



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 07:18 PM EDT

PDB ID : 1PO5
Title : Structure of mammalian cytochrome P450 2B4
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Deposited on : 2003-06-13
Resolution : 1.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

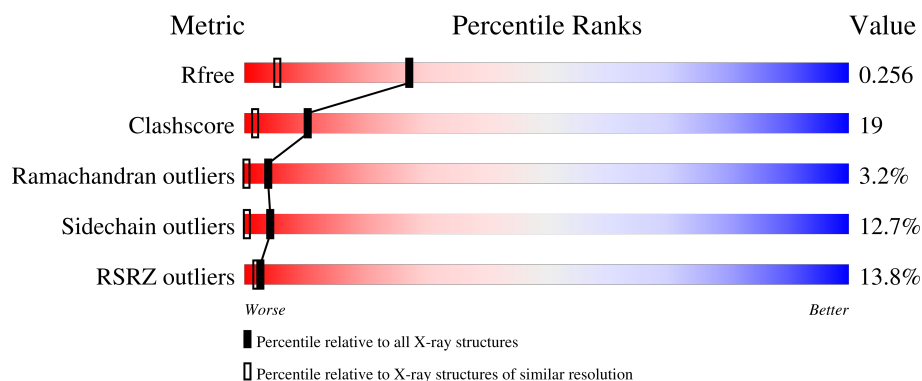
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	476	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4036 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3732	2402	651	668	11			

There are 32 discrepancies between the modelled and reference sequences:

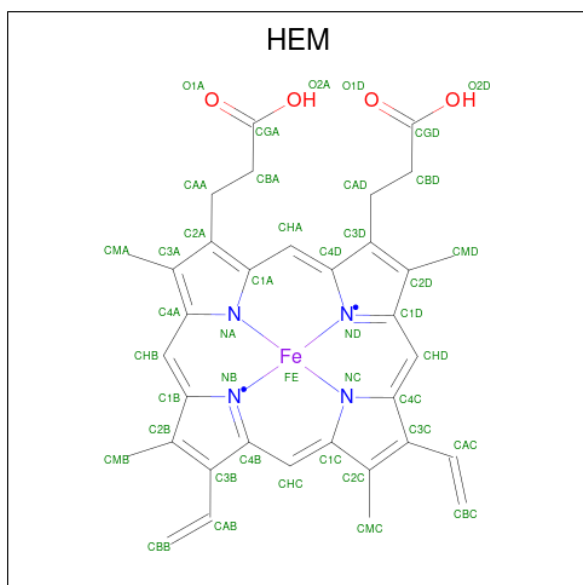
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178

