CBD-CAD	2.14	1.59	1.51
2	A	501	HEM	C4C-NC	-2.14	1.35	1.39
2	A	501	HEM	O1A-CGA	2.13	1.29	1.22
2	C	501	HEM	CMD-C2D	2.13	1.55	1.50
2	D	501	HEM	CAC-C3C	2.09	1.53	1.47
2	C	501	HEM	CBD-CGD	2.08	1.55	1.50
2	A	501	HEM	CAC-C3C	2.04	1.52	1.47
2	B	501	HEM	CAA-C2A	2.03	1.56	1.51
2	D	501	HEM	CBD-CAD	2.01	1.58	1.51

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	506	TWO	C9-O4-C3	5.36	125.38	117.51
2	D	501	HEM	CBD-CAD-C3D	-5.10	98.43	112.53
2	B	501	HEM	C1B-NB-C4B	4.86	110.97	105.21
2	D	501	HEM	C4D-ND-C1D	4.80	110.90	105.21
2	B	501	HEM	CBD-CAD-C3D	-4.47	100.18	112.53
2	A	501	HEM	CHB-C1B-NB	4.30	129.69	124.37
2	A	501	HEM	CBD-CAD-C3D	-4.21	100.88	112.53
2	B	501	HEM	C4D-ND-C1D	4.16	110.13	105.21
2	A	501	HEM	C1B-NB-C4B	4.13	110.10	105.21
5	A	504	TWO	C9-O4-C3	4.07	123.49	117.51
2	B	501	HEM	C3B-C4B-NB	-4.07	106.54	109.47
2	D	501	HEM	C1B-NB-C4B	3.90	109.82	105.21
2	A	501	HEM	C2B-C1B-NB	-3.81	105.46	109.84
