



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:06 AM UTC

PDB ID : 4DO1 / pdb_00004do1
Title : The crystal structures of 4-methoxybenzoate bound CYP19A4
Authors : Zhou, W.; Bell, S.G.; Yang, W.; Tan, A.B.H.; Zhou, R.; Johnson, E.O.D.;
Zhang, A.; Rao, Z.; Wong, L.-L.
Deposited on : 2012-02-09
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

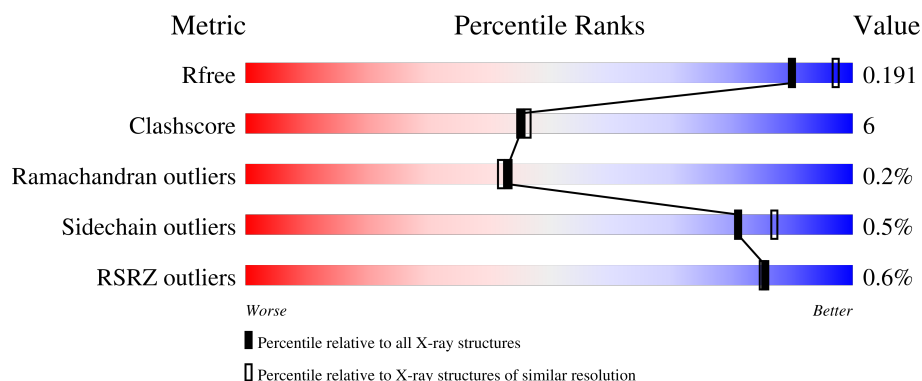
1 Overall quality at a glance

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	% 81% 13% ..
1	B	410	82% 13% ..
1	C	410	85% 10% ..
1	D	410	% 80% 15% ..

2 Entry composition [i](#)

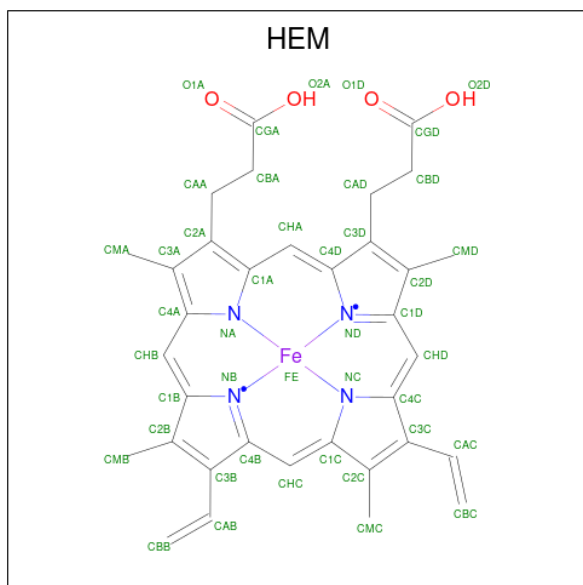
There are 7 unique types of molecules in this entry. The entry contains 14553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0
			3021	1912	534	564	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: $C_{34}H_{32}FeN_4O_4$).



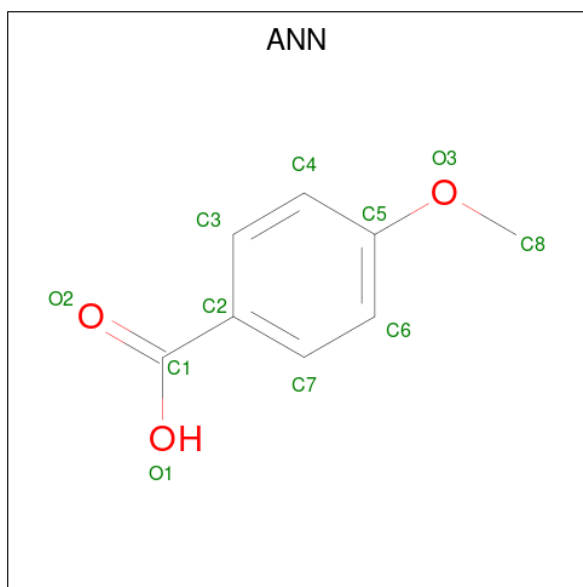
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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

- Molecule 3 is 4-METHOXYBENZOIC ACID (CCD ID: ANN) (formula: C₈H₈O₃).



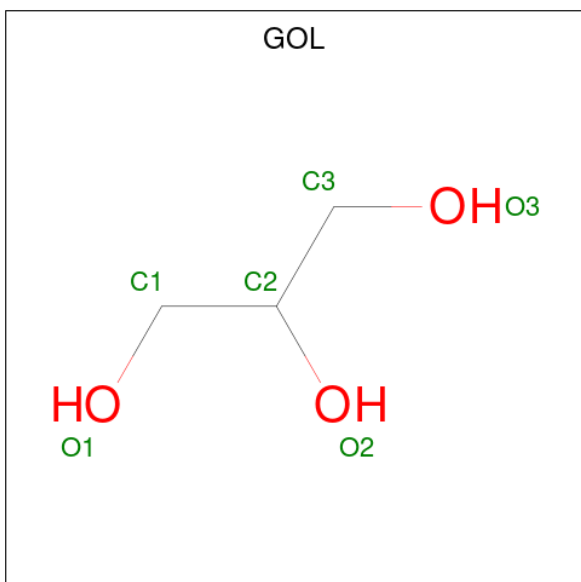
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	8	3		
3	B	1	Total	C	O	0	0
			11	8	3		
3	C	1	Total	C	O	0	0
			11	8	3		
3	D	1	Total	C	O	0	0
			11	8	3		

- 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	B	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	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 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	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

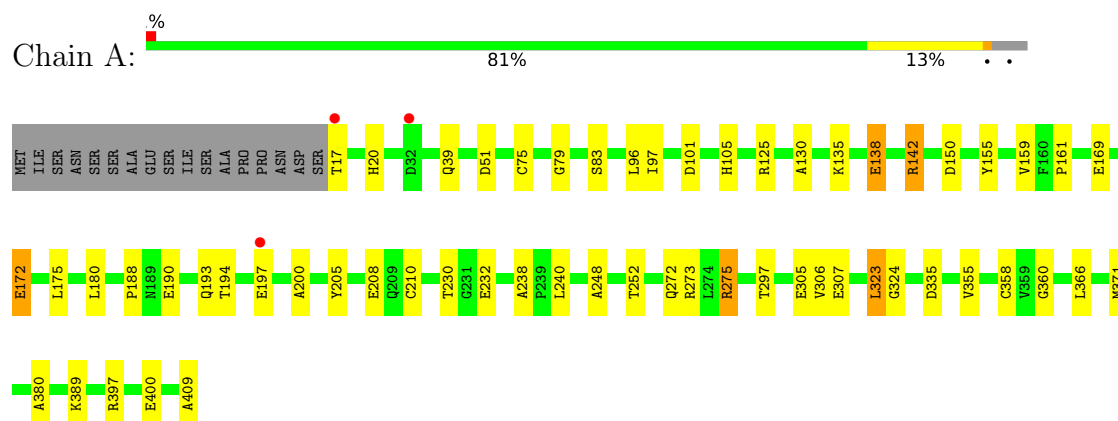
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	567	Total O 567 567	0	0
7	B	542	Total O 542 542	0	0
7	C	563	Total O 563 563	0	0
7	D	525	Total O 525 525	0	0

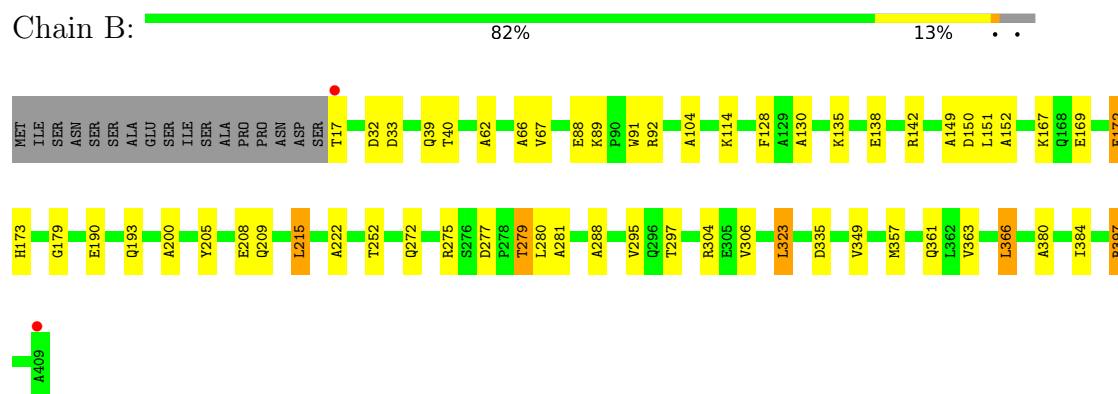
3 Residue-property plots [i](#)

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.

