



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:54 PM UTC

PDB ID : 4G1X / pdb_00004g1x
Title : Crystal structure of Mycobacterium tuberculosis CYP121 in complex with 4-(1H-1,2,4-triazol-1-yl)quinolin-6-amine
Authors : Hudson, S.A.
Deposited on : 2012-07-11
Resolution : 1.30 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

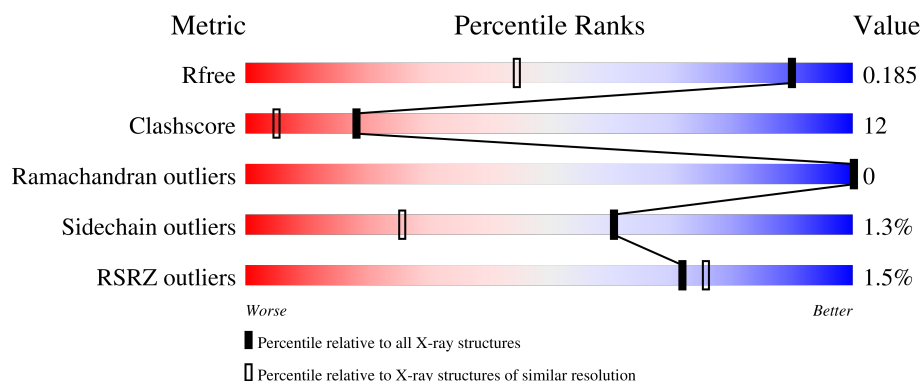
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

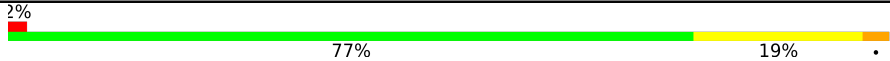
The reported resolution of this entry is 1.30 Å.

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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	395	

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
4	DMS	A	405	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	A	406	-	-	X	-
5	TQU	A	410	-	-	X	-

2 Entry composition [i](#)

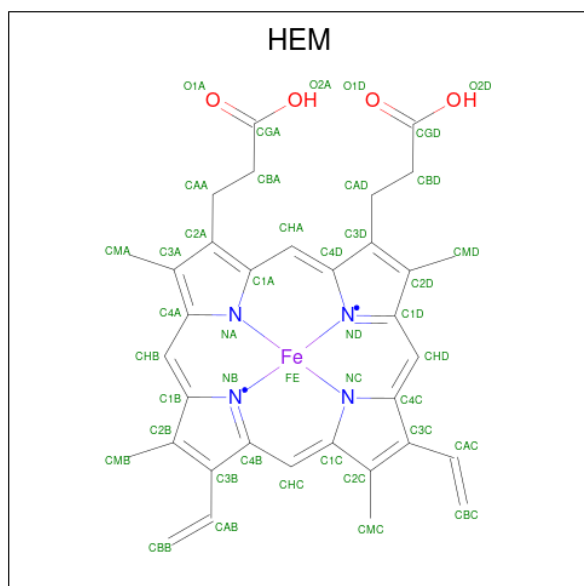
There are 6 unique types of molecules in this entry. The entry contains 4073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 121.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	26	1
			3089	1975	540	563	11			

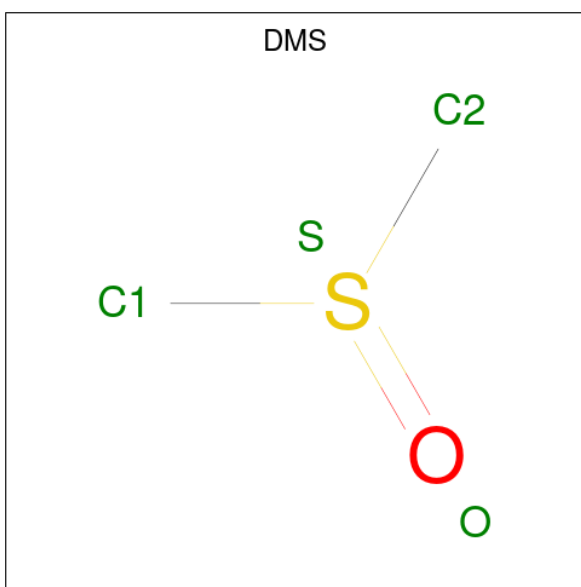
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	1
			10	8	2		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



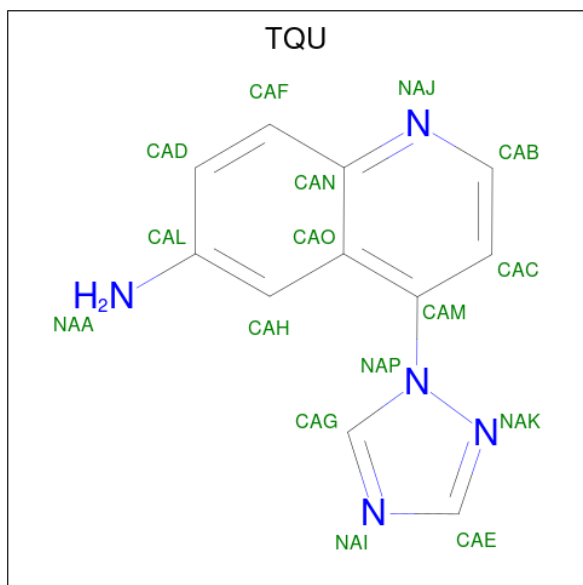
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 4-(1H-1,2,4-triazol-1-yl)quinolin-6-amine (CCD ID: TQU) (formula: C₁₁H₉N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			16	11	5		
5	A	1	Total	C	N	0	0
			16	11	5		