5	B	505	TWO	C1-C2-C3	3.72	124.64	119.71
5	A	504	TWO	O4-C3-C2	3.63	120.33	115.40
2	B	501	HEM	C4C-NC-C1C	3.57	111.64	105.82
5	B	505	TWO	O3-C2-C1	-3.52	118.36	124.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	506	TWO	O2-C7-C5	3.47	123.74	114.84
2	B	501	HEM	C2B-C1B-NB	-3.44	105.89	109.84
2	D	501	HEM	C4C-NC-C1C	3.35	111.28	105.82
4	B	503	GOL	O1-C1-C2	-3.20	95.95	110.38
2	C	501	HEM	CMD-C2D-C1D	3.19	130.02	125.03
2	B	501	HEM	CHB-C1B-NB	3.15	128.26	124.37
2	A	501	HEM	C3B-C2B-C1B	3.15	108.78	106.41
5	B	505	TWO	C9-O4-C3	3.09	122.05	117.51
2	D	501	HEM	CAA-CBA-CGA	-3.09	105.47	113.67
2	A	501	HEM	C3B-C4B-NB	-3.06	107.27	109.47
5	D	506	TWO	C4-C3-C2	3.04	123.73	119.83
2	B	501	HEM	CHD-C1D-ND	3.02	127.67	124.42
2	A	501	HEM	C4C-NC-C1C	2.97	110.67	105.82
5	B	505	TWO	C6-C1-C2	-2.96	114.45	120.06
2	B	501	HEM	C4B-C3B-C2B	2.95	109.99	107.28
2	D	501	HEM	C3B-C4B-NB	-2.94	107.35	109.47