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



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

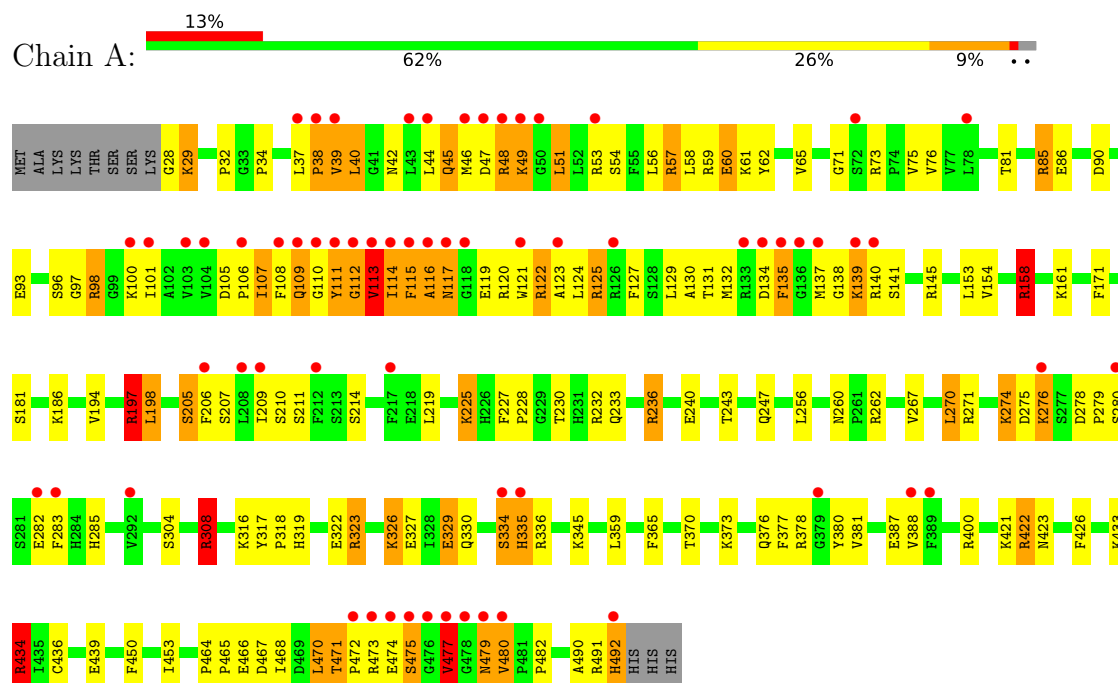
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	261	Total	O		
			261	261	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 2B4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	57.09Å 114.20Å 133.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.70 – 1.60 21.73 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (21.70-1.60) 94.2 (21.73-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.60Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.217 , 0.289 0.192 , 0.256	Depositor DCC
R_{free} test set	2931 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 92.6	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	0.95	EDS
Total number of atoms	4036	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: 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	0.42	0/3826	1.15	22/5178 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ARG	NE-CZ-NH2	10.05	125.33	120.30
1	A	158	ARG	CD-NE-CZ	10.00	137.59	123.60
1	A	434	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	A	38	PRO	C-N-CA	6.95	139.08	121.70
1	A	262	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	A	85	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	85	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	232	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	308	ARG	CD-NE-CZ	6.23	132.32	123.60
1	A	197	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	A	236	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	336	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	378	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	422	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	323	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	317	TYR	CB-CG-CD2	5.50	124.30	121.00
1	A	158	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	450	PHE	O-C-N	-5.37	114.11	122.70
1	A	111	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	135	PHE	CB-CG-CD1	5.11	124.38	120.80
1	A	109	GLN	C-N-CA	5.08	132.96	122.30
1	A	59	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	3732	0	3742	140	0
2	A	43	0	30	2	0
3	A	261	0	0	9	0
All	All	4036	0	3772	140	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 19.