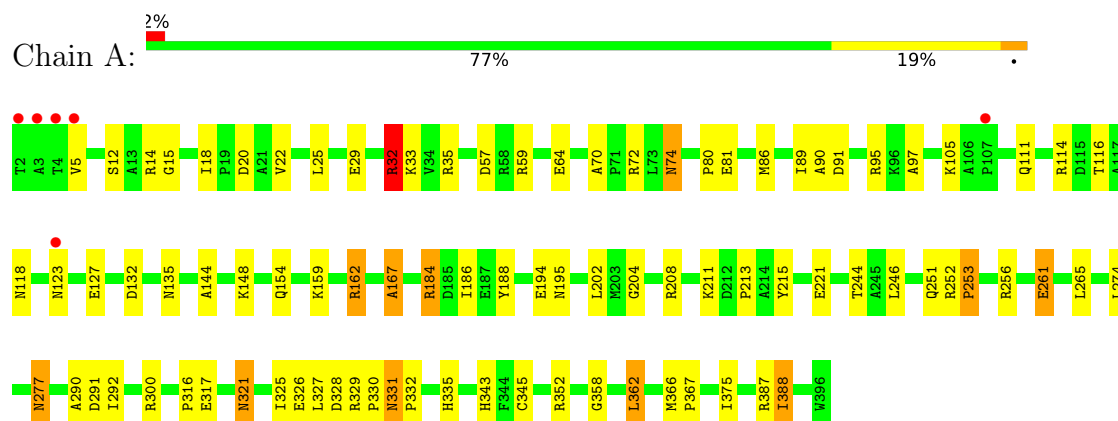
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	789	Total	O	0	41
			830	830		

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 121



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.41 Å 77.41 Å 263.95 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.14 – 1.30 37.14 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.14-1.30) 99.6 (37.14-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.30 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.186 0.161 , 0.185	Depositor DCC
R_{free} test set	5795 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4073	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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: TQU, SO4, DMS, HEM

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	1.98	60/3265 (1.8%)	1.60	30/4439 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	ARG	CA-CB	-11.89	1.32	1.53
1	A	321	ASN	C-O	-11.45	1.18	1.23
1	A	25	LEU	N-CA	-10.18	1.34	1.46
1	A	116	THR	CA-C	8.59	1.63	1.52
1	A	388	ILE	CA-CB	-8.25	1.43	1.54
1	A	118	ASN	CA-C	-8.18	1.42	1.52
1	A	105	LYS	CA-C	-8.11	1.41	1.52
1	A	32	ARG	CB-CG	-7.89	1.28	1.52
1	A	345	CYS	C-N	-7.86	1.25	1.34
1	A	335	HIS	CG-CD2	7.71	1.44	1.35
1	A	215	TYR	N-CA	7.25	1.54	1.46
1	A	18	ILE	CA-C	7.09	1.60	1.52
1	A	261	GLU	N-CA	6.72	1.54	1.46
1	A	188	TYR	C-O	6.67	1.31	1.24
1	A	89	ILE	C-O	6.63	1.31	1.24
1	A	57	ASP	C-O	6.47	1.31	1.24
1	A	290	ALA	C-O	6.43	1.31	1.23
1	A	70	ALA	N-CA	6.42	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	ILE	C-O	6.31	1.31	1.24
1	A	32	ARG	NE-CZ	6.30	1.40	1.33
1	A	204	GLY	N-CA	6.28	1.53	1.45
1	A	274	LEU	CA-C	-6.19	1.45	1.52
1	A	15	GLY	C-O	6.13	1.28	1.24
1	A	81	GLU	CD-OE1	6.07	1.36	1.25
1	A	252	ARG	N-CA	6.05	1.53	1.46
1	A	291	ASP	N-CA	-6.00	1.38	1.46
1	A	105	LYS	N-CA	5.99	1.54	1.46
1	A	35	ARG	CZ-NH2	5.93	1.41	1.33
1	A	90	ALA	C-O	5.87	1.31	1.24
1	A	321	ASN	CA-CB	5.87	1.56	1.52
1	A	116	THR	C-N	-5.86	1.26	1.33
1	A	335	HIS	CE1-NE2	5.80	1.38	1.32
1	A	184	ARG	C-O	5.78	1.30	1.24
1	A	367	PRO	CA-CB	5.65	1.62	1.53
1	A	91	ASP	C-O	5.64	1.31	1.24
1	A	256	ARG	CZ-NH2	5.60	1.40	1.33
1	A	328	ASP	CA-C	-5.59	1.45	1.53
1	A	343	HIS	ND1-CE1	5.57	1.38	1.32
1	A	332	PRO	C-O	5.56	1.30	1.24
1	A	59	ARG	CZ-NH1	5.52	1.40	1.32
1	A	184	ARG	CZ-NH1	5.51	1.40	1.32
1	A	325	ILE	N-CA	-5.49	1.40	1.46
1	A	14	ARG	NE-CZ	5.48	1.39	1.33
1	A	329	ARG	CA-C	5.47	1.59	1.53
1	A	97	ALA	N-CA	-5.42	1.39	1.46
1	A	132	ASP	C-O	5.38	1.30	1.23
1	A	195	ASN	C-N	5.35	1.40	1.34
1	A	253	PRO	CA-C	5.35	1.60	1.52
1	A	81	GLU	CD-OE2	5.26	1.35	1.25
1	A	329	ARG	C-O	-5.23	1.17	1.23
1	A	292	ILE	C-O	5.19	1.29	1.24
1	A	387	ARG	C-O	5.18	1.30	1.24
1	A	330	PRO	N-CD	-5.17	1.40	1.47
1	A	300	ARG	CA-C	-5.14	1.46	1.52
1	A	162	ARG	C-O	5.14	1.30	1.24
1	A	204	GLY	C-O	5.14	1.29	1.23
1	A	211	LYS	N-CA	5.12	1.52	1.46
1	A	135	ASN	C-O	5.12	1.30	1.24
1	A	253	PRO	C-O	-5.08	1.17	1.24
1	A	135	ASN	CA-C	-5.04	1.46	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ARG	CB-CG-CD	-11.00	86.00	111.30
1	A	208	ARG	NE-CZ-NH1	-8.67	112.83	121.50
1	A	195	ASN	CA-C-O	8.35	125.50	119.32
1	A	321	ASN	CA-C-O	8.19	126.78	120.48
1	A	329	ARG	O-C-N	6.76	128.96	121.53
1	A	105	LYS	CA-C-O	-6.47	111.70	119.27
1	A	59	ARG	N-CA-C	-6.31	105.44	113.01
1	A	352	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	A	25	LEU	CA-C-O	6.05	127.17	120.82
1	A	59	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	15	GLY	CA-C-O	-5.92	113.66	119.04
1	A	22	VAL	O-C-N	5.80	127.59	121.91
1	A	366	MET	O-C-N	-5.73	116.59	121.23
1	A	362[A]	LEU	CB-CA-C	-5.65	102.02	110.88
1	A	362[B]	LEU	CB-CA-C	-5.65	102.02	110.88
1	A	265	LEU	CA-C-O	-5.48	112.65	119.28
1	A	274	LEU	O-C-N	-5.43	116.48	122.07
1	A	388	ILE	N-CA-CB	5.33	118.67	111.21
1	A	25	LEU	N-CA-CB	-5.25	102.39	110.01
1	A	327	LEU	O-C-N	5.21	129.56	122.37
1	A	277	ASN	CB-CG-ND2	5.20	124.20	116.40
1	A	290	ALA	O-C-N	-5.15	117.85	123.26
1	A	345	CYS	O-C-N	5.14	125.78	121.31
1	A	358	GLY	CA-C-O	-5.12	115.48	120.75
1	A	202	LEU	CA-C-O	-5.06	115.50	120.82
1	A	167	ALA	N-CA-C	5.05	117.52	111.71
1	A	329	ARG	CA-C-N	-5.05	114.59	120.04
1	A	329	ARG	C-N-CA	-5.05	114.59	120.04
1	A	213	PRO	CA-C-O	-5.04	111.98	119.18
1	A	32	ARG	CD-NE-CZ	-5.00	117.39	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ARG	Sidechain