4	B	503	GOL	O3-C3-C2	-2.90	97.31	110.38
2	C	501	HEM	C4C-NC-C1C	2.85	110.47	105.82
5	B	505	TWO	O4-C3-C2	2.79	119.19	115.40
2	D	501	HEM	CHC-C4B-NB	2.79	127.42	124.42
2	C	501	HEM	C1D-C2D-C3D	-2.78	104.05	106.98
2	B	501	HEM	CAD-C3D-C4D	2.74	129.47	124.70
2	A	501	HEM	CAD-C3D-C4D	2.73	129.46	124.70
2	D	501	HEM	O2A-CGA-CBA	2.70	122.54	114.00
5	B	505	TWO	C8-O3-C2	2.66	121.41	117.51
2	B	501	HEM	C2C-C1C-NC	-2.63	104.78	109.64
2	C	501	HEM	CBD-CAD-C3D	-2.61	105.33	112.53
2	D	501	HEM	O1A-CGA-CBA	-2.59	114.88	123.09
5	C	506	TWO	O1-C7-C5	-2.58	114.69	121.46
2	B	501	HEM	O2A-CGA-CBA	2.55	122.07	114.00
2	C	501	HEM	O2A-CGA-CBA	2.52	121.96	114.00
2	B	501	HEM	O1A-CGA-CBA	-2.52	115.10	123.09
5	B	505	TWO	O2-C7-C5	2.49	121.22	114.84
5	C	506	TWO	C6-C1-C2	-2.48	115.36	120.06
2	A	501	HEM	CMC-C2C-C1C	-2.48	120.36	124.73
5	D	506	TWO	O3-C2-C3	2.46	118.74	115.40
2	C	501	HEM	CHC-C1C-NC	2.44	127.11	124.45