All (140) 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:A:129:LEU:HA	1:A:132:MET:HE3	1.53	0.91
1:A:260:ASN:HB2	3:A:9210:HOH:O	1.72	0.89
1:A:37:LEU:HD23	1:A:38:PRO:HD2	1.67	0.77
1:A:131:THR:HG23	1:A:267:VAL:HG12	1.66	0.76
1:A:335:HIS:HB2	3:A:9075:HOH:O	1.86	0.76
1:A:37:LEU:HD13	1:A:40:LEU:HD11	1.68	0.75
1:A:47:ASP:HB3	1:A:49:LYS:HG2	1.66	0.75
1:A:211:SER:HA	1:A:480:VAL:HG11	1.68	0.73
1:A:243:THR:O	1:A:247:GLN:HG3	1.87	0.73
1:A:37:LEU:HD13	1:A:40:LEU:HD21	1.72	0.71
1:A:194:VAL:HA	1:A:197:ARG:NH1	2.05	0.71
1:A:464:PRO:HG2	1:A:467:ASP:OD2	1.92	0.70
1:A:119:GLU:O	1:A:122:ARG:HG2	1.92	0.68
1:A:171:PHE:HD2	1:A:308:ARG:HG3	1.59	0.68
1:A:326:LYS:HE2	1:A:327:GLU:N	2.09	0.67
1:A:86:GLU:O	1:A:90:ASP:HB2	1.95	0.67
1:A:194:VAL:HG22	1:A:197:ARG:HH12	1.59	0.66
1:A:304:SER:O	1:A:308:ARG:HD3	1.96	0.65
1:A:473:ARG:O	1:A:474:GLU:HB3	1.95	0.65
1:A:125:ARG:HD2	3:A:9160:HOH:O	1.97	0.65
1:A:65:VAL:HG21	1:A:377:PHE:HE2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:HIS:O	1:A:323:ARG:HG3	1.97	0.64
1:A:40:LEU:HA	1:A:71:GLY:HA2	1.79	0.63
1:A:422:ARG:NH1	1:A:423:ASN:H	1.97	0.63
1:A:479:ASN:O	1:A:480:VAL:HB	1.96	0.63
1:A:270:LEU:O	1:A:274:LYS:HG2	1.98	0.63
1:A:28:GLY:HA3	1:A:381:VAL:HG23	1.81	0.63
1:A:194:VAL:HA	1:A:197:ARG:HH12	1.63	0.62
1:A:137:MET:HB2	1:A:139:LYS:HE3	1.82	0.62
1:A:38:PRO:O	1:A:39:VAL:HG22	2.01	0.61
1:A:316:LYS:HD3	1:A:470:LEU:HD11	1.84	0.60
1:A:129:LEU:HD23	1:A:132:MET:CE	2.32	0.60
1:A:434:ARG:HG2	2:A:500:HEM:CGD	2.33	0.59
1:A:112:GLY:O	1:A:113:VAL:HG23	2.03	0.58
1:A:209:ILE:HD13	1:A:480:VAL:HG22	1.86	0.58
1:A:434:ARG:HB2	1:A:434:ARG:NH1	2.19	0.58
1:A:205:SER:O	1:A:206:PHE:HB2	2.04	0.57
1:A:40:LEU:HD23	1:A:44:LEU:HG	1.87	0.56
1:A:120:ARG:O	1:A:123:ALA:HB3	2.05	0.56
1:A:318:PRO:O	1:A:322:GLU:HG3	2.05	0.56
1:A:42:ASN:HD22	1:A:45:GLN:NE2	2.04	0.55
1:A:473:ARG:HD2	1:A:482:PRO:HB3	1.87	0.55
1:A:474:GLU:O	1:A:474:GLU:HG3	2.06	0.55
1:A:171:PHE:CD2	1:A:308:ARG:HG3	2.41	0.55
1:A:129:LEU:HD23	1:A:132:MET:HE1	1.88	0.55
1:A:326:LYS:O	1:A:330:GLN:HG3	2.07	0.55
1:A:28:GLY:HA2	1:A:29:LYS:HE2	1.88	0.55
1:A:197:ARG:NE	1:A:240:GLU:HG3	2.22	0.54
1:A:471:THR:HG22	1:A:472:PRO:HD2	1.90	0.54
1:A:81:THR:O	1:A:85:ARG:HG3	2.09	0.53
1:A:37:LEU:HD23	1:A:38:PRO:CD	2.35	0.52
1:A:51:LEU:HD13	1:A:365:PHE:CZ	2.44	0.52
1:A:154:VAL:O	1:A:158:ARG:HG3	2.09	0.52
1:A:28:GLY:HA3	1:A:381:VAL:CG2	2.39	0.52
1:A:100:LYS:HD2	1:A:370:THR:HG21	1.90	0.52
1:A:400:ARG:HA	1:A:400:ARG:CZ	2.40	0.51
1:A:137:MET:HG3	1:A:138:GLY:H	1.74	0.51
1:A:475:SER:HB2	1:A:477:VAL:O	2.10	0.51
1:A:473:ARG:HD2	1:A:482:PRO:CB	2.40	0.51
1:A:491:ARG:O	1:A:492:HIS:O	2.29	0.51
1:A:278:ASP:OD1	1:A:279:PRO:HD2	2.11	0.50
1:A:308:ARG:HH11	1:A:308:ARG:HG2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HA	1:A:233:GLN:NE2	2.27	0.50
1:A:40:LEU:HD13	1:A:40:LEU:H	1.77	0.49
1:A:42:ASN:HD22	1:A:45:GLN:HE22	1.60	0.49
1:A:120:ARG:HD2	1:A:283:PHE:CE2	2.48	0.49
1:A:115:PHE:O	1:A:116:ALA:O	2.30	0.48
1:A:93:GLU:CD	1:A:433:LYS:HZ2	2.16	0.48
1:A:76:VAL:HB	1:A:388:VAL:HG22	1.95	0.48
1:A:209:ILE:HD13	1:A:480:VAL:CG2	2.44	0.48