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	3089	0	3110	62	0
2	A	86	0	60	3	0
3	A	20	0	0	0	0
4	A	16	0	24	16	0
5	A	32	0	18	13	0
6	A	830	0	0	43	5
All	All	4073	0	3212	79	5

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 12.

All (79) 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)
5:A:410:TQU:H7	6:A:1075:HOH:O	1.29	1.28
1:A:251[A]:GLN:NE2	1:A:375:ILE:HD13	1.48	1.28
1:A:388:ILE:HG22	6:A:832:HOH:O	1.35	1.23
5:A:410:TQU:H8	6:A:1127:HOH:O	1.37	1.18
5:A:410:TQU:H4	6:A:616:HOH:O	1.39	1.17
1:A:162:ARG:HG3	6:A:912:HOH:O	1.41	1.16
4:A:407:DMS:H22	6:A:1097:HOH:O	1.49	1.12
1:A:251[A]:GLN:NE2	1:A:375:ILE:CD1	2.15	1.09
1:A:251[B]:GLN:OE1	6:A:1067:HOH:O	1.74	1.03
1:A:111:GLN:NE2	1:A:114[B]:ARG:HH21	1.60	1.00
1:A:251[A]:GLN:HE22	1:A:375:ILE:HD13	1.27	0.94
1:A:184:ARG:CZ	6:A:1088:HOH:O	2.16	0.93
5:A:410:TQU:H5	6:A:603:HOH:O	1.67	0.93
1:A:123:ASN:ND2	6:A:1167[B]:HOH:O	1.81	0.87
1:A:244:THR:HG23	6:A:832:HOH:O	1.77	0.84
5:A:410:TQU:CAF	6:A:603:HOH:O	2.23	0.83
1:A:80[A]:PRO:HG3	6:A:1007:HOH:O	1.81	0.79
1:A:194[B]:GLU:OE2	6:A:810:HOH:O	2.00	0.79
1:A:162:ARG:HH12	4:A:406:DMS:C2	1.95	0.79
1:A:321:ASN:HA	4:A:407:DMS:H23	1.65	0.79
1:A:148:LYS:HE2	6:A:870:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLN:HE22	1:A:114[B]:ARG:HH21	1.32	0.77
1:A:251[A]:GLN:HE21	1:A:375:ILE:HD13	1.42	0.77
1:A:221:GLU:OE2	6:A:896:HOH:O	2.04	0.76
4:A:405:DMS:H22	6:A:1229[B]:HOH:O	1.87	0.75
5:A:410:TQU:CAD	6:A:603:HOH:O	2.33	0.75
1:A:162:ARG:HH12	4:A:406:DMS:H23	1.52	0.74
1:A:20:ASP:H	4:A:405:DMS:C1	2.00	0.73
5:A:410:TQU:H4	6:A:603:HOH:O	1.90	0.71
5:A:409:TQU:H1	5:A:409:TQU:NAK	2.05	0.71
1:A:162:ARG:HH22	4:A:406:DMS:H11	1.56	0.70
5:A:410:TQU:CAD	6:A:616:HOH:O	2.10	0.69
1:A:12[B]:SER:HB3	6:A:1189:HOH:O	1.94	0.68
1:A:5:VAL:HG22	4:A:408:DMS:H12	1.74	0.68
1:A:20:ASP:H	4:A:405:DMS:H12	1.59	0.67
1:A:159:LYS:CD	6:A:1037:HOH:O	2.43	0.67
1:A:127[B]:GLU:CG	6:A:1018:HOH:O	2.43	0.65
1:A:162:ARG:HH22	4:A:406:DMS:C1	2.09	0.65
1:A:162:ARG:NH1	6:A:912:HOH:O	2.30	0.65
1:A:326:GLU:OE2	6:A:918:HOH:O	2.14	0.64
1:A:29:GLU:HG2	1:A:32:ARG:HB3	1.80	0.64
1:A:194[B]:GLU:CD	6:A:810:HOH:O	2.41	0.63
1:A:74:ASN:C	1:A:74:ASN:HD22	2.07	0.62
1:A:261:GLU:CG	6:A:1091:HOH:O	2.47	0.61
1:A:251[A]:GLN:HE21	1:A:375:ILE:CD1	2.03	0.60
1:A:317:GLU:CG	6:A:1050:HOH:O	2.50	0.58
1:A:144:ALA:HA	1:A:154:GLN:HE22	1.71	0.56
1:A:162:ARG:HH12	4:A:406:DMS:H21	1.69	0.56
2:A:401[B]:HEM:CBB	2:A:401[B]:HEM:HHC	2.36	0.54
1:A:64[B]:GLU:OE2	6:A:661:HOH:O	2.18	0.53
1:A:127[A]:GLU:CG	6:A:1018:HOH:O	2.56	0.53
1:A:162:ARG:NH1	4:A:406:DMS:H21	2.25	0.51