5	C	506	TWO	C5-C4-C3	-2.43	116.34	119.60
2	D	501	HEM	C2B-C1B-NB	-2.43	107.05	109.84
2	A	501	HEM	C4C-C3C-C2C	2.43	108.92	106.81
5	C	506	TWO	C1-C2-C3	2.42	122.92	119.71
5	C	506	TWO	C6-C5-C4	2.39	122.01	119.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CHD-C4C-NC	2.36	127.02	124.45
2	D	501	HEM	C4A-NA-C1A	2.35	109.66	105.82
2	A	501	HEM	C4A-C3A-C2A	2.34	109.50	106.82
2	C	501	HEM	C2A-C1A-NA	-2.32	107.58	110.15
2	A	501	HEM	O2D-CGD-CBD	2.28	121.21	114.00
2	A	501	HEM	CHC-C4B-NB	2.25	126.84	124.42
4	C	505	GOL	O1-C1-C2	-2.23	100.34	110.38
5	B	505	TWO	O4-C3-C4	-2.19	120.31	124.08
2	C	501	HEM	O2D-CGD-CBD	2.14	120.75	114.00
2	D	501	HEM	CAD-CBD-CGD	-2.13	108.02	113.67
2	D	501	HEM	C4C-C3C-C2C	2.11	108.65	106.81
2	D	501	HEM	CMA-C3A-C4A	-2.11	122.20	125.42
5	C	506	TWO	O3-C2-C1	-2.10	120.76	124.30
2	C	501	HEM	CHB-C4A-NA	2.06	127.60	123.86
2	D	501	HEM	C4C-CHD-C1D	2.06	130.39	126.02
2	A	501	HEM	O1A-CGA-CBA	-2.04	116.61	123.09