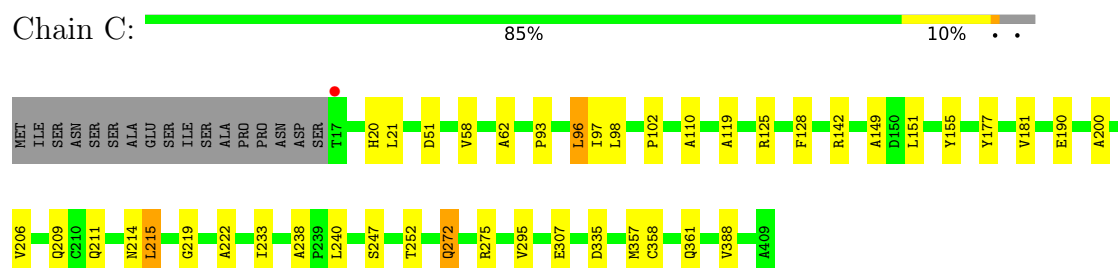
• Molecule 1: Cytochrome P450



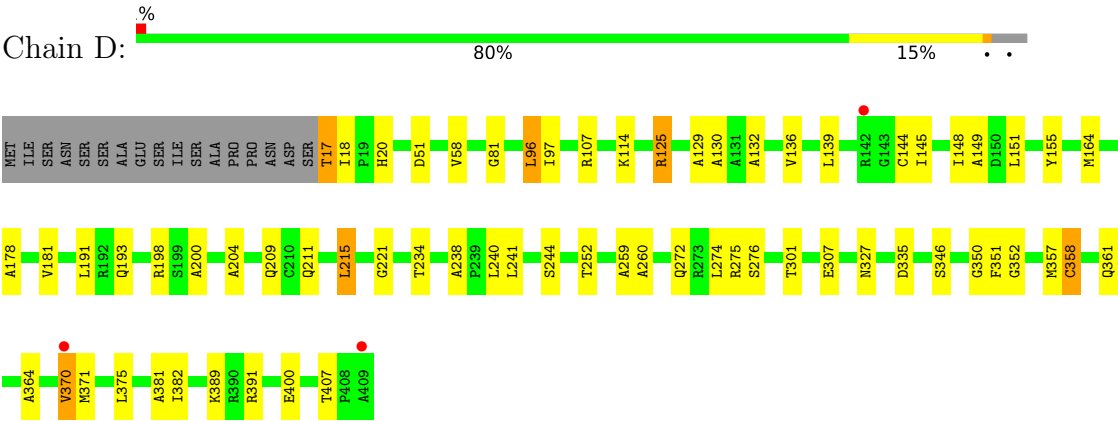
• Molecule 1: Cytochrome P450



• 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	107.02Å 143.48Å 172.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 2.00 43.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.67-2.00) 99.4 (43.67-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.154 , 0.189 0.157 , 0.191	Depositor DCC
R_{free} test set	8967 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtrriage
Anisotropy	0.410	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14553	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 40.69 % 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 2.6363e-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

5.1 Standard geometry

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

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	1.74	24/3099 (0.8%)	1.25	6/4217 (0.1%)
1	B	1.67	28/3093 (0.9%)	1.20	2/4209 (0.0%)
1	C	1.65	21/3093 (0.7%)	1.22	5/4209 (0.1%)
1	D	1.72	31/3093 (1.0%)	1.28	10/4209 (0.2%)
All	All	1.69	104/12378 (0.8%)	1.24	23/16844 (0.1%)

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	PRO	N-CD	-14.53	1.27	1.47
1	D	58	VAL	CA-CB	8.85	1.66	1.54
1	D	81	GLY	N-CA	8.49	1.52	1.44
1	B	62	ALA	CA-CB	8.47	1.66	1.53
1	D	178	ALA	CA-CB	-7.96	1.41	1.53
1	B	323	LEU	CG-CD2	-7.88	1.26	1.52
1	B	104	ALA	CA-CB	7.63	1.65	1.53
1	D	335	ASP	N-CA	7.62	1.51	1.46
1	A	323	LEU	CG-CD2	-7.62	1.27	1.52
1	A	335	ASP	CA-CB	7.59	1.57	1.52
1	D	238	ALA	C-O	-7.37	1.17	1.24
1	A	305	GLU	CA-C	7.05	1.61	1.52
1	B	397	ARG	CZ-NH2	-6.87	1.24	1.33
1	C	149	ALA	CA-CB	6.78	1.64	1.53
1	C	200	ALA	CA-CB	6.60	1.61	1.53
1	A	200	ALA	CA-CB	6.43	1.62	1.53
1	B	179	GLY	N-CA	6.41	1.54	1.45
1	D	301	THR	C-O	6.40	1.31	1.24
1	B	349	VAL	CA-C	6.24	1.60	1.53
1	C	62	ALA	CA-CB	6.21	1.63	1.53
1	A	297	THR	N-CA	6.20	1.53	1.45
1	B	222	ALA	N-CA	6.19	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	LEU	CG-CD2	-6.17	1.32	1.52
1	B	288	ALA	N-CA	6.16	1.53	1.46
1	D	370	VAL	CB-CG2	-6.13	1.32	1.52
1	A	306	VAL	CA-CB	6.10	1.63	1.54
1	D	200	ALA	CA-CB	6.08	1.61	1.53
1	D	234	THR	C-O	6.05	1.32	1.23
1	A	366	LEU	C-O	-6.04	1.17	1.24
1	C	102	PRO	CA-C	6.02	1.57	1.52
1	B	306	VAL	CA-CB	6.02	1.63	1.54
1	B	130	ALA	CA-CB	6.01	1.62	1.53
1	C	295	VAL	N-CA	6.01	1.53	1.46
1	D	155	TYR	CA-C	6.00	1.59	1.52
1	D	191	LEU	CA-C	5.95	1.60	1.52
1	D	107	ARG	C-O	-5.95	1.18	1.24
1	B	66	ALA	CA-CB	5.93	1.62	1.53
1	D	149	ALA	CA-CB	5.92	1.63	1.53
1	B	335	ASP	C-O	5.90	1.26	1.23
1	A	125	ARG	CZ-NH2	5.81	1.41	1.33
1	B	200	ALA	CA-CB	5.80	1.61	1.53
1	C	190	GLU	C-O	5.79	1.30	1.24
1	C	295	VAL	CA-CB	5.79	1.60	1.53
1	C	238	ALA	CA-C	5.79	1.59	1.52
1	D	181	VAL	CA-CB	5.75	1.61	1.54
1	B	88	GLU	CD-OE1	5.74	1.36	1.25
1	A	188	PRO	CA-C	5.71	1.58	1.52
1	D	204	ALA	CA-CB	5.67	1.62	1.53
1	C	98	LEU	N-CA	5.65	1.53	1.46
1	C	272	GLN	N-CA	5.61	1.53	1.46
1	B	152	ALA	CA-CB	5.59	1.62	1.53
1	A	155	TYR	CA-CB	5.58	1.60	1.53
1	D	351	PHE	N-CA	5.57	1.52	1.46
1	C	110	ALA	CA-CB	5.57	1.62	1.53
1	C	58	VAL	CA-CB	5.56	1.61	1.54
1	C	128	PHE	N-CA	5.52	1.52	1.46
1	B	297	THR	N-CA	5.51	1.52	1.45
1	B	363	VAL	CA-CB	5.49	1.60	1.54
1	D	370	VAL	CA-CB	5.49	1.61	1.54
1	B	130	ALA	N-CA	5.48	1.53	1.46
1	B	281	ALA	N-CA	5.47	1.52	1.46
1	C	222	ALA	CA-CB	5.46	1.62	1.53
1	A	324	GLY	N-CA	5.45	1.52	1.45
1	C	155	TYR	CA-C	5.45	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	GLY	N-CA	5.45	1.51	1.45
1	C	119	ALA	CA-CB	5.43	1.61	1.53
1	B	295	VAL	CA-CB	5.42	1.59	1.53
1	A	130	ALA	CA-CB	5.38	1.61	1.53
1	B	384	ILE	CA-CB	5.38	1.59	1.54
1	A	155	TYR	CA-C	5.37	1.58	1.52
1	B	67	VAL	CA-C	5.35	1.59	1.52
1	B	149	ALA	CA-CB	5.35	1.61	1.53
1	D	130	ALA	CA-CB	5.35	1.61	1.53
1	B	40	THR	CA-C	5.34	1.59	1.52
1	C	272	GLN	CG-CD	5.30	1.65	1.52
1	A	275	ARG	N-CA	5.29	1.52	1.46
1	A	172	GLU	CG-CD	5.28	1.65	1.52
1	D	241	LEU	CA-CB	5.27	1.61	1.53
1	D	381	ALA	CA-CB	5.27	1.62	1.53
1	B	33	ASP	CG-OD1	5.27	1.35	1.25
1	D	260	ALA	N-CA	-5.27	1.40	1.46
1	A	159	VAL	N-CA	5.24	1.51	1.46
1	C	93	PRO	CA-C	5.23	1.57	1.52
1	A	138	GLU	N-CA	5.22	1.52	1.46
1	D	352	GLY	CA-C	5.22	1.58	1.52
1	A	248	ALA	CA-CB	5.20	1.62	1.53
1	A	371	MET	CG-SD	5.20	1.93	1.80
1	D	274	LEU	CA-C	5.20	1.59	1.52
1	D	382	ILE	CA-CB	5.19	1.60	1.54
1	C	388	VAL	CA-CB	-5.17	1.47	1.54
1	A	238	ALA	CA-CB	5.15	1.60	1.53
1	A	79	GLY	N-CA	5.14	1.51	1.45
1	D	164	MET	C-O	5.13	1.30	1.24
1	D	211	GLN	N-CA	5.12	1.52	1.46
1	A	210	CYS	N-CA	5.09	1.52	1.46
1	D	18	ILE	CA-C	5.09	1.57	1.53
1	D	244	SER	N-CA	5.09	1.52	1.46
1	B	380	ALA	CA-CB	5.09	1.61	1.53
1	A	83	SER	CA-C	5.09	1.59	1.52
1	D	114	LYS	N-CA	5.08	1.52	1.46
1	C	233	ILE	CG1-CD1	5.05	1.71	1.51
1	D	259	ALA	CA-CB	5.01	1.61	1.53
1	D	276	SER	N-CA	-5.01	1.39	1.46
1	B	172	GLU	CG-CD	5.00	1.64	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	LEU	CD1-CG-CD2	-11.55	85.39	110.80
1	A	323	LEU	CD1-CG-CD2	-8.42	92.28	110.80
1	D	17	THR	CA-C-N	-7.99	117.17	122.60
1	D	17	THR	C-N-CA	-7.99	117.17	122.60
1	B	323	LEU	CD1-CG-CD2	-7.60	94.08	110.80
1	A	273	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	C	96	LEU	CA-C-N	-5.86	116.95	123.16
1	C	96	LEU	C-N-CA	-5.86	116.95	123.16
1	D	125	ARG	CG-CD-NE	-5.78	99.28	112.00
1	A	39	GLN	CB-CG-CD	-5.67	102.96	112.60
1	A	175	LEU	CA-C-N	-5.66	113.19	119.19
1	A	175	LEU	C-N-CA	-5.66	113.19	119.19
1	D	335	ASP	O-C-N	5.42	124.02	121.53
1	D	132	ALA	N-CA-C	-5.38	105.32	111.14
1	B	304	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	D	335	ASP	CB-CA-C	-5.25	107.47	111.20
1	D	346	SER	N-CA-CB	5.08	117.76	109.69
1	D	96	LEU	CA-C-N	-5.06	117.80	123.16
1	D	96	LEU	C-N-CA	-5.06	117.80	123.16
1	C	335	ASP	CB-CA-C	-5.05	107.62	111.20
1	C	247	SER	N-CA-C	-5.04	105.25	111.40
1	C	181	VAL	CB-CA-C	-5.03	105.35	112.14
1	A	142	ARG	N-CA-C	-5.00	106.35	112.90