1:A:95:ARG:NE	6:A:1191:HOH:O	2.43	0.51
1:A:80[A]:PRO:CG	6:A:1007:HOH:O	2.50	0.50
1:A:167:ALA:HB1	5:A:410:TQU:CAH	2.41	0.50
1:A:64[A]:GLU:CG	6:A:661:HOH:O	2.59	0.49
1:A:184:ARG:NH2	6:A:1088:HOH:O	2.39	0.49
5:A:410:TQU:CAC	6:A:1075:HOH:O	2.14	0.49
1:A:331:ASN:H	1:A:331:ASN:HD22	1.60	0.48
1:A:127[A]:GLU:CB	6:A:1018:HOH:O	2.61	0.48
1:A:127[A]:GLU:HB2	6:A:1018:HOH:O	2.15	0.47
1:A:127[B]:GLU:CB	6:A:1018:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PRO:HB3	4:A:407:DMS:H12	1.96	0.46
4:A:405:DMS:C2	6:A:1229[B]:HOH:O	2.54	0.46
1:A:246:LEU:HD22	1:A:362[B]:LEU:CD2	2.46	0.46
2:A:401[B]:HEM:HHC	2:A:401[B]:HEM:HBB2	1.97	0.45
1:A:251[A]:GLN:C	1:A:253:PRO:HD3	2.42	0.44
1:A:388:ILE:CG2	6:A:832:HOH:O	2.20	0.44
1:A:86[B]:MET:HG3	6:A:1252:HOH:O	2.18	0.43
1:A:167:ALA:HB1	5:A:410:TQU:CAL	2.48	0.43
1:A:33[B]:LYS:HB2	1:A:33[B]:LYS:HE3	1.83	0.42
5:A:409:TQU:NAK	5:A:409:TQU:CAH	2.67	0.42
2:A:401[B]:HEM:CBB	2:A:401[B]:HEM:CHC	2.97	0.42
1:A:246:LEU:HD22	1:A:362[B]:LEU:HD22	2.01	0.41
1:A:326:GLU:HG2	6:A:918:HOH:O	2.21	0.41
1:A:184:ARG:NE	6:A:1088:HOH:O	2.41	0.41
1:A:162:ARG:NH2	4:A:406:DMS:H11	2.31	0.40
1:A:331:ASN:HD22	1:A:331:ASN:N	2.17	0.40
1:A:162:ARG:NH1	4:A:406:DMS:C2	2.73	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:703:HOH:O	6:A:1272:HOH:O[10_555]	1.72	0.48
6:A:879:HOH:O	6:A:1119:HOH:O[6_554]	1.84	0.36
6:A:838:HOH:O	6:A:1266:HOH:O[5_555]	2.04	0.16
6:A:838:HOH:O	6:A:1064:HOH:O[10_555]	2.13	0.07
6:A:738:HOH:O	6:A:1102:HOH:O[10_555]	2.19	0.01

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	419/395 (106%)	414 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	330/325 (102%)	326 (99%)	4 (1%)	63	29

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	74	ASN
1	A	277	ASN
1	A	331	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	111	GLN
1	A	154	GLN
1	A	331	ASN
1	A	342	GLN
1	A	356	GLN

5.3.3 RNA ⓘ

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	401[B]	5,1	50,50,50	1.97	16 (32%)	67,82,82	1.94	21 (31%)
4	DMS	A	407	-	3,3,3	0.58	0	3,3,3	1.29	1 (33%)
5	TQU	A	410	-	18,18,18	3.52	2 (11%)	23,25,25	1.58	7 (30%)
3	SO4	A	403	-	4,4,4	1.52	1 (25%)	6,6,6	0.74	0
3	SO4	A	402[A]	-	4,4,4	0.99	0	6,6,6	1.06	1 (16%)
4	DMS	A	406	-	3,3,3	0.39	0	3,3,3	2.20	1 (33%)
2	HEM	A	401[A]	5,1	50,50,50	1.61	9 (18%)	67,82,82	1.82	16 (23%)
4	DMS	A	405	-	3,3,3	0.72	0	3,3,3	1.85	1 (33%)
3	SO4	A	404	-	4,4,4	0.79	0	6,6,6	0.31	0
4	DMS	A	408	-	3,3,3	0.31	0	3,3,3	1.36	0
3	SO4	A	402[B]	-	4,4,4	0.81	0	6,6,6	1.78	1 (16%)
5	TQU	A	409	2	18,18,18	3.52	2 (11%)	23,25,25	1.58	7 (30%)