2	C	501	HEM	C3B-C2B-C1B	2.04	107.94	106.41
5	B	505	TWO	C6-C5-C4	2.03	121.60	119.25
5	C	506	TWO	C8-O3-C2	2.02	120.48	117.51
2	C	501	HEM	O2A-CGA-O1A	-2.00	118.18	123.33

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-O2
4	A	503	GOL	O1-C1-C2-C3
4	D	505	GOL	O1-C1-C2-C3
5	A	504	TWO	C2-C3-O4-C9
5	A	504	TWO	C4-C3-O4-C9
5	D	506	TWO	C2-C3-O4-C9
5	B	505	TWO	C2-C3-O4-C9
5	B	505	TWO	C4-C3-O4-C9
4	B	503	GOL	C1-C2-C3-O3
5	D	506	TWO	C4-C3-O4-C9
4	D	505	GOL	O1-C1-C2-O2
4	B	504	GOL	O1-C1-C2-C3
4	B	503	GOL	O2-C2-C3-O3
2	D	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

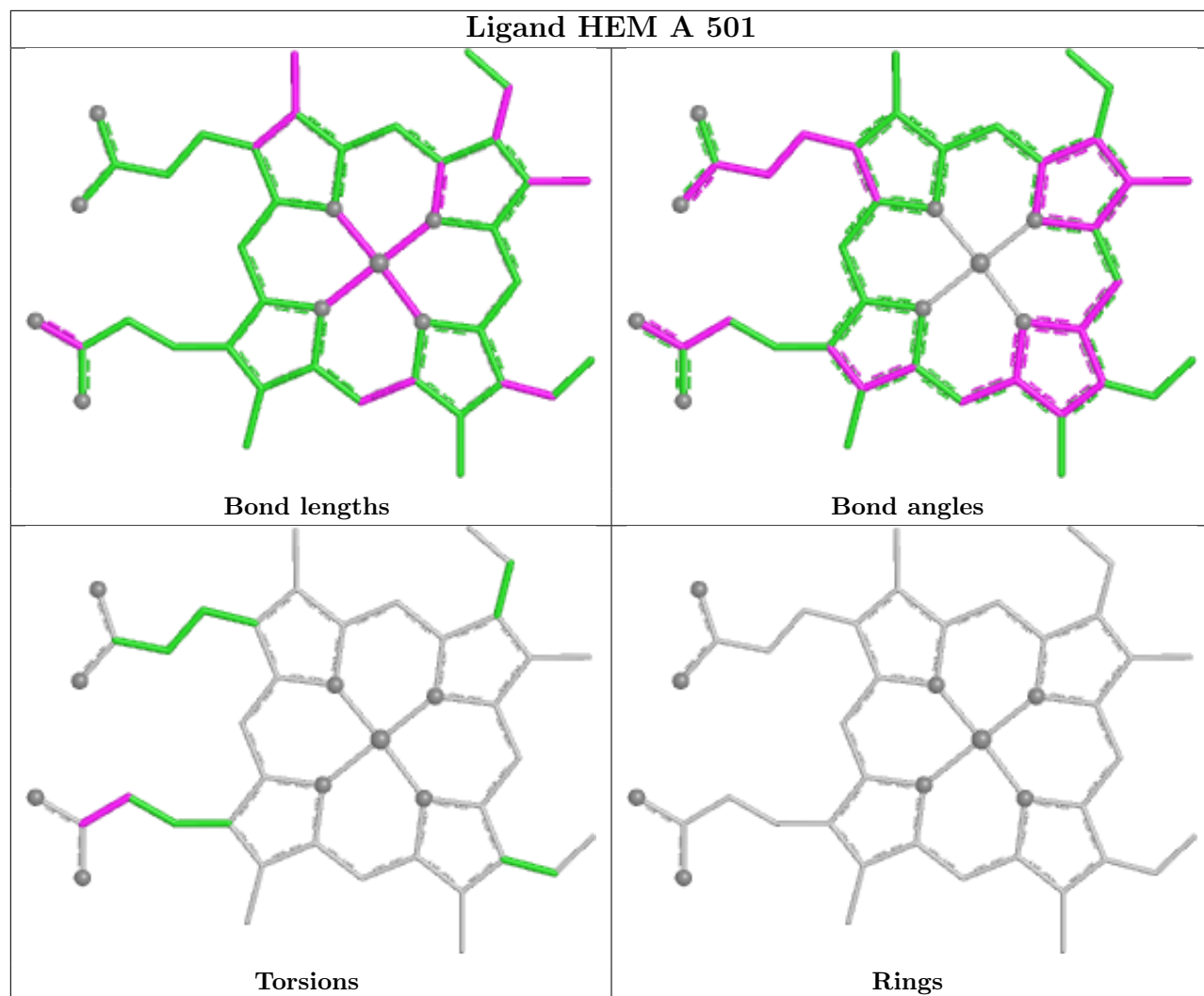
Mol	Chain	Res	Type	Atoms
2	D	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D

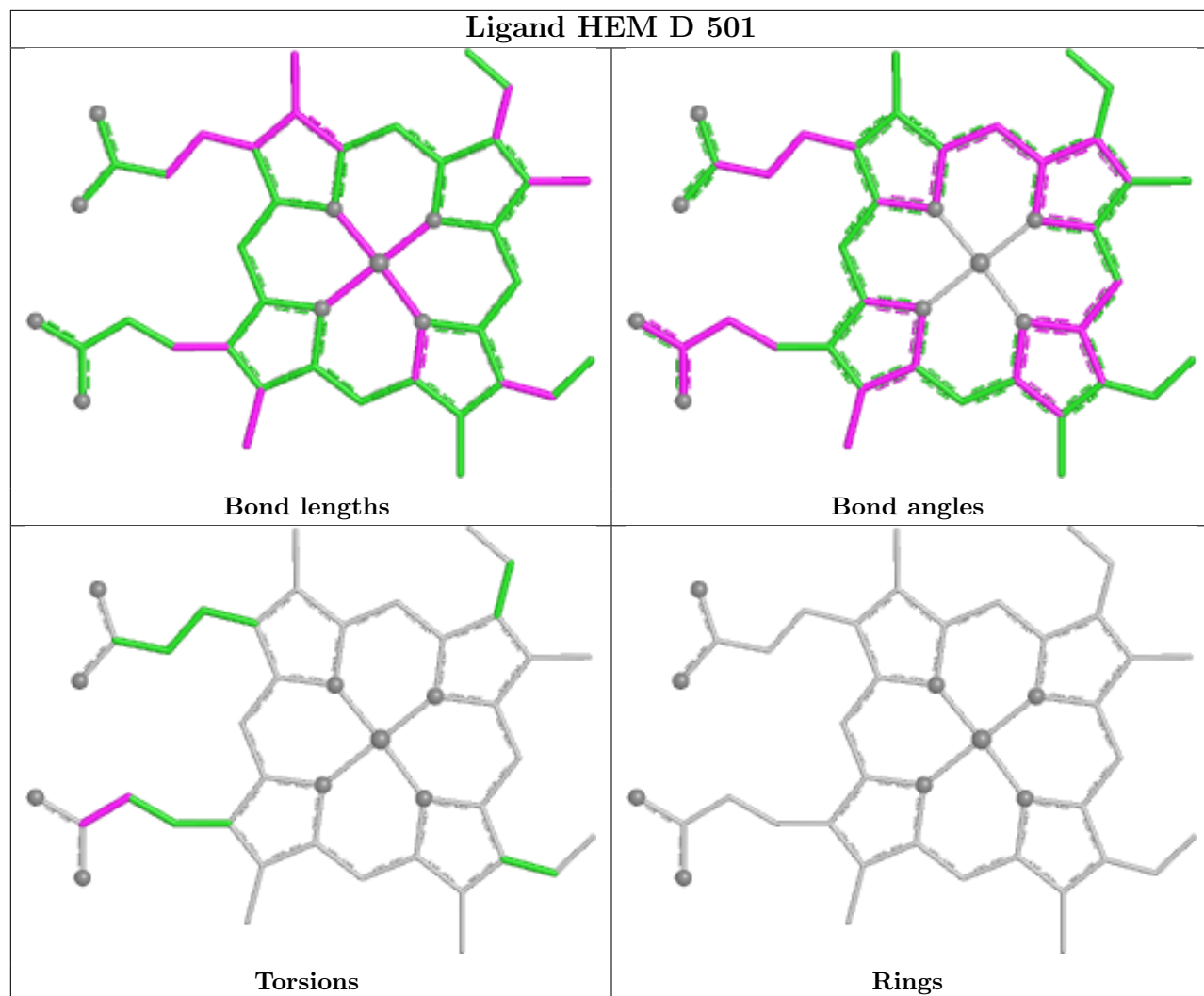
There are no ring outliers.

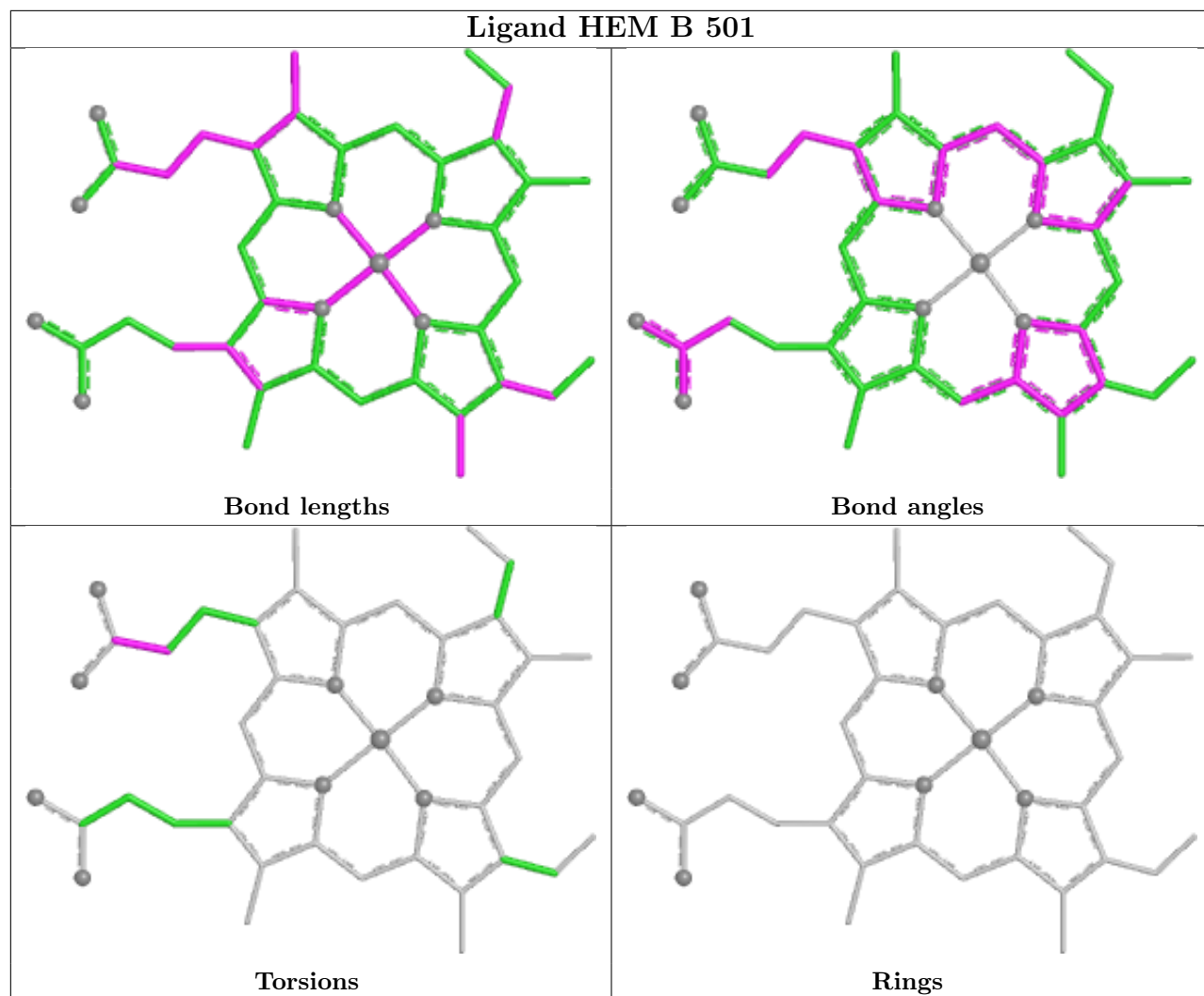
6 monomers are involved in 21 short contacts:

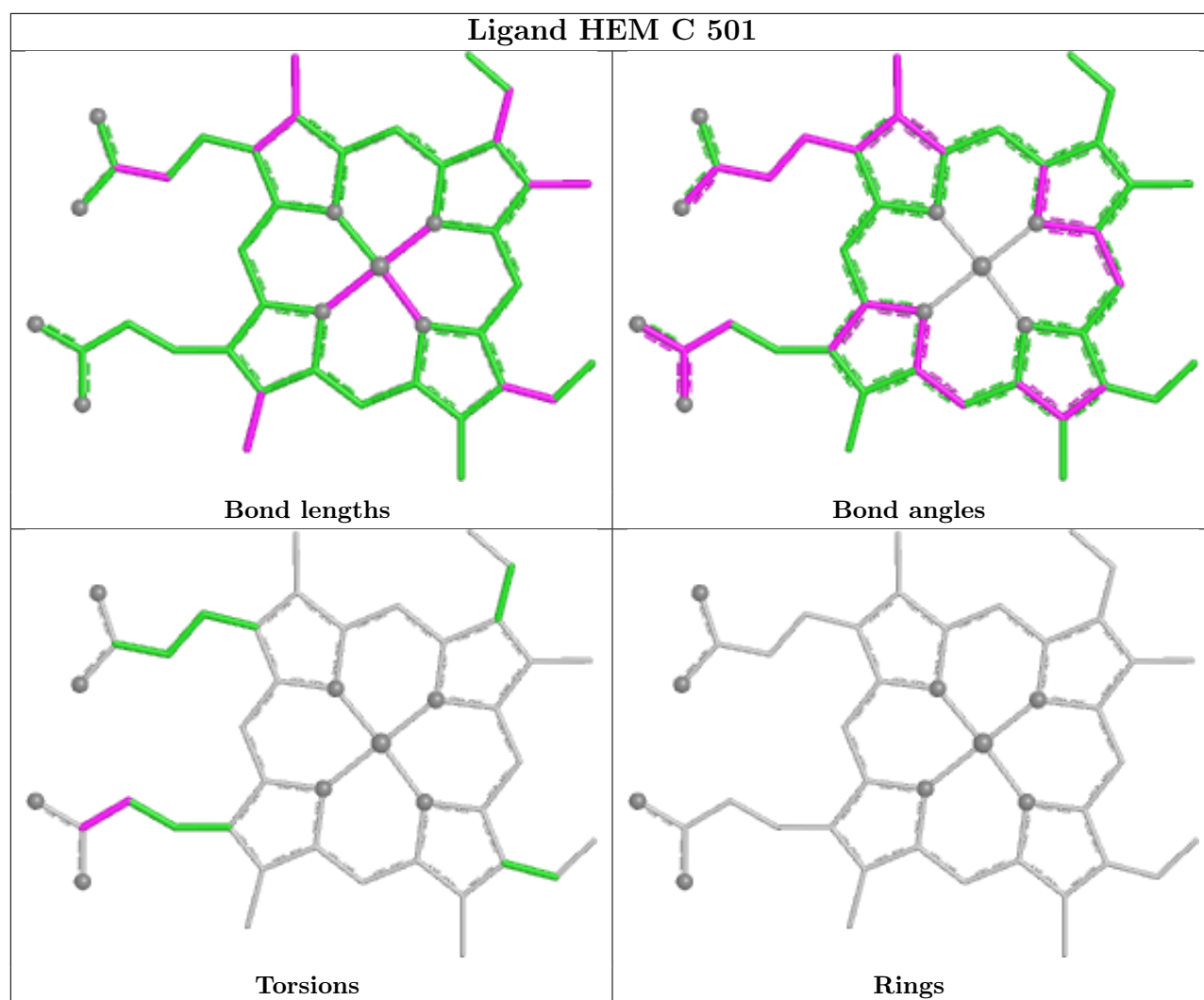
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	506	TWO	3	0
5	D	506	TWO	2	0
2	A	501	HEM	3	0
2	D	501	HEM	4	0
2	B	501	HEM	6	0
2	C	501	HEM	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/410 (95%)	-0.75	1 (0%) 90 89	12, 19, 29, 39	1 (0%)
1	B	393/410 (95%)	-0.72	1 (0%) 90 89	13, 19, 30, 42	1 (0%)
1	C	393/410 (95%)	-0.57	1 (0%) 90 89	15, 22, 33, 43	1 (0%)
1	D	393/410 (95%)	-0.22	2 (0%) 87 87	16, 26, 40, 55	1 (0%)
All	All	1572/1640 (95%)	-0.57	5 (0%) 90 89	12, 21, 35, 55	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	THR	3.2
1	B	17	THR	2.8
1	D	366	LEU	2.6
1	C	17	THR	2.6
1	D	409	ALA	2.2

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,

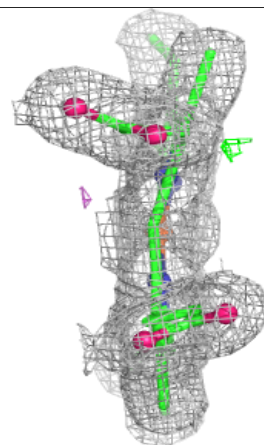
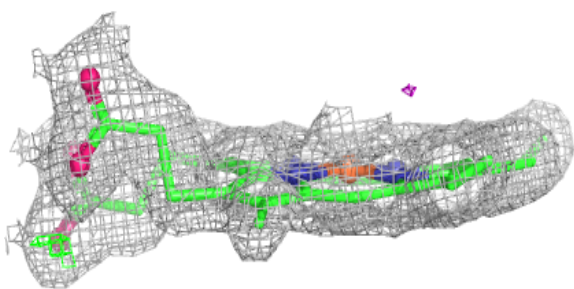
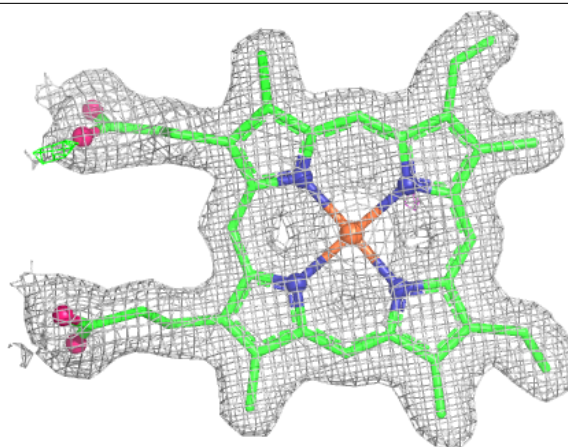
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	504	5/5	0.78	0.14	64,66,70,70	0