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	3024	0	2998	41	0
1	B	3021	0	2993	39	0
1	C	3021	0	2993	28	0
1	D	3021	0	2993	40	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	4	0
3	A	11	0	7	0	0
3	B	11	0	7	0	0
3	C	11	0	7	0	0
3	D	11	0	7	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	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	567	0	0	12	0
7	B	542	0	0	12	0
7	C	563	0	0	4	0
7	D	525	0	0	8	0
All	All	14553	0	12157	145	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 6.

All (145) 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:190:GLU:HG2	7:B:679:HOH:O	1.39	1.20
1:D:129:ALA:HA	1:D:370:VAL:CG1	1.74	1.17
1:D:193:GLN:HG3	7:D:1119:HOH:O	1.56	1.02
1:C:209:GLN:O	1:C:215:LEU:HD11	1.61	1.01
1:B:167:LYS:HE3	1:B:169:GLU:HG2	1.46	0.97
1:D:129:ALA:HA	1:D:370:VAL:HG11	1.46	0.97
1:C:272:GLN:HE22	1:C:275:ARG:HH11	1.18	0.91
1:B:17:THR:HG21	7:B:631:HOH:O	1.72	0.89
1:A:135:LYS:HE2	1:A:150:ASP:O	1.75	0.87
1:C:214:ASN:C	1:C:215:LEU:HD12	1.99	0.87
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.22	0.87
1:D:215:LEU:HD23	1:D:221:GLY:HA3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLU:HG2	7:A:856:HOH:O	1.76	0.85
1:D:96:LEU:HD21	1:D:240:LEU:HD13	1.56	0.85
1:B:366:LEU:HD13	1:B:366:LEU:C	2.01	0.85
1:A:190:GLU:HG2	7:A:1098:HOH:O	1.79	0.83
1:A:96:LEU:HD21	1:A:240:LEU:HD13	1.61	0.82
1:B:272:GLN:HE22	1:B:275:ARG:HH21	1.22	0.82
1:D:129:ALA:HA	1:D:370:VAL:HG13	1.60	0.82
1:B:135:LYS:HE2	1:B:150:ASP:O	1.80	0.81
1:B:209:GLN:O	1:B:215:LEU:HD21	1.82	0.79
1:D:272:GLN:HE22	1:D:275:ARG:HH11	1.30	0.79
1:D:144:CYS:SG	7:D:1017:HOH:O	2.40	0.79
1:A:96:LEU:CD2	1:A:240:LEU:HD13	2.16	0.76
1:D:129:ALA:CA	1:D:370:VAL:HG11	2.16	0.75
1:C:215:LEU:HD12	1:C:215:LEU:N	2.01	0.74
1:C:215:LEU:N	1:C:215:LEU:CD1	2.51	0.74
1:D:129:ALA:CA	1:D:370:VAL:CG1	2.63	0.73
1:D:96:LEU:CD2	1:D:240:LEU:HD13	2.18	0.73
1:C:96:LEU:HD21	1:C:240:LEU:HD13	1.70	0.72
1:D:215:LEU:HD23	1:D:221:GLY:CA	2.21	0.70
1:C:272:GLN:HE22	1:C:275:ARG:NH1	1.89	0.70
1:D:96:LEU:HD21	1:D:240:LEU:CD1	2.24	0.68
1:D:209:GLN:O	1:D:215:LEU:HD11	1.94	0.66
1:B:172:GLU:H	1:B:172:GLU:CD	2.04	0.65
1:B:167:LYS:CE	1:B:169:GLU:HG2	2.25	0.64
1:D:125:ARG:NH1	7:D:1104:HOH:O	2.26	0.64
1:A:138:GLU:OE1	1:B:167:LYS:NZ	2.27	0.64
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.81	0.63
1:B:135:LYS:CE	1:B:150:ASP:O	2.46	0.63
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.79	0.62
1:B:277:ASP:OD1	1:B:279:THR:HB	1.99	0.62
1:D:389:LYS:HE3	1:D:400:GLU:OE1	2.00	0.62
1:A:105:HIS:HE1	2:A:501:HEM:O1D	1.82	0.61
1:A:193:GLN:HB2	7:A:910:HOH:O	2.02	0.60
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.83	0.59
1:B:17:THR:CG2	7:B:631:HOH:O	2.42	0.59
1:B:366:LEU:C	1:B:366:LEU:CD1	2.75	0.59
1:A:96:LEU:HD21	1:A:240:LEU:CD1	2.30	0.59
1:B:114:LYS:HG2	7:B:989:HOH:O	2.03	0.59
1:D:391:ARG:NH2	7:D:881:HOH:O	2.36	0.59
1:D:307:GLU:HG2	7:D:670:HOH:O	2.04	0.58
1:D:357:MET:HE3	1:D:361:GLN:HE22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:VAL:HG21	1:D:375:LEU:HD22	1.85	0.58
1:A:142:ARG:HD3	1:B:205:TYR:HA	1.86	0.58
1:A:389:LYS:HD3	1:A:400:GLU:OE1	2.03	0.58
1:A:105:HIS:HD2	7:A:615:HOH:O	1.87	0.57
1:D:209:GLN:O	1:D:215:LEU:CD1	2.53	0.57
1:C:357:MET:HE3	1:C:361:GLN:HE22	1.70	0.56
1:A:172:GLU:H	1:A:172:GLU:CD	2.13	0.56
1:D:20:HIS:HD2	1:D:51:ASP:OD1	1.87	0.56
1:B:89:LYS:HE2	7:B:1116:HOH:O	2.06	0.55
1:A:355:VAL:HG12	7:A:1167:HOH:O	2.06	0.55
1:A:194:THR:O	1:A:197:GLU:HG2	2.07	0.54
1:C:214:ASN:C	1:C:215:LEU:CD1	2.77	0.54
1:A:272:GLN:HE22	1:A:275:ARG:NH1	1.99	0.54
1:B:151:LEU:HD23	1:B:151:LEU:C	2.33	0.54
1:B:208:GLU:HB2	7:B:1104:HOH:O	2.08	0.54
1:C:20:HIS:HD2	1:C:51:ASP:OD1	1.89	0.54
1:C:96:LEU:HD22	1:C:96:LEU:N	2.22	0.53
1:D:389:LYS:HE3	1:D:400:GLU:CD	2.35	0.52
1:D:125:ARG:HD2	7:D:803:HOH:O	2.10	0.52
1:C:307:GLU:HG2	7:C:725:HOH:O	2.09	0.52
1:A:190:GLU:CG	7:A:1098:HOH:O	2.48	0.51
1:B:366:LEU:HD13	1:B:366:LEU:O	2.09	0.51
1:C:252:THR:HB	2:C:501:HEM:C3B	2.46	0.50
1:A:389:LYS:HE2	1:A:400:GLU:OE2	2.11	0.50
1:C:97:ILE:HG12	2:C:501:HEM:CGD	2.42	0.49
1:A:193:GLN:NE2	7:A:1116:HOH:O	2.45	0.49
1:D:215:LEU:HD23	1:D:221:GLY:C	2.38	0.49
1:A:138:GLU:HG3	1:B:169:GLU:HG3	1.94	0.48
1:D:407:THR:HG23	7:D:806:HOH:O	2.14	0.48
1:A:252:THR:HB	2:A:501:HEM:C3B	2.48	0.48
1:A:230:THR:OG1	1:A:232:GLU:OE1	2.29	0.48
1:C:142:ARG:NH1	7:C:897:HOH:O	2.46	0.48
1:A:397:ARG:NH2	7:A:893:HOH:O	2.43	0.47
1:D:252:THR:HB	2:D:501:HEM:C3B	2.49	0.47
1:D:151:LEU:C	1:D:151:LEU:HD23	2.39	0.47
1:D:17:THR:CG2	7:D:1113:HOH:O	2.62	0.47
1:C:96:LEU:HD23	1:C:240:LEU:HB3	1.96	0.47
1:C:211:GLN:O	1:C:215:LEU:HD13	2.15	0.47
1:C:151:LEU:C	1:C:151:LEU:HD23	2.39	0.47
1:B:357:MET:HE3	1:B:361:GLN:HE22	1.80	0.46
1:C:214:ASN:O	1:C:215:LEU:HD12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:HG12	2:D:501:HEM:CGD	2.46	0.46
1:A:135:LYS:CE	1:A:150:ASP:O	2.57	0.46
1:B:167:LYS:NZ	1:B:208:GLU:OE1	2.49	0.46
1:D:129:ALA:N	1:D:370:VAL:HG11	2.31	0.46
1:B:193:GLN:HB2	7:B:1085:HOH:O	2.15	0.46
1:A:97:ILE:HG12	2:A:501:HEM:CGD	2.46	0.45
1:C:125:ARG:NH1	7:C:1132:HOH:O	2.48	0.45
1:A:17:THR:HG21	7:A:1159:HOH:O	2.16	0.45
1:B:397:ARG:NH2	7:B:970:HOH:O	2.43	0.45
1:B:128:PHE:CD2	1:B:366:LEU:HD12	2.51	0.45
1:A:360:GLY:HA3	2:A:501:HEM:C3C	2.52	0.45
1:B:39:GLN:HG2	7:B:769:HOH:O	2.17	0.45
1:B:91:TRP:CZ2	1:B:92:ARG:HD3	2.53	0.44
1:C:358:CYS:HA	2:C:501:HEM:CHA	2.47	0.44
1:D:129:ALA:CA	1:D:370:VAL:HG13	2.39	0.44
1:A:96:LEU:HD23	1:A:240:LEU:HB3	2.00	0.44
1:A:169:GLU:HG3	1:B:138:GLU:HG3	1.99	0.44
1:A:172:GLU:CD	7:A:997:HOH:O	2.61	0.44
1:A:205:TYR:HA	1:B:142:ARG:HD3	2.00	0.44
1:B:167:LYS:HD3	7:B:930:HOH:O	2.18	0.44
1:B:17:THR:HG23	7:B:1025:HOH:O	2.18	0.44
1:A:20:HIS:HD2	1:A:51:ASP:OD1	2.01	0.43
1:C:177:TYR:CD2	1:C:206:VAL:HG21	2.53	0.43
1:C:142:ARG:NH2	7:C:826:HOH:O	2.30	0.43
1:C:20:HIS:CD2	1:C:51:ASP:OD1	2.70	0.43
1:D:96:LEU:HD13	1:D:96:LEU:HA	1.74	0.43
1:B:252:THR:HB	2:B:501:HEM:C3B	2.54	0.43
1:B:323:LEU:HD22	1:B:323:LEU:N	2.33	0.43
1:A:150:ASP:CG	1:B:173:HIS:HE2	2.27	0.43
1:B:272:GLN:HE22	1:B:275:ARG:HD3	1.84	0.43
1:A:75:CYS:HB2	1:A:101:ASP:OD2	2.19	0.42
1:D:327:ASN:HD21	1:D:350:GLY:N	2.16	0.42
1:A:389:LYS:CE	1:A:400:GLU:OE2	2.67	0.42
1:C:20:HIS:C	1:C:21:LEU:HD12	2.45	0.42
1:D:139:LEU:HD13	1:D:145:ILE:HD13	2.01	0.42
1:A:307:GLU:HG2	7:A:622:HOH:O	2.20	0.42
1:D:136:VAL:CG2	1:D:375:LEU:HD22	2.50	0.42
1:B:272:GLN:HE22	1:B:275:ARG:NH2	2.02	0.41
1:D:97:ILE:HD13	1:D:97:ILE:HG21	1.66	0.41
1:A:17:THR:HB	7:A:1159:HOH:O	2.20	0.41
1:B:128:PHE:CD2	1:B:366:LEU:CD1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD11	7:B:901:HOH:O	2.20	0.41
1:A:323:LEU:HD22	1:A:323:LEU:N	2.36	0.41
1:A:380:ALA:HB2	1:A:409:ALA:HA	2.03	0.41
1:D:357:MET:O	1:D:358:CYS:C	2.64	0.41
1:C:215:LEU:N	1:C:215:LEU:HD13	2.33	0.41
1:C:357:MET:HE2	1:C:357:MET:HB3	1.88	0.41
1:D:371:MET:SD	1:D:375:LEU:CD2	3.09	0.40
1:A:96:LEU:HD13	1:A:96:LEU:HA	1.94	0.40
1:C:357:MET:O	1:C:358:CYS:C	2.63	0.40
1:D:364:ALA:HB2	2:D:501:HEM:HHC	2.02	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	392/410 (96%)	384 (98%)	7 (2%)	1 (0%)	36	35
1	B	391/410 (95%)	383 (98%)	8 (2%)	0	100	100
1	C	391/410 (95%)	384 (98%)	7 (2%)	0	100	100
1	D	391/410 (95%)	386 (99%)	3 (1%)	2 (0%)	24	21
All	All	1565/1640 (95%)	1537 (98%)	25 (2%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	CYS
1	A	358	CYS
1	D	148	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	320/334 (96%)	319 (100%)	1 (0%)	86	91
1	B	319/334 (96%)	316 (99%)	3 (1%)	70	78
1	C	319/334 (96%)	318 (100%)	1 (0%)	86	91
1	D	319/334 (96%)	318 (100%)	1 (0%)	86	91
All	All	1277/1336 (96%)	1271 (100%)	6 (0%)	81	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	B	32	ASP
1	B	279	THR
1	B	366	LEU
1	C	215	LEU
1	D	198	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	105	HIS
1	A	209	GLN
1	A	214	ASN
1	A	272	GLN
1	B	203	GLN
1	B	272	GLN
1	C	20	HIS
1	C	209	GLN
1	C	214	ASN
1	C	272	GLN
1	C	296	GLN
1	D	20	HIS