1:A:275:ASP:O	1:A:276:LYS:HB2	2.14	0.48
1:A:113:VAL:HG12	1:A:115:PHE:HD2	1.77	0.47
1:A:236:ARG:HG2	1:A:236:ARG:HH11	1.80	0.47
1:A:480:VAL:O	1:A:480:VAL:HG12	2.14	0.47
1:A:466:GLU:HG2	3:A:9131:HOH:O	2.13	0.47
1:A:34:PRO:HD3	1:A:58:LEU:HD22	1.96	0.47
1:A:37:LEU:HD22	1:A:40:LEU:CD1	2.44	0.47
1:A:158:ARG:NH2	1:A:490:ALA:HB1	2.30	0.47
1:A:256:LEU:HD21	1:A:270:LEU:HD13	1.97	0.47
1:A:29:LYS:O	1:A:380:TYR:HB3	2.14	0.47
1:A:114:ILE:O	1:A:114:ILE:HG22	2.15	0.46
1:A:207:SER:HB2	3:A:9046:HOH:O	2.13	0.46
1:A:207:SER:O	1:A:207:SER:OG	2.30	0.46
1:A:32:PRO:HD3	1:A:380:TYR:CZ	2.51	0.46
1:A:73:ARG:HA	1:A:73:ARG:HD3	1.46	0.46
1:A:116:ALA:HB1	1:A:121:TRP:CG	2.50	0.46
1:A:422:ARG:HH22	1:A:426:PHE:HB3	1.81	0.46
1:A:57:ARG:NH1	1:A:60:GLU:OE2	2.49	0.45
1:A:98:ARG:NH2	1:A:434:ARG:HD2	2.31	0.45
1:A:130:ALA:O	1:A:134:ASP:N	2.50	0.45
1:A:96:SER:O	1:A:434:ARG:NH1	2.49	0.45
1:A:129:LEU:HD23	1:A:132:MET:HE3	1.98	0.45
1:A:115:PHE:O	1:A:116:ALA:HB3	2.17	0.44
1:A:105:ASP:HA	1:A:106:PRO:HD2	1.82	0.44
1:A:119:GLU:HG2	1:A:120:ARG:N	2.31	0.44
1:A:145:ARG:HD3	1:A:181:SER:OG	2.17	0.44
1:A:473:ARG:O	1:A:479:ASN:O	2.36	0.44
1:A:137:MET:HB2	1:A:139:LYS:CE	2.47	0.44
1:A:40:LEU:CA	1:A:71:GLY:HA2	2.48	0.44
1:A:131:THR:O	1:A:135:PHE:HB2	2.18	0.44
1:A:274:LYS:N	1:A:274:LYS:HD3	2.32	0.43
1:A:138:GLY:O	1:A:141:SER:N	2.50	0.43
1:A:198:LEU:HG	3:A:9212:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HA	1:A:233:GLN:HE22	1.83	0.43
1:A:113:VAL:HG12	1:A:115:PHE:CD2	2.52	0.43
1:A:439:GLU:HG3	3:A:9135:HOH:O	2.18	0.43
1:A:464:PRO:HA	1:A:465:PRO:HD3	1.85	0.43
1:A:61:LYS:HG2	1:A:62:TYR:CE2	2.54	0.43
1:A:198:LEU:HB2	3:A:9212:HOH:O	2.19	0.43
1:A:326:LYS:HE2	1:A:326:LYS:C	2.39	0.43
1:A:329:GLU:HG3	1:A:330:GLN:N	2.33	0.42
1:A:120:ARG:HB3	1:A:283:PHE:HE2	1.84	0.42
1:A:270:LEU:HD12	1:A:274:LYS:NZ	2.34	0.42
1:A:107:ILE:N	1:A:107:ILE:HD13	2.34	0.42
1:A:145:ARG:NH1	1:A:181:SER:OG	2.52	0.42
1:A:48:ARG:H	1:A:48:ARG:HG2	1.26	0.42
1:A:49:LYS:HE3	1:A:53:ARG:HB3	2.00	0.42
1:A:479:ASN:HB3	1:A:480:VAL:H	1.68	0.42
1:A:37:LEU:HD13	1:A:40:LEU:CD2	2.47	0.42
1:A:227:PHE:HA	1:A:228:PRO:HA	1.81	0.42
1:A:127:PHE:CE2	1:A:271:ARG:HG2	2.55	0.42
1:A:97:GLY:O	1:A:434:ARG:NH2	2.53	0.42
1:A:42:ASN:HD22	1:A:45:GLN:CD	2.23	0.42
1:A:125:ARG:O	1:A:129:LEU:HG	2.20	0.41
1:A:37:LEU:HD13	1:A:40:LEU:CD1	2.45	0.41
1:A:119:GLU:C	1:A:122:ARG:HG2	2.39	0.41
1:A:75:VAL:HG22	1:A:387:GLU:HB3	2.02	0.41
1:A:400:ARG:HA	1:A:400:ARG:NE	2.35	0.41
1:A:434:ARG:NH2	3:A:9080:HOH:O	2.49	0.41
1:A:40:LEU:HD21	1:A:44:LEU:HD12	2.03	0.41
1:A:119:GLU:N	1:A:119:GLU:OE1	2.54	0.41
1:A:141:SER:O	1:A:145:ARG:HG3	2.20	0.41
1:A:225:LYS:HB3	1:A:225:LYS:HE2	1.51	0.41
1:A:436:CYS:HB2	2:A:500:HEM:NA	2.36	0.41
1:A:465:PRO:HA	1:A:468:ILE:HD12	2.03	0.41
1:A:125:ARG:O	1:A:125:ARG:HG3	2.15	0.41
1:A:153:LEU:HD21	1:A:453:ILE:HD11	2.03	0.41
1:A:422:ARG:HA	1:A:422:ARG:HD2	1.75	0.40
1:A:49:LYS:CE	1:A:53:ARG:HB3	2.52	0.40
1:A:106:PRO:O	1:A:108:PHE:N	2.52	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	463/476 (97%)	426 (92%)	22 (5%)	15 (3%)	4 0