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
5	TQU	A	410	-	-	0/4/4/4	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	401[B]	5,1	-	0/14/54/54	-
2	HEM	A	401[A]	5,1	-	0/14/54/54	-
5	TQU	A	409	2	-	0/4/4/4	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	409	TQU	CAM-NAP	-11.05	1.33	1.43
5	A	410	TQU	CAM-NAP	-10.98	1.33	1.43
5	A	410	TQU	NAP-NAK	-9.13	1.23	1.36
5	A	409	TQU	NAP-NAK	-9.06	1.23	1.36
2	A	401[B]	HEM	C4D-ND	-5.06	1.31	1.40
2	A	401[B]	HEM	FE-ND	4.40	2.08	1.94
2	A	401[B]	HEM	C3C-C2C	4.25	1.45	1.37
2	A	401[A]	HEM	C4D-ND	-4.14	1.33	1.40
2	A	401[A]	HEM	C1B-NB	-3.75	1.33	1.40
2	A	401[B]	HEM	FE-NB	3.62	2.06	1.94
2	A	401[B]	HEM	C4B-NB	-3.37	1.32	1.38
2	A	401[A]	HEM	FE-ND	3.23	2.04	1.94
2	A	401[B]	HEM	C3D-C2D	3.19	1.43	1.36
2	A	401[B]	HEM	C1B-NB	-3.11	1.34	1.40
2	A	401[B]	HEM	C4C-NC	2.98	1.45	1.39
2	A	401[B]	HEM	C1A-NA	2.91	1.45	1.39
2	A	401[B]	HEM	CHC-C4B	2.90	1.45	1.39
2	A	401[A]	HEM	FE-NB	2.76	2.03	1.94
2	A	401[A]	HEM	C3C-C2C	2.65	1.42	1.37
2	A	401[A]	HEM	C4C-NC	2.62	1.44	1.39
2	A	401[B]	HEM	CHD-C1D	2.49	1.44	1.39
2	A	401[A]	HEM	C1B-C2B	-2.44	1.39	1.44
2	A	401[B]	HEM	O1D-CGD	2.36	1.29	1.22
2	A	401[A]	HEM	CMA-C3A	-2.26	1.46	1.50
2	A	401[B]	HEM	CHB-C1B	2.20	1.42	1.38
2	A	401[B]	HEM	C1D-ND	-2.16	1.34	1.38
2	A	401[A]	HEM	CMB-C2B	-2.06	1.46	1.50
2	A	401[B]	HEM	C3B-C2B	2.05	1.41	1.37
2	A	401[B]	HEM	CHA-C4D	2.01	1.42	1.38
3	A	403	SO4	O4-S	-2.01	1.31	1.48

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	HEM	C3B-C4B-NB	5.08	113.12	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	HEM	O1D-CGD-CBD	-4.84	107.73	123.09
2	A	401[A]	HEM	CHC-C4B-NB	4.66	129.43	124.42
2	A	401[B]	HEM	C3B-C2B-C1B	-4.42	103.09	106.41
2	A	401[A]	HEM	C4B-C3B-C2B	-4.29	103.34	107.28
2	A	401[B]	HEM	C1D-C2D-C3D	-3.94	102.83	106.98
3	A	402[B]	SO4	O3-S-O2	3.85	129.69	109.56
2	A	401[B]	HEM	C2B-C1B-NB	3.85	114.26	109.84
2	A	401[A]	HEM	CMC-C2C-C1C	3.79	131.40	124.73
2	A	401[A]	HEM	C1C-CHC-C4B	-3.48	118.63	126.02
2	A	401[A]	HEM	C1D-C2D-C3D	-3.37	103.44	106.98
4	A	406	DMS	C2-S-C1	3.34	115.52	98.42
2	A	401[B]	HEM	C4A-CHB-C1B	-3.31	118.46	126.25
2	A	401[A]	HEM	O2D-CGD-CBD	3.24	124.23	114.00
2	A	401[B]	HEM	CHC-C4B-NB	3.20	127.87	124.42
2	A	401[A]	HEM	C3B-C4B-NB	3.15	111.73	109.47
2	A	401[A]	HEM	CHC-C4B-C3B	-3.13	118.83	125.07
2	A	401[B]	HEM	C3C-C2C-C1C	-3.12	104.09	107.05
2	A	401[A]	HEM	CHC-C1C-NC	3.12	127.85	124.45
5	A	410	TQU	CAE-NAK-NAP	3.06	108.89	102.32
5	A	409	TQU	CAE-NAK-NAP	3.04	108.85	102.32
2	A	401[B]	HEM	CHC-C4B-C3B	-3.04	119.00	125.07
5	A	409	TQU	CAB-NAJ-CAN	2.99	121.45	116.93
5	A	410	TQU	CAB-NAJ-CAN	2.98	121.44	116.93
2	A	401[B]	HEM	CHA-C1A-NA	2.94	129.18	123.86
2	A	401[B]	HEM	C3D-C4D-ND	2.94	113.39	110.17
2	A	401[B]	HEM	C2C-C1C-NC	2.93	115.05	109.64
2	A	401[B]	HEM	CHB-C1B-C2B	-2.89	118.74	126.95
2	A	401[B]	HEM	CHA-C1A-C2A	-2.87	119.02	125.30
2	A	401[A]	HEM	C2D-C1D-ND	2.73	113.06	109.90
2	A	401[B]	HEM	C2D-C1D-ND	2.72	113.04	109.90
2	A	401[A]	HEM	CHC-C1C-C2C	-2.70	119.86	125.49
2	A	401[A]	HEM	C2B-C1B-NB	2.67	112.91	109.84
5	A	410	TQU	NAK-CAE-NAI	-2.57	107.57	114.90
2	A	401[B]	HEM	C4C-NC-C1C	-2.55	101.66	105.82
5	A	409	TQU	NAK-CAE-NAI	-2.55	107.63	114.90
2	A	401[B]	HEM	C4B-C3B-C2B	-2.53	104.95	107.28
5	A	409	TQU	CAC-CAB-NAJ	-2.52	120.86	124.60
5	A	410	TQU	CAC-CAB-NAJ	-2.51	120.86	124.60
5	A	409	TQU	CAM-CAO-CAN	2.49	119.32	116.98
5	A	410	TQU	CAM-CAO-CAN	2.44	119.28	116.98
5	A	409	TQU	CAO-CAN-NAJ	-2.35	120.33	122.82
3	A	402[A]	SO4	O4-S-O3	-2.30	95.83	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	DMS	O-S-C1	2.30	117.99	106.49
5	A	410	TQU	CAO-CAN-NAJ	-2.29	120.39	122.82
4	A	407	DMS	C2-S-C1	2.24	109.89	98.42
2	A	401[B]	HEM	C1C-CHC-C4B	-2.20	121.35	126.02
2	A	401[B]	HEM	C1A-CHA-C4D	-2.15	121.19	126.25
2	A	401[B]	HEM	CMA-C3A-C4A	2.13	128.66	125.42
2	A	401[B]	HEM	CHB-C1B-NB	2.13	127.00	124.37
2	A	401[A]	HEM	CMC-C2C-C3C	-2.10	123.34	128.43
5	A	410	TQU	CAC-CAM-NAP	2.07	120.60	118.09
5	A	409	TQU	CAC-CAM-NAP	2.06	120.59	118.09
2	A	401[B]	HEM	CHC-C1C-C2C	-2.04	121.24	125.49
2	A	401[A]	HEM	CHD-C4C-NC	-2.02	122.25	124.45
2	A	401[A]	HEM	CHB-C1B-C2B	-2.00	121.26	126.95