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Mol	Chain	Res	Type
1	D	168	GLN
1	D	203	GLN
1	D	209	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 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\# Z > 2$
2	HEM	D	501	1	50,50,50	2.45	19 (38%)	67,82,82	1.92	14 (20%)
5	GOL	D	504	-	5,5,5	0.35	0	5,5,5	1.18	1 (20%)
3	ANN	D	502	-	11,11,11	1.52	4 (36%)	14,14,14	1.42	4 (28%)
4	SO4	B	503	-	4,4,4	0.54	0	6,6,6	0.82	0
4	SO4	C	503	-	4,4,4	0.33	0	6,6,6	0.58	0
4	SO4	D	503	-	4,4,4	0.38	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	504	-	5,5,5	0.77	0	5,5,5	1.07	0
3	ANN	A	502	-	11,11,11	1.39	1 (9%)	14,14,14	1.98	5 (35%)
2	HEM	A	501	1	50,50,50	2.10	13 (26%)	67,82,82	1.69	11 (16%)
3	ANN	C	502	-	11,11,11	1.58	3 (27%)	14,14,14	1.55	3 (21%)
5	GOL	C	504	-	5,5,5	0.64	0	5,5,5	1.21	1 (20%)
2	HEM	C	501	1	50,50,50	2.11	13 (26%)	67,82,82	1.59	16 (23%)
4	SO4	B	504	-	4,4,4	1.09	0	6,6,6	0.47	0
5	GOL	B	505	-	5,5,5	0.62	0	5,5,5	1.57	1 (20%)
4	SO4	A	503	-	4,4,4	0.60	0	6,6,6	0.73	0
3	ANN	B	502	-	11,11,11	1.47	1 (9%)	14,14,14	1.36	2 (14%)
2	HEM	B	501	1	50,50,50	1.96	12 (24%)	67,82,82	1.39	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
2	HEM	D	501	1	-	2/14/54/54	-
5	GOL	D	504	-	-	2/4/4/4	-
3	ANN	D	502	-	-	0/6/6/6	0/1/1/1
5	GOL	A	504	-	-	0/4/4/4	-
3	ANN	A	502	-	-	0/6/6/6	0/1/1/1
2	HEM	A	501	1	-	1/14/54/54	-
3	ANN	C	502	-	-	0/6/6/6	0/1/1/1
5	GOL	C	504	-	-	0/4/4/4	-
2	HEM	C	501	1	-	2/14/54/54	-
5	GOL	B	505	-	-	2/4/4/4	-
3	ANN	B	502	-	-	0/6/6/6	0/1/1/1
2	HEM	B	501	1	-	1/14/54/54	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NB	5.95	2.13	1.94
2	A	501	HEM	FE-ND	5.95	2.13	1.94
2	A	501	HEM	FE-NA	5.63	2.13	1.95
2	C	501	HEM	C3D-C2D	5.59	1.48	1.36
2	B	501	HEM	C3D-C2D	5.55	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NC	5.41	2.13	1.95
2	D	501	HEM	C3D-C2D	5.20	1.48	1.36
2	B	501	HEM	FE-NC	5.18	2.12	1.95
2	C	501	HEM	FE-NC	5.01	2.11	1.95
2	D	501	HEM	FE-NA	4.92	2.11	1.95
2	A	501	HEM	C3D-C2D	4.88	1.47	1.36
2	C	501	HEM	FE-NB	4.80	2.09	1.94
2	D	501	HEM	FE-ND	4.60	2.09	1.94
2	D	501	HEM	CBD-CGD	4.12	1.60	1.50
2	C	501	HEM	CMA-C3A	4.02	1.59	1.50
2	B	501	HEM	FE-NA	3.96	2.08	1.95
2	D	501	HEM	CAC-C3C	3.83	1.57	1.47
2	C	501	HEM	CMC-C2C	3.77	1.58	1.50
2	A	501	HEM	FE-NC	3.76	2.07	1.95
2	C	501	HEM	FE-NA	3.59	2.07	1.95
2	A	501	HEM	CMA-C3A	3.54	1.58	1.50
2	A	501	HEM	CMD-C2D	3.49	1.57	1.50
2	D	501	HEM	CMC-C2C	3.43	1.57	1.50
2	B	501	HEM	CMA-C3A	3.42	1.57	1.50
2	C	501	HEM	FE-ND	3.41	2.05	1.94
2	A	501	HEM	CAC-C3C	3.40	1.56	1.47
2	C	501	HEM	CMB-C2B	3.40	1.57	1.50
2	B	501	HEM	CMC-C2C	3.35	1.57	1.50
2	D	501	HEM	CMD-C2D	3.32	1.57	1.50
2	B	501	HEM	C4A-C3A	3.30	1.50	1.43
2	A	501	HEM	CMB-C2B	3.28	1.57	1.50
2	D	501	HEM	CBD-CAD	3.28	1.63	1.51
2	B	501	HEM	CMB-C2B	3.24	1.57	1.50
2	B	501	HEM	CAB-C3B	3.23	1.56	1.47
2	A	501	HEM	CAB-C3B	3.16	1.55	1.47
2	D	501	HEM	CAB-C3B	3.15	1.55	1.47
3	A	502	ANN	C4-C5	3.15	1.44	1.38
2	C	501	HEM	CBD-CGD	3.14	1.57	1.50
2	B	501	HEM	CMD-C2D	3.12	1.57	1.50
2	D	501	HEM	CMA-C3A	3.04	1.57	1.50
2	D	501	HEM	CMB-C2B	3.01	1.57	1.50
2	D	501	HEM	C1C-NC	-2.91	1.34	1.39
2	A	501	HEM	FE-NB	2.91	2.03	1.94
2	D	501	HEM	C1B-NB	-2.90	1.35	1.40
3	C	502	ANN	C4-C3	2.79	1.43	1.38
3	D	502	ANN	O2-C1	2.63	1.30	1.22
2	C	501	HEM	CAC-C3C	2.57	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CAC-C3C	2.55	1.54	1.47
2	D	501	HEM	C1A-NA	-2.54	1.34	1.39
2	D	501	HEM	CBA-CGA	2.47	1.56	1.50
2	C	501	HEM	C4C-NC	-2.42	1.35	1.39
3	B	502	ANN	O3-C5	-2.32	1.32	1.37
2	A	501	HEM	CBD-CAD	2.27	1.59	1.51
2	D	501	HEM	CHC-C4B	2.26	1.44	1.39
2	A	501	HEM	C4A-C3A	2.26	1.48	1.43
2	A	501	HEM	C2A-C3A	-2.25	1.33	1.38
3	D	502	ANN	C2-C1	2.18	1.54	1.49
3	D	502	ANN	O3-C8	2.13	1.48	1.42
3	D	502	ANN	C7-C2	2.12	1.42	1.39
3	C	502	ANN	C4-C5	2.09	1.42	1.38
2	B	501	HEM	O1D-CGD	2.09	1.28	1.22
3	C	502	ANN	O3-C8	2.07	1.48	1.42
2	C	501	HEM	CMD-C2D	2.06	1.55	1.50
2	D	501	HEM	C1D-C2D	2.05	1.48	1.44
2	B	501	HEM	CBD-CGD	2.03	1.55	1.50
2	C	501	HEM	C1B-NB	-2.02	1.36	1.40