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	113	VAL
1	A	117	ASN
1	A	335	HIS
1	A	479	ASN
1	A	112	GLY
1	A	114	ILE
1	A	110	GLY
1	A	116	ALA
1	A	480	VAL
1	A	111	TYR
1	A	475	SER
1	A	334	SER
1	A	477	VAL
1	A	107	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	411/421 (98%)	359 (87%)	52 (13%)	4 0

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	40	LEU
1	A	45	GLN
1	A	46	MET
1	A	48	ARG
1	A	49	LYS
1	A	51	LEU
1	A	54	SER
1	A	56	LEU
1	A	57	ARG
1	A	60	GLU
1	A	98	ARG
1	A	101	ILE
1	A	109	GLN
1	A	113	VAL
1	A	115	PHE
1	A	117	ASN
1	A	122	ARG
1	A	124	LEU
1	A	125	ARG
1	A	139	LYS
1	A	140	ARG
1	A	158	ARG
1	A	161	LYS
1	A	186	LYS
1	A	197	ARG
1	A	198	LEU
1	A	205	SER
1	A	210	SER
1	A	214	SER
1	A	219	LEU
1	A	225	LYS
1	A	270	LEU
1	A	274	LYS
1	A	276	LYS
1	A	280	SER
1	A	282	GLU
1	A	285	HIS
1	A	308	ARG
1	A	326	LYS
1	A	329	GLU
1	A	334	SER

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Mol	Chain	Res	Type
1	A	345	LYS
1	A	359	LEU
1	A	373	LYS
1	A	376	GLN
1	A	421	LYS
1	A	434	ARG
1	A	470	LEU
1	A	471	THR
1	A	477	VAL
1	A	492	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	242	ASN
1	A	260	ASN
1	A	492	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	500	1	27,50,50	1.57	6 (22%)	17,82,82	1.30	4 (23%)

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	A	500	1	-	0/6/54/54	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-CAC	-3.69	1.40	1.47
2	A	500	HEM	CBB-CAB	2.79	1.47	1.29
2	A	500	HEM	CMA-C3A	2.75	1.57	1.51
2	A	500	HEM	C1D-ND	-2.54	1.30	1.36
2	A	500	HEM	C1D-CHD	-2.12	1.35	1.41
2	A	500	HEM	CAD-C3D	2.09	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	CAA-CBA-CGA	-2.54	108.41	112.67
2	A	500	HEM	CMB-C2B-C3B	2.39	129.15	124.68
2	A	500	HEM	CMD-C2D-C1D	-2.13	125.18	128.46
2	A	500	HEM	C4A-C3A-C2A	-2.07	105.56	107.00

There are no chirality outliers.

There are no torsion outliers.