3	SO4	D	504	5/5	0.79	0.16	76,77,78,79	0
4	GOL	B	503	6/6	0.84	0.17	31,47,47,49	0
3	SO4	D	503	5/5	0.91	0.13	51,52,54,55	0
4	GOL	D	505	6/6	0.94	0.09	27,37,42,45	0
6	CL	D	507	1/1	0.95	0.10	36,36,36,36	0
3	SO4	C	503	5/5	0.96	0.10	34,37,44,48	0
4	GOL	B	504	6/6	0.96	0.06	17,21,23,33	0
4	GOL	C	505	6/6	0.96	0.07	20,25,29,35	0
3	SO4	D	502	5/5	0.96	0.11	36,39,44,45	0
4	GOL	A	503	6/6	0.96	0.07	21,26,30,35	0
3	SO4	A	502	5/5	0.97	0.08	28,34,38,41	0
5	TWO	B	505	13/13	0.98	0.04	12,16,18,20	0
5	TWO	C	506	13/13	0.98	0.04	17,19,23,24	0
5	TWO	D	506	13/13	0.98	0.05	15,21,25,25	0
6	CL	B	506	1/1	0.98	0.04	21,21,21,21	0
2	HEM	D	501	43/43	0.98	0.05	13,19,22,26	0
2	HEM	B	501	43/43	0.99	0.04	10,14,17,18	0
3	SO4	C	502	5/5	0.99	0.05	22,22,24,27	0
2	HEM	C	501	43/43	0.99	0.04	12,16,20,22	0