There are no chirality outliers.

There are no torsion outliers.

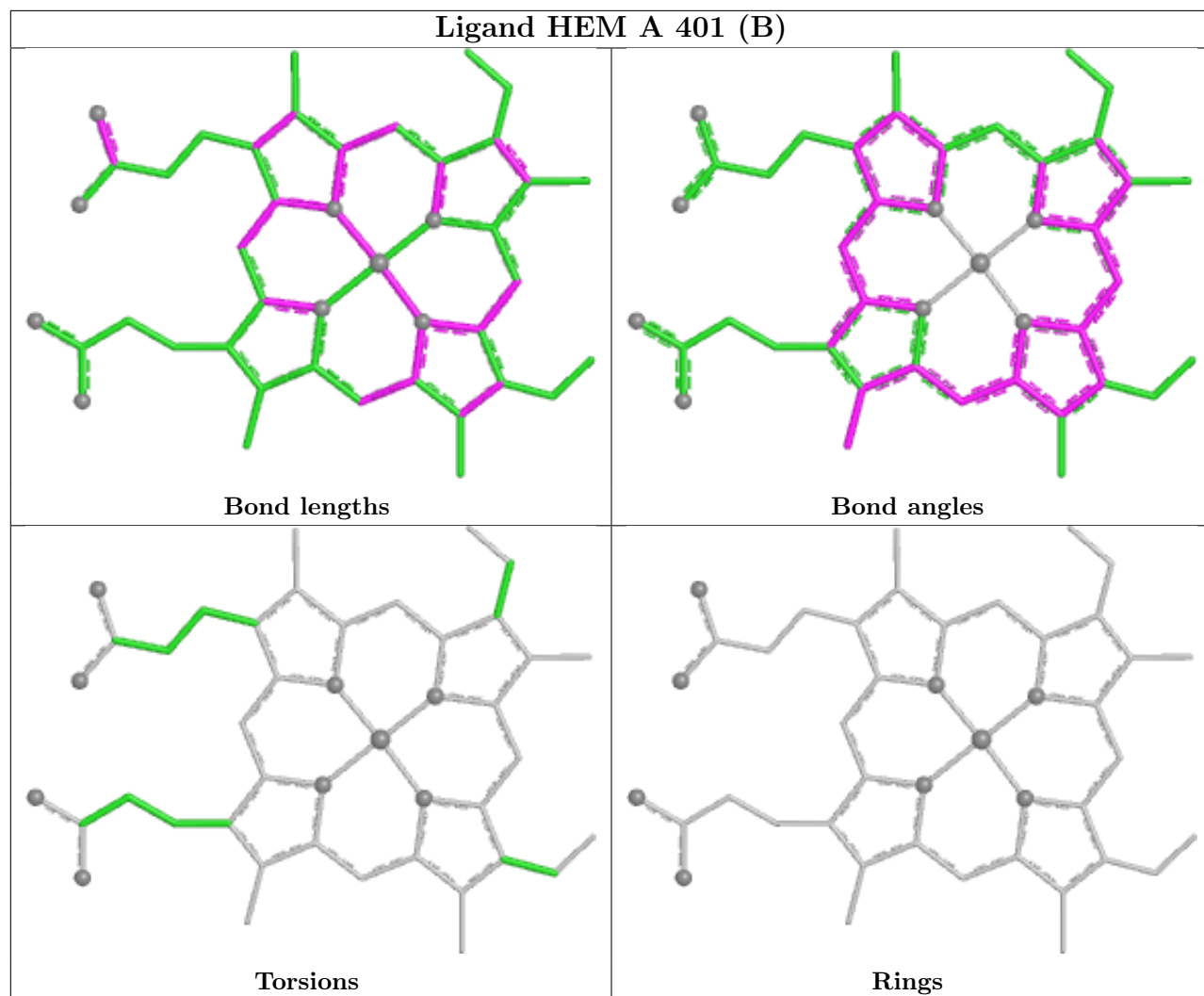
There are no ring outliers.