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4D-ND-C1D	6.70	113.14	105.21
2	D	501	HEM	C1B-NB-C4B	6.46	112.86	105.21
2	D	501	HEM	C3B-C4B-NB	-6.00	105.16	109.47
2	D	501	HEM	CBD-CAD-C3D	-4.70	99.55	112.53
3	A	502	ANN	C3-C4-C5	-4.55	114.53	119.73
2	A	501	HEM	C3D-C4D-ND	-4.19	105.58	110.17
2	D	501	HEM	C4D-ND-C1D	4.18	110.16	105.21
2	C	501	HEM	CMD-C2D-C1D	3.80	130.98	125.03
2	B	501	HEM	CHD-C4C-NC	3.71	128.50	124.45
2	C	501	HEM	C4D-ND-C1D	3.67	109.55	105.21
2	D	501	HEM	CAD-CBD-CGD	-3.63	104.04	113.67
2	C	501	HEM	C1B-NB-C4B	3.61	109.48	105.21
2	A	501	HEM	CBD-CAD-C3D	-3.58	102.64	112.53
2	B	501	HEM	CBD-CAD-C3D	-3.52	102.80	112.53
2	A	501	HEM	CHA-C4D-ND	3.39	128.57	124.37
2	C	501	HEM	CBD-CAD-C3D	-3.28	103.46	112.53
2	C	501	HEM	C3B-C4B-NB	-3.20	107.17	109.47
2	D	501	HEM	CHC-C4B-NB	3.09	127.75	124.42
3	C	502	ANN	C3-C4-C5	-3.09	116.21	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHD-C1D-ND	3.08	127.73	124.42
2	B	501	HEM	C4C-NC-C1C	2.96	110.65	105.82
2	A	501	HEM	C4C-NC-C1C	2.95	110.63	105.82
3	A	502	ANN	C4-C5-C6	2.95	124.46	120.16
2	D	501	HEM	C2B-C1B-NB	-2.88	106.53	109.84
2	C	501	HEM	C1D-C2D-C3D	-2.86	103.97	106.98
3	B	502	ANN	O1-C1-O2	-2.85	117.23	123.35
3	D	502	ANN	C3-C4-C5	-2.82	116.51	119.73
2	B	501	HEM	CMB-C2B-C1B	2.74	129.31	125.03
2	A	501	HEM	O2A-CGA-CBA	2.73	122.63	114.00
2	D	501	HEM	C4C-NC-C1C	2.72	110.26	105.82
2	A	501	HEM	CHD-C4C-NC	2.69	127.38	124.45
2	C	501	HEM	O2A-CGA-CBA	2.68	122.45	114.00
2	B	501	HEM	CAD-C3D-C4D	2.67	129.35	124.70
2	A	501	HEM	CHC-C1C-NC	2.67	127.36	124.45
2	B	501	HEM	CHC-C4B-NB	2.65	127.28	124.42
2	B	501	HEM	O2D-CGD-CBD	2.61	122.23	114.00
2	D	501	HEM	CMD-C2D-C1D	2.59	129.07	125.03
2	D	501	HEM	CHD-C4C-NC	2.58	127.26	124.45
3	A	502	ANN	C3-C2-C7	2.57	121.83	118.57
3	C	502	ANN	C4-C5-C6	2.57	123.90	120.16
3	C	502	ANN	O1-C1-C2	2.57	121.42	114.84
2	C	501	HEM	CAD-CBD-CGD	-2.53	106.96	113.67
2	D	501	HEM	O2D-CGD-CBD	2.51	121.93	114.00
2	C	501	HEM	C3B-C2B-C1B	2.51	108.29	106.41
2	C	501	HEM	C4C-NC-C1C	2.49	109.88	105.82
2	C	501	HEM	O2D-CGD-O1D	-2.48	116.96	123.33
5	B	505	GOL	C3-C2-C1	-2.45	102.80	111.80
2	C	501	HEM	C4C-C3C-C2C	2.45	108.94	106.81
3	D	502	ANN	C4-C5-C6	2.41	123.67	120.16
2	D	501	HEM	CMB-C2B-C1B	2.34	128.69	125.03
3	A	502	ANN	O1-C1-O2	-2.33	118.34	123.35
2	B	501	HEM	C4C-C3C-C2C	2.32	108.83	106.81
2	D	501	HEM	O2A-CGA-CBA	2.29	121.22	114.00
2	C	501	HEM	C2B-C1B-NB	-2.25	107.25	109.84
5	C	504	GOL	O1-C1-C2	-2.23	100.33	110.38
3	A	502	ANN	O1-C1-C2	2.22	120.53	114.84
3	B	502	ANN	C3-C4-C5	-2.22	117.20	119.73
2	C	501	HEM	O2A-CGA-O1A	-2.15	117.81	123.33
3	D	502	ANN	C6-C7-C2	-2.14	118.51	120.80
2	C	501	HEM	CHD-C4C-NC	2.13	126.77	124.45
2	A	501	HEM	O1A-CGA-CBA	-2.12	116.36	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CMB-C2B-C3B	-2.11	123.31	128.43
2	A	501	HEM	C4C-C3C-C2C	2.11	108.64	106.81
3	D	502	ANN	C3-C2-C7	2.05	121.17	118.57
2	B	501	HEM	C1D-C2D-C3D	-2.04	104.83	106.98
2	B	501	HEM	C1C-CHC-C4B	-2.04	121.69	126.02
5	D	504	GOL	O2-C2-C3	-2.01	100.86	109.18
2	C	501	HEM	C3A-C4A-NA	-2.00	106.93	110.14
2	D	501	HEM	CMC-C2C-C1C	-2.00	121.20	124.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	505	GOL	O1-C1-C2-C3
5	B	505	GOL	O1-C1-C2-O2
5	D	504	GOL	C1-C2-C3-O3
2	C	501	HEM	CAA-CBA-CGA-O2A
5	D	504	GOL	O2-C2-C3-O3
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D