6	CL	A	505	1/1	0.99	0.03	22,22,22,22	0
2	HEM	A	501	43/43	0.99	0.03	10,13,15,17	0
6	CL	C	507	1/1	0.99	0.04	27,27,27,27	0
5	TWO	A	504	13/13	0.99	0.03	10,14,20,20	0
3	SO4	B	502	5/5	1.00	0.03	20,21,21,24	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.

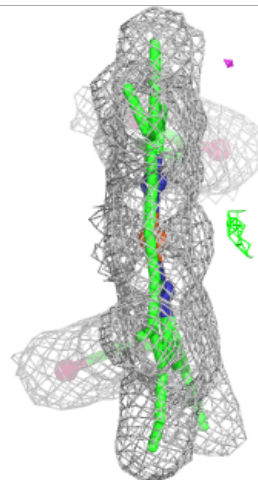
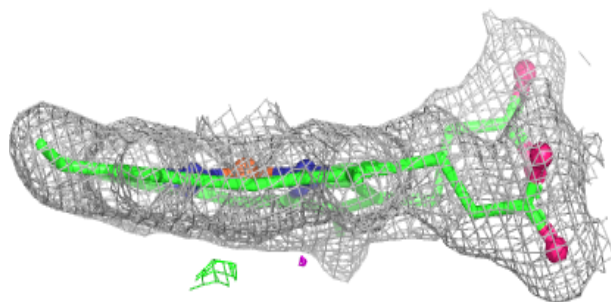
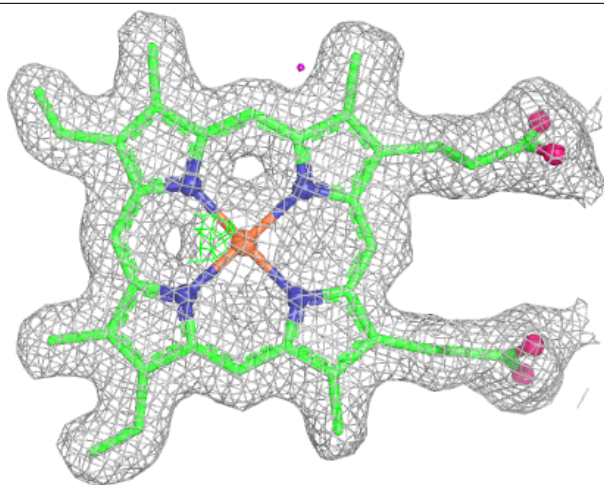
Electron density around HEM D 501:

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



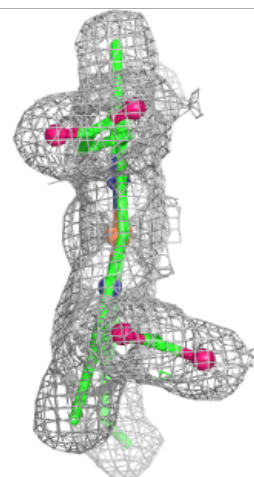
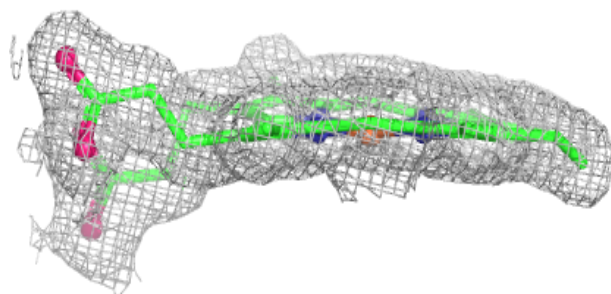
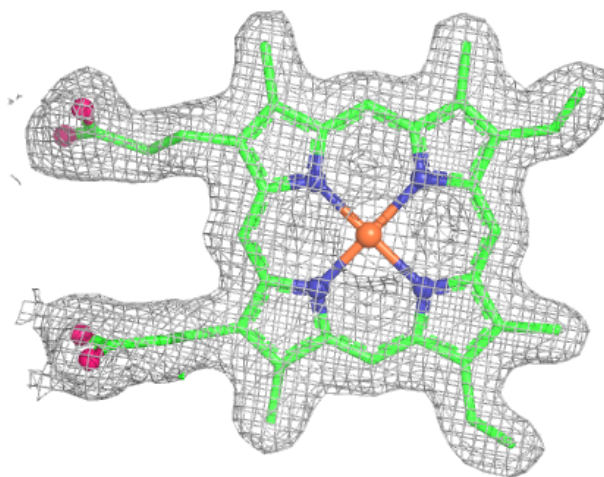
Electron density around HEM B 501:

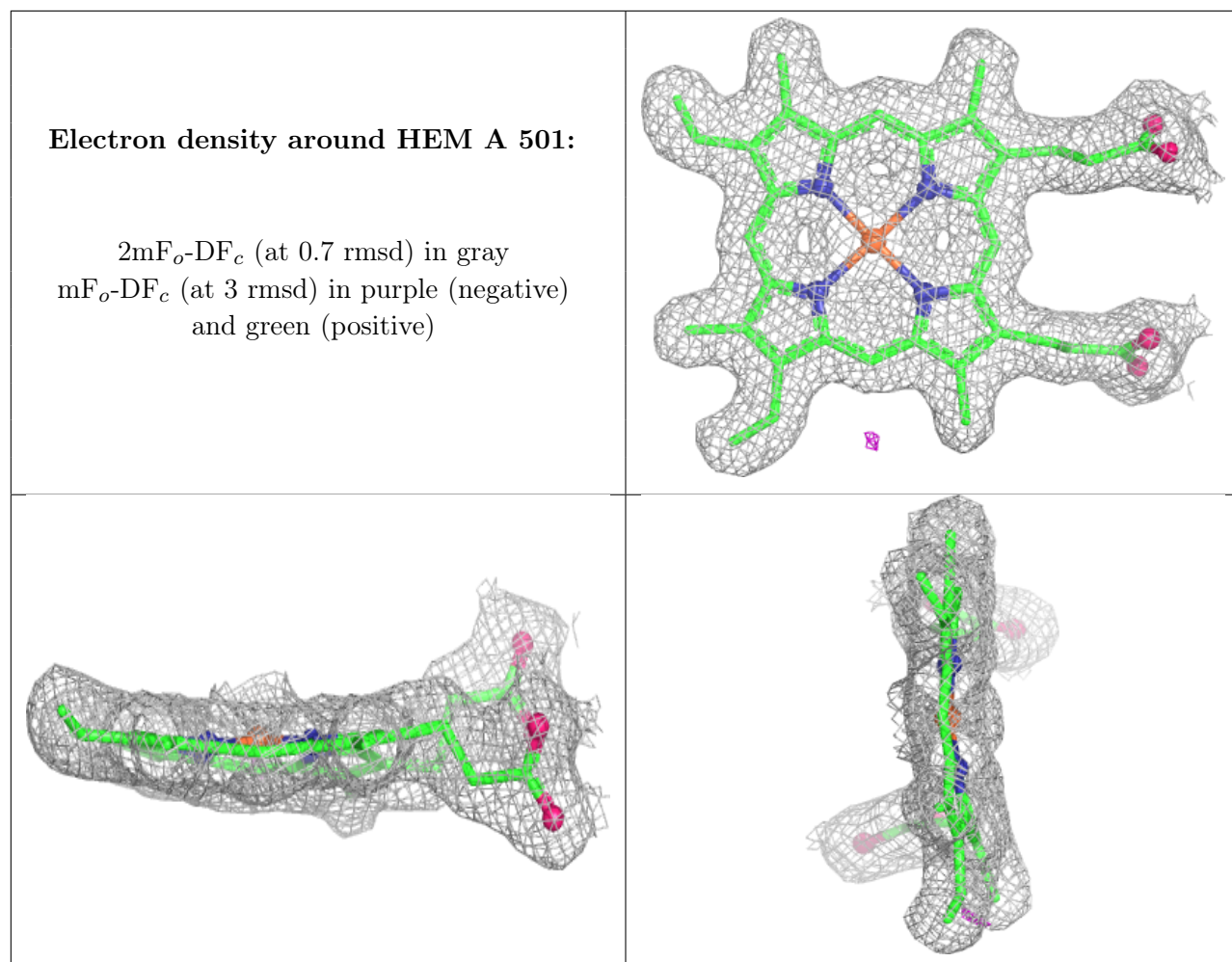
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 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.