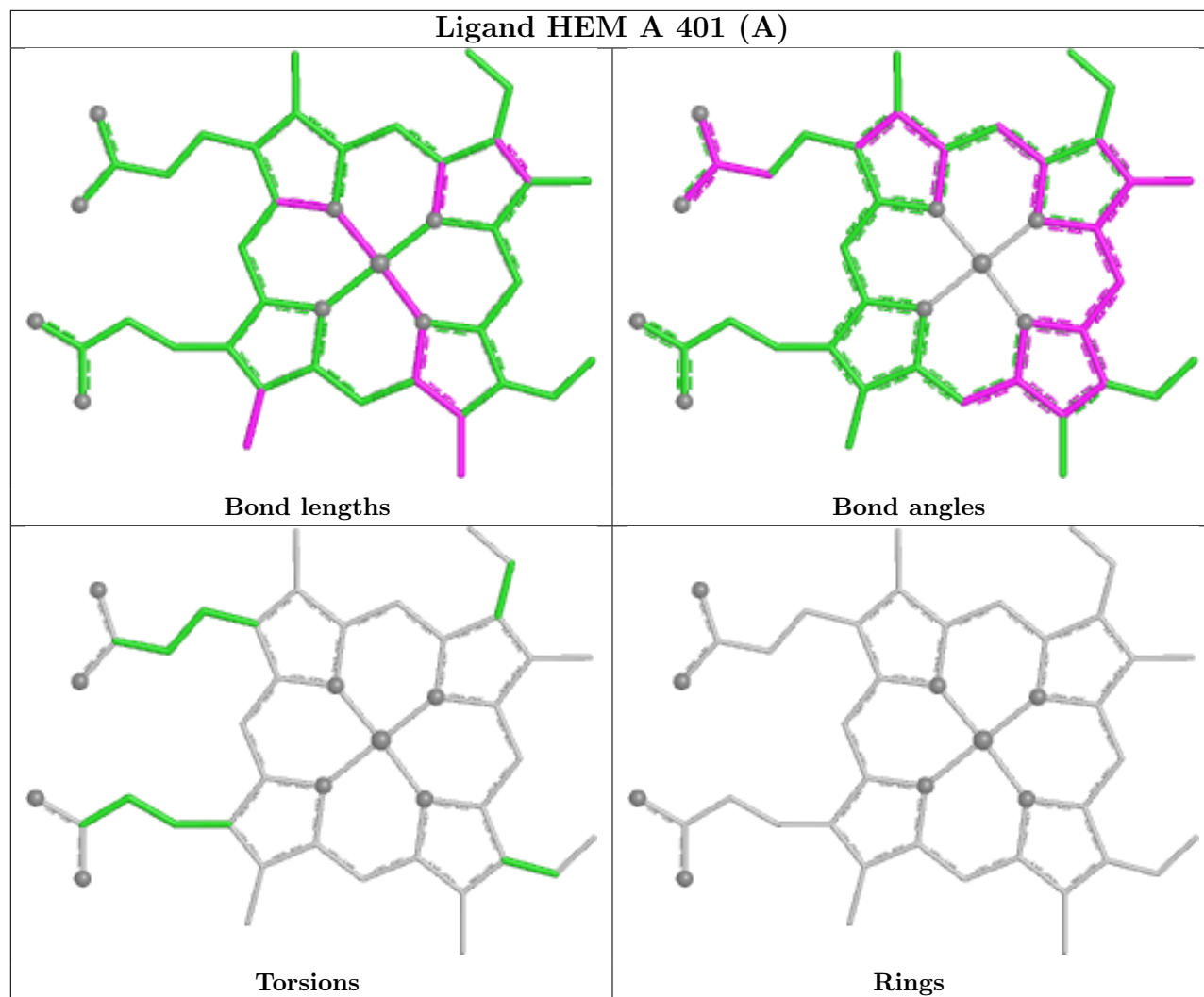
7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401[B]	HEM	3	0
4	A	407	DMS	3	0
5	A	410	TQU	11	0
4	A	406	DMS	8	0
4	A	405	DMS	4	0
4	A	408	DMS	1	0
5	A	409	TQU	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.

Ligand HEM A 401 (B)





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	395/395 (100%)	-0.19	6 (1%) 72 76	4, 10, 20, 48	27 (6%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	THR	4.1
1	A	2	THR	3.7
1	A	107	PRO	2.9
1	A	3	ALA	2.5
1	A	5	VAL	2.3
1	A	123	ASN	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(Å ²)	Q<0.9
5	TQU	A	410	16/16	0.68	0.22	9,10,13,16	16