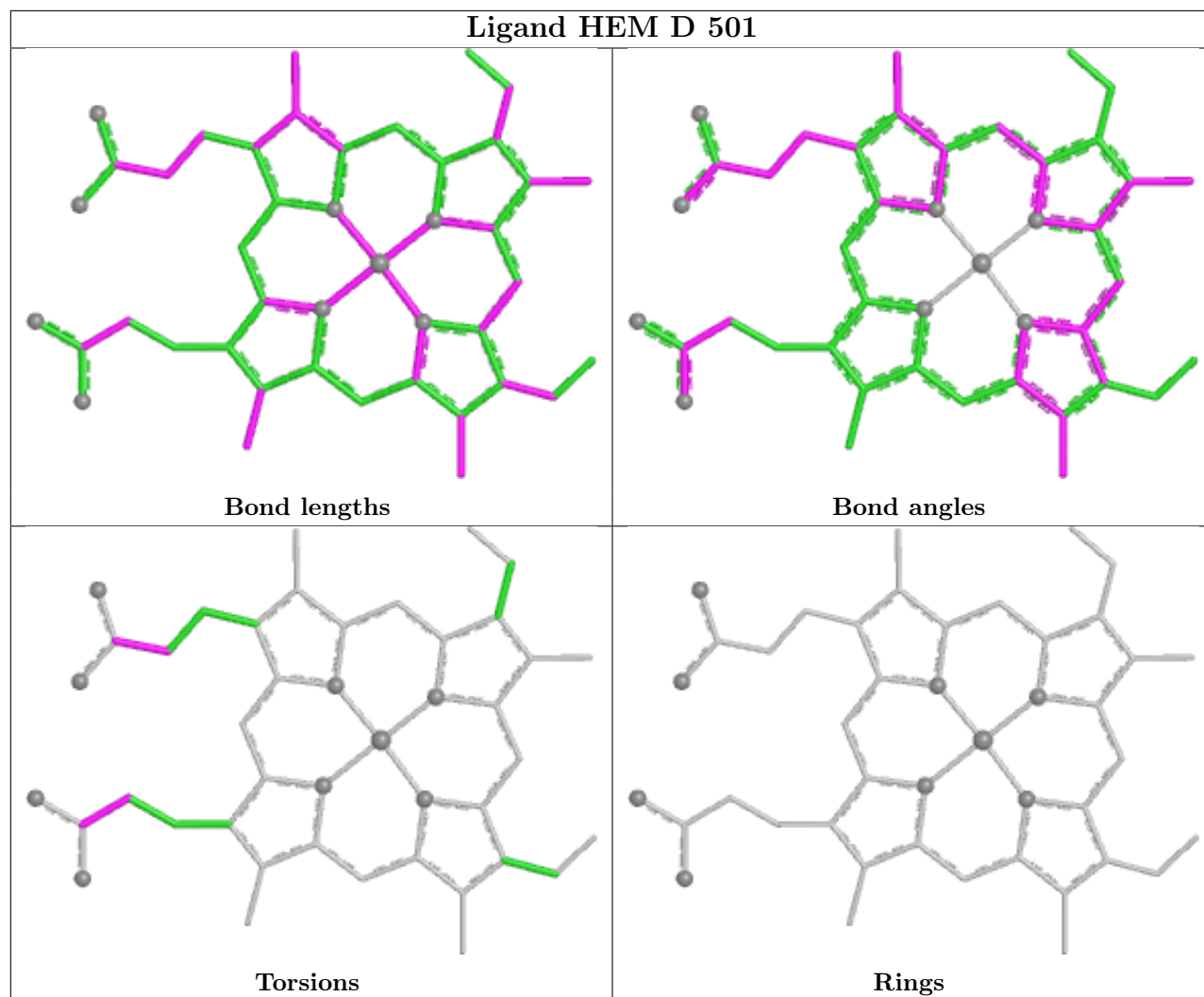
There are no ring outliers.

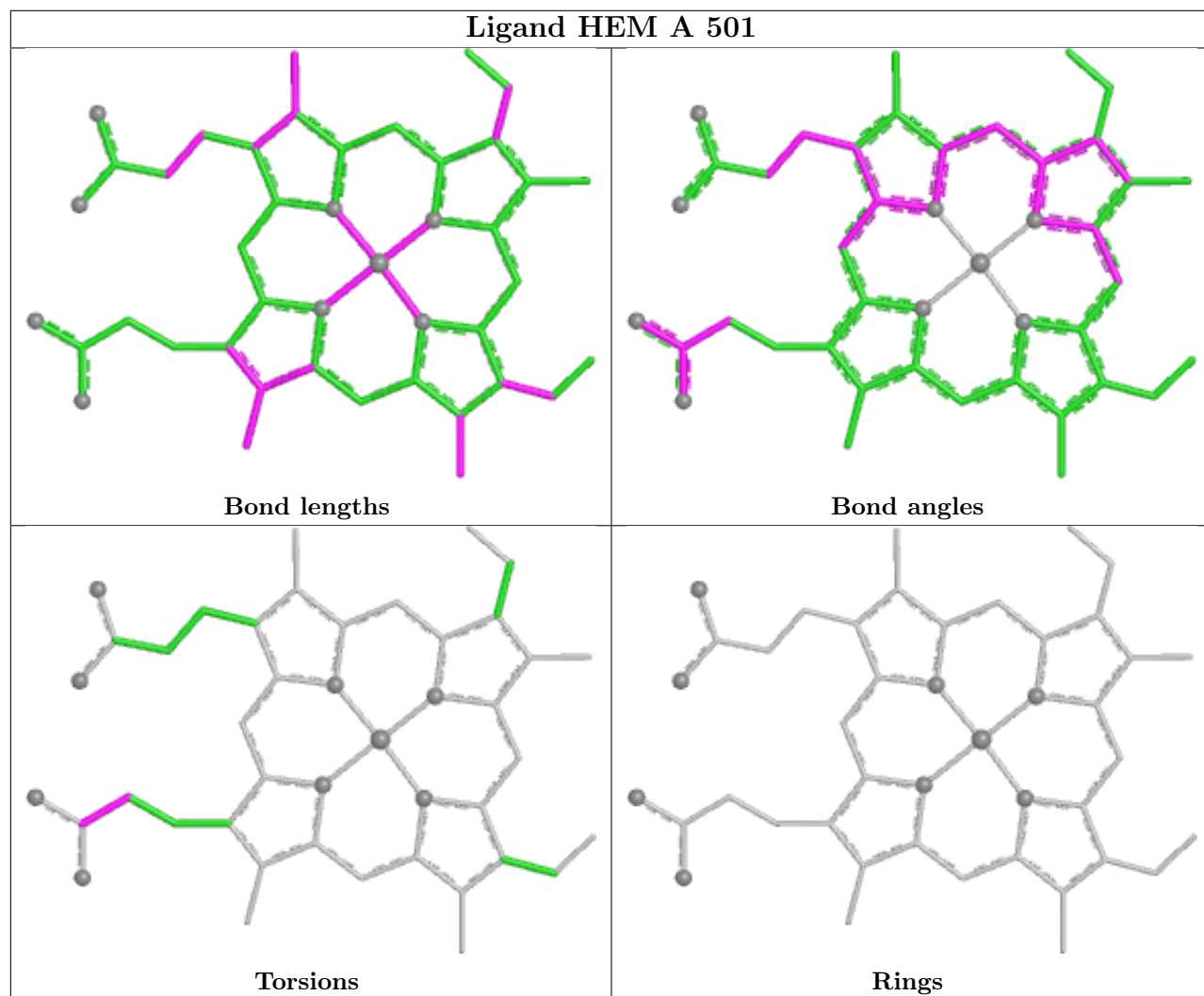
4 monomers are involved in 14 short contacts:

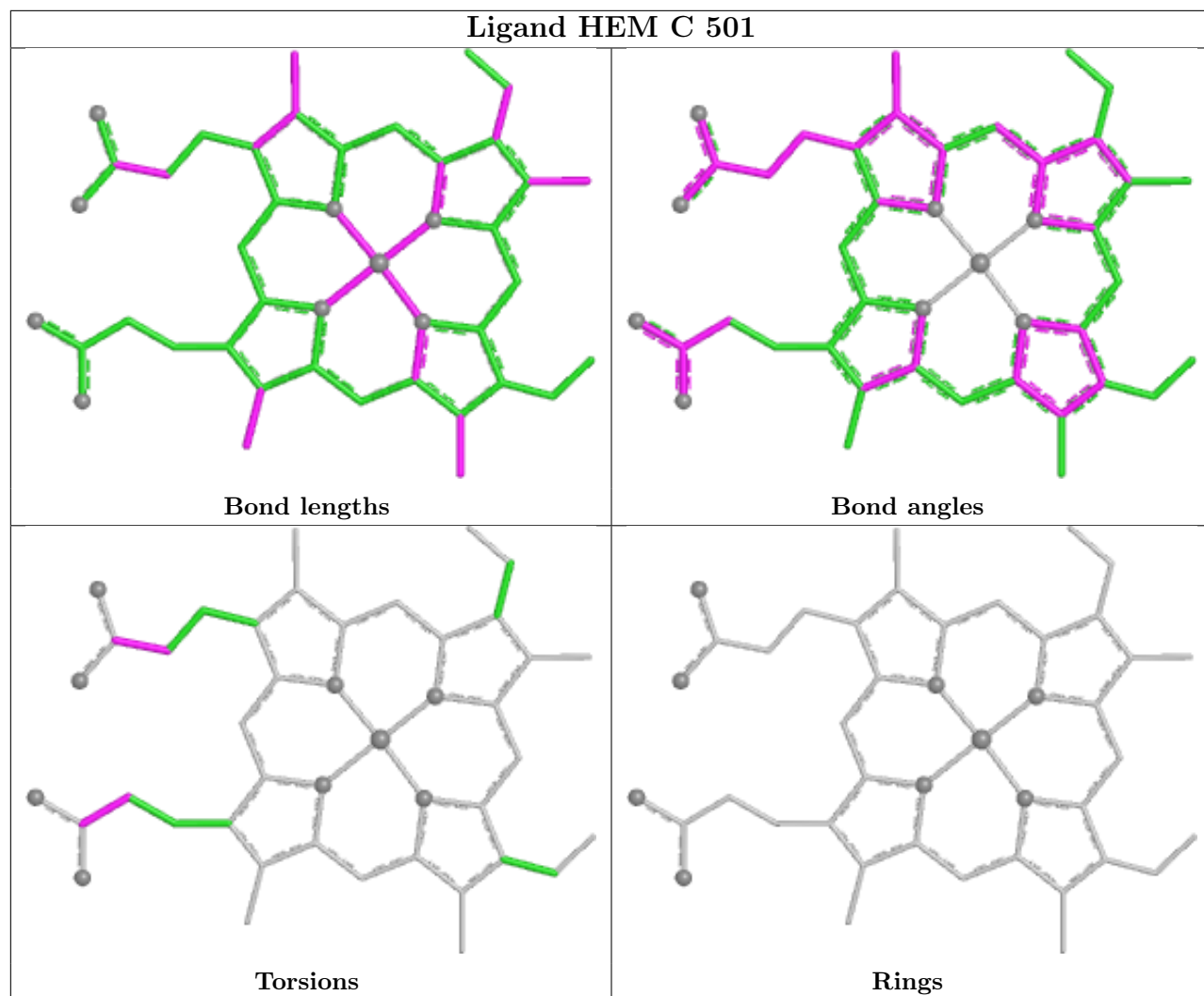
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	HEM	4	0
2	A	501	HEM	5	0
2	C	501	HEM	3	0
2	B	501	HEM	2	0

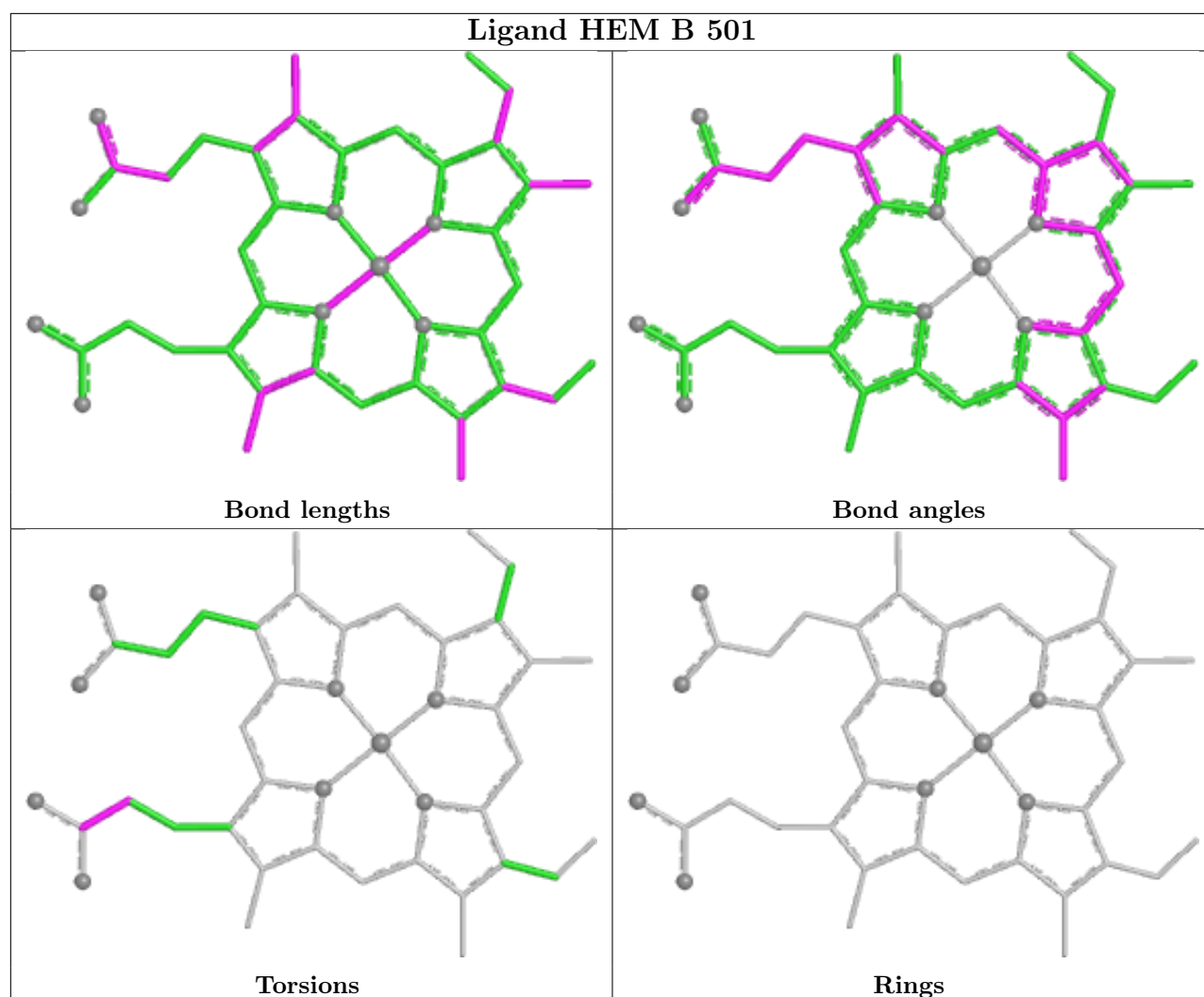
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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%)	-0.76	3 (0%) 82 82	13, 19, 31, 43	1 (0%)
1	B	393/410 (95%)	-0.75	2 (0%) 87 87	12, 19, 31, 41	0
1	C	393/410 (95%)	-0.76	1 (0%) 90 89	14, 19, 31, 42	0
1	D	393/410 (95%)	-0.54	3 (0%) 82 82	15, 22, 35, 48	0
All	All	1572/1640 (95%)	-0.70	9 (0%) 85 85	12, 20, 32, 48	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	THR	3.6
1	D	142	ARG	3.5
1	C	17	THR	3.1
1	B	17	THR	2.5
1	B	409	ALA	2.3
1	D	409	ALA	2.2
1	D	370	VAL	2.1
1	A	197	GLU	2.1
1	A	32	ASP	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 ⓘ

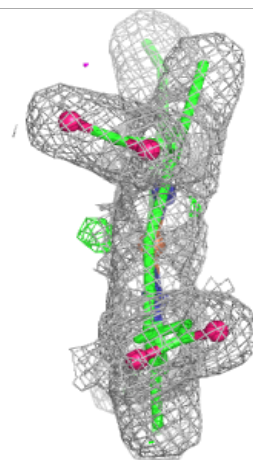
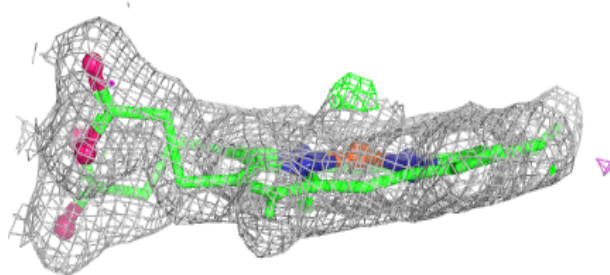
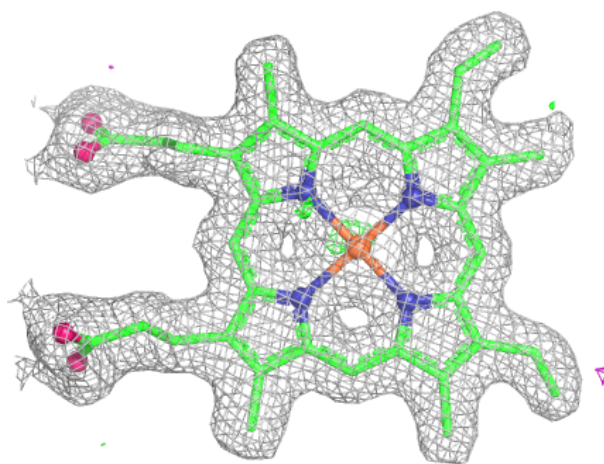
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	D	504	6/6	0.94	0.09	23,32,35,40	0
4	SO4	B	504	5/5	0.95	0.14	25,33,35,38	0
5	GOL	A	504	6/6	0.96	0.07	16,19,24,35	0
4	SO4	B	503	5/5	0.96	0.09	30,33,37,40	0
5	GOL	C	504	6/6	0.97	0.06	19,21,26,33	0
5	GOL	B	505	6/6	0.97	0.07	20,28,29,37	0
3	ANN	D	502	11/11	0.98	0.05	14,17,18,19	0
4	SO4	D	503	5/5	0.98	0.08	36,38,42,42	0
3	ANN	A	502	11/11	0.98	0.04	10,13,14,14	0
6	CL	D	505	1/1	0.98	0.06	27,27,27,27	0
4	SO4	C	503	5/5	0.99	0.04	18,21,23,23	0
2	HEM	A	501	43/43	0.99	0.04	10,13,15,16	0
3	ANN	B	502	11/11	0.99	0.03	12,13,15,15	0
3	ANN	C	502	11/11	0.99	0.04	10,13,15,16	0
2	HEM	B	501	43/43	0.99	0.04	9,13,16,16	0
2	HEM	C	501	43/43	0.99	0.04	10,14,17,19	0
6	CL	A	505	1/1	0.99	0.03	19,19,19,19	0
6	CL	B	506	1/1	0.99	0.03	20,20,20,20	0
6	CL	C	505	1/1	0.99	0.03	23,23,23,23	0
2	HEM	D	501	43/43	0.99	0.04	11,16,18,19	0
4	SO4	A	503	5/5	1.00	0.03	19,19,21,22	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.