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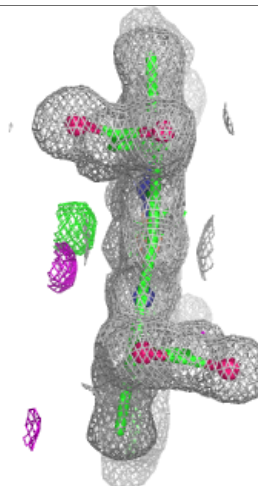
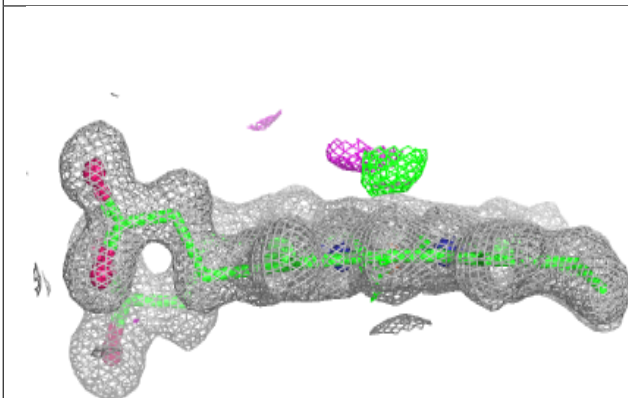
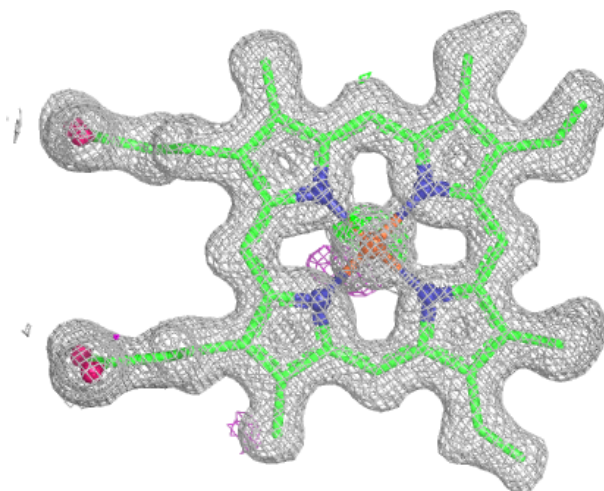
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	407	4/4	0.70	0.20	28,45,57,67	0
4	DMS	A	405	4/4	0.70	0.18	33,41,42,50	0
4	DMS	A	408	4/4	0.79	0.18	48,52,55,55	0
4	DMS	A	406	4/4	0.79	0.16	37,39,42,53	0
5	TQU	A	409	16/16	0.87	0.10	7,10,13,14	0
3	SO4	A	402[A]	5/5	0.96	0.07	9,10,13,14	5
3	SO4	A	402[B]	5/5	0.96	0.07	11,13,15,15	5
3	SO4	A	404	5/5	0.96	0.10	13,18,26,26	0
3	SO4	A	403	5/5	0.97	0.18	14,16,17,21	0
2	HEM	A	401[A]	43/43	0.99	0.04	6,7,12,15	43
2	HEM	A	401[B]	43/43	0.99	0.04	4,5,5,6	43

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.

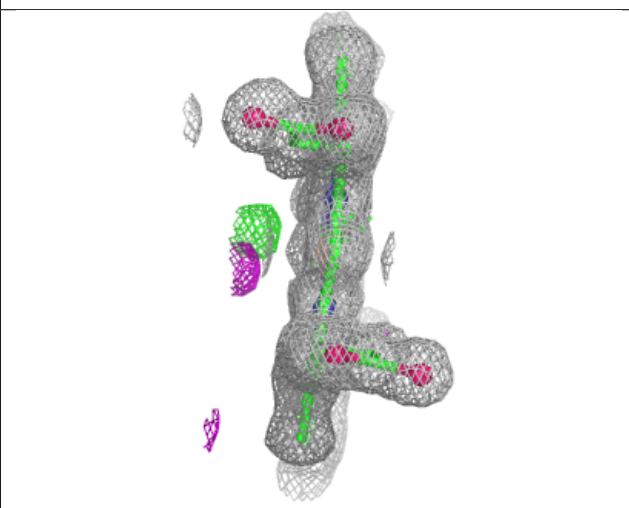
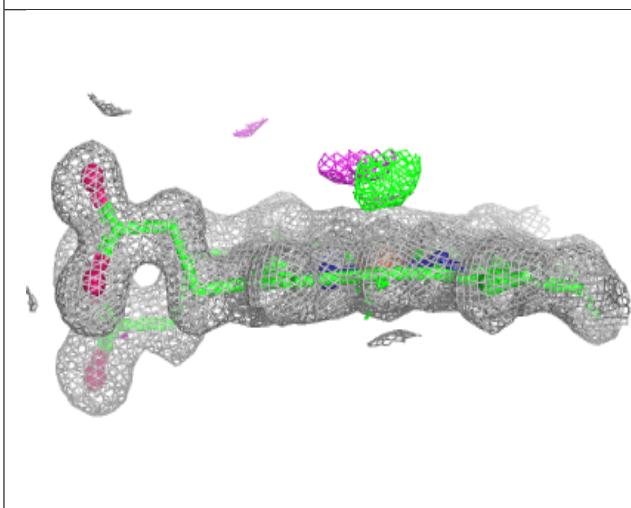
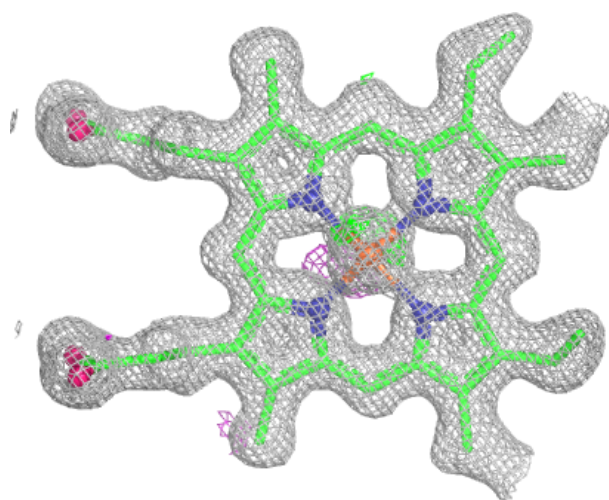
Electron density around HEM A 401 (A):

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 401 (B):

$2mF_o-DF_c$ (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.