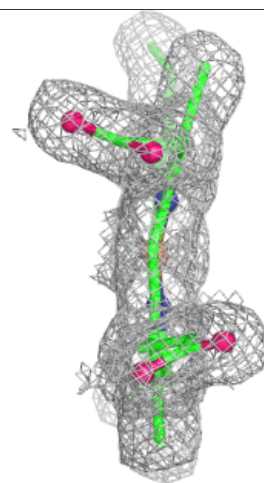
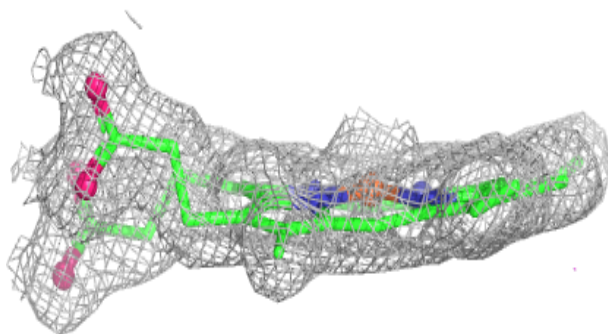
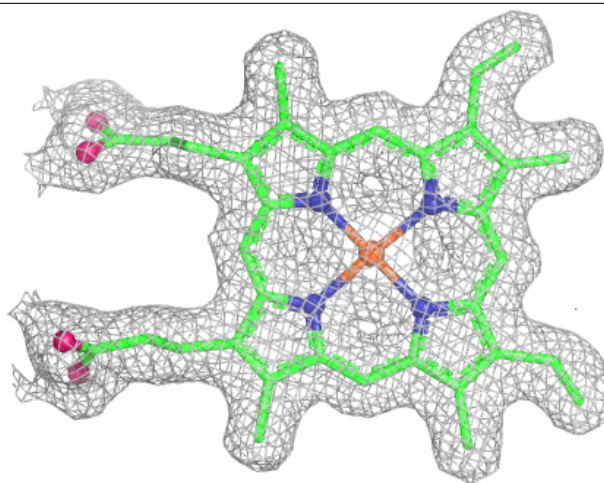
Electron density around HEM A 501:

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



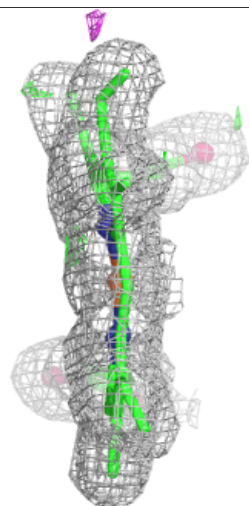
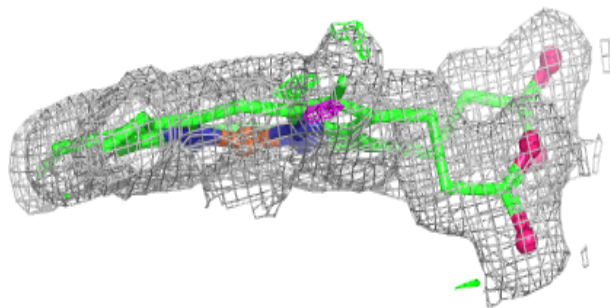
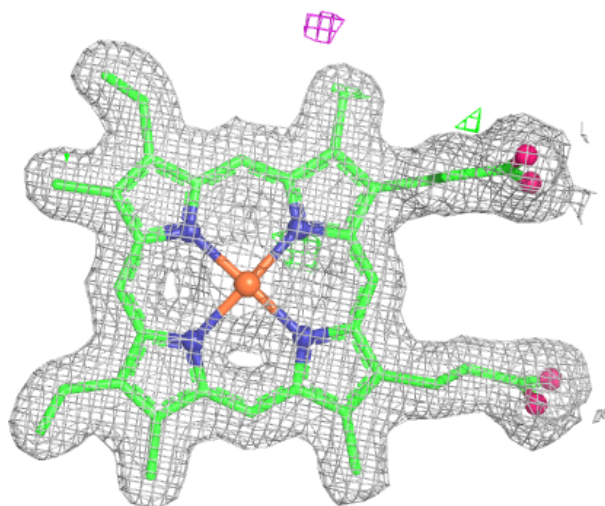
Electron density around HEM B 501:

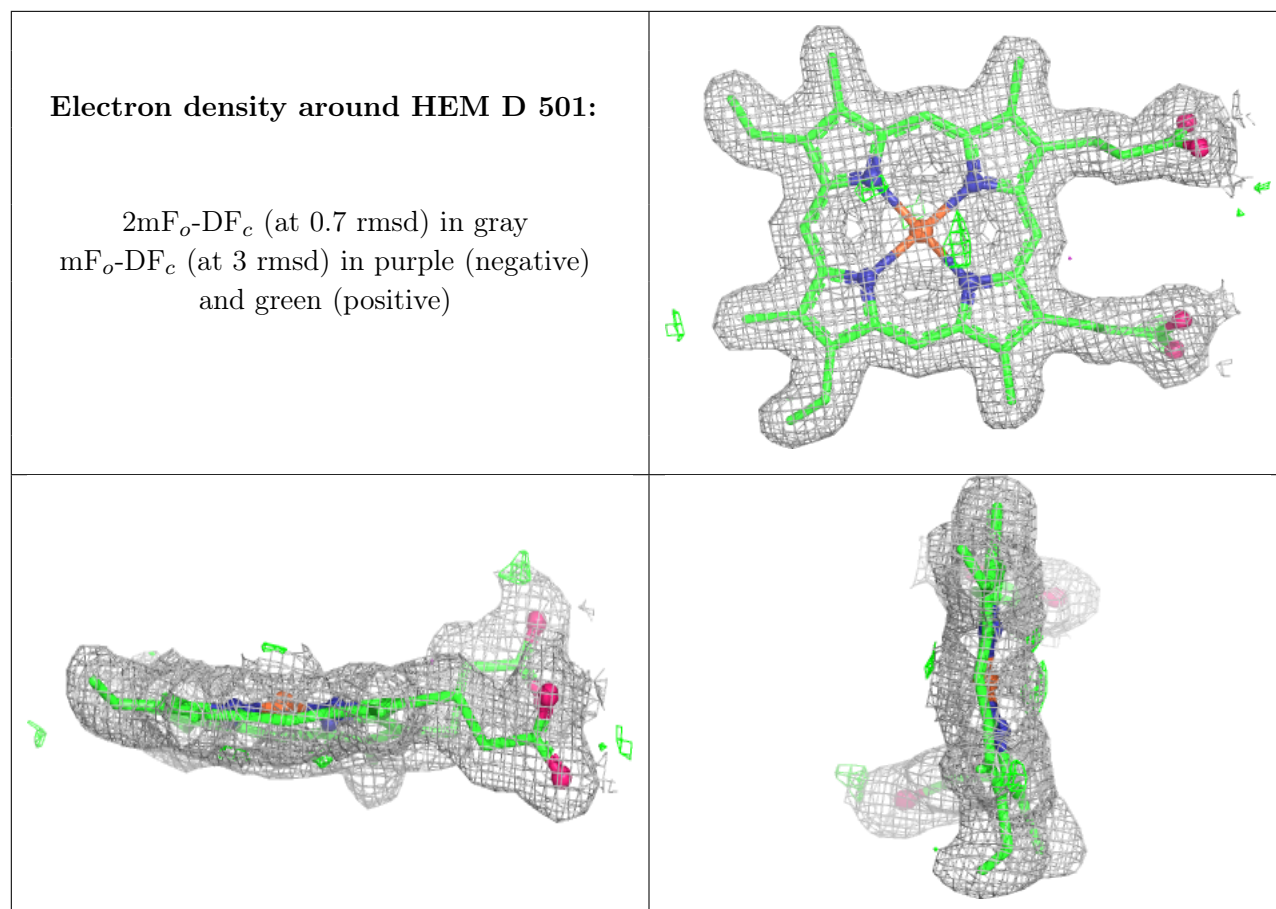
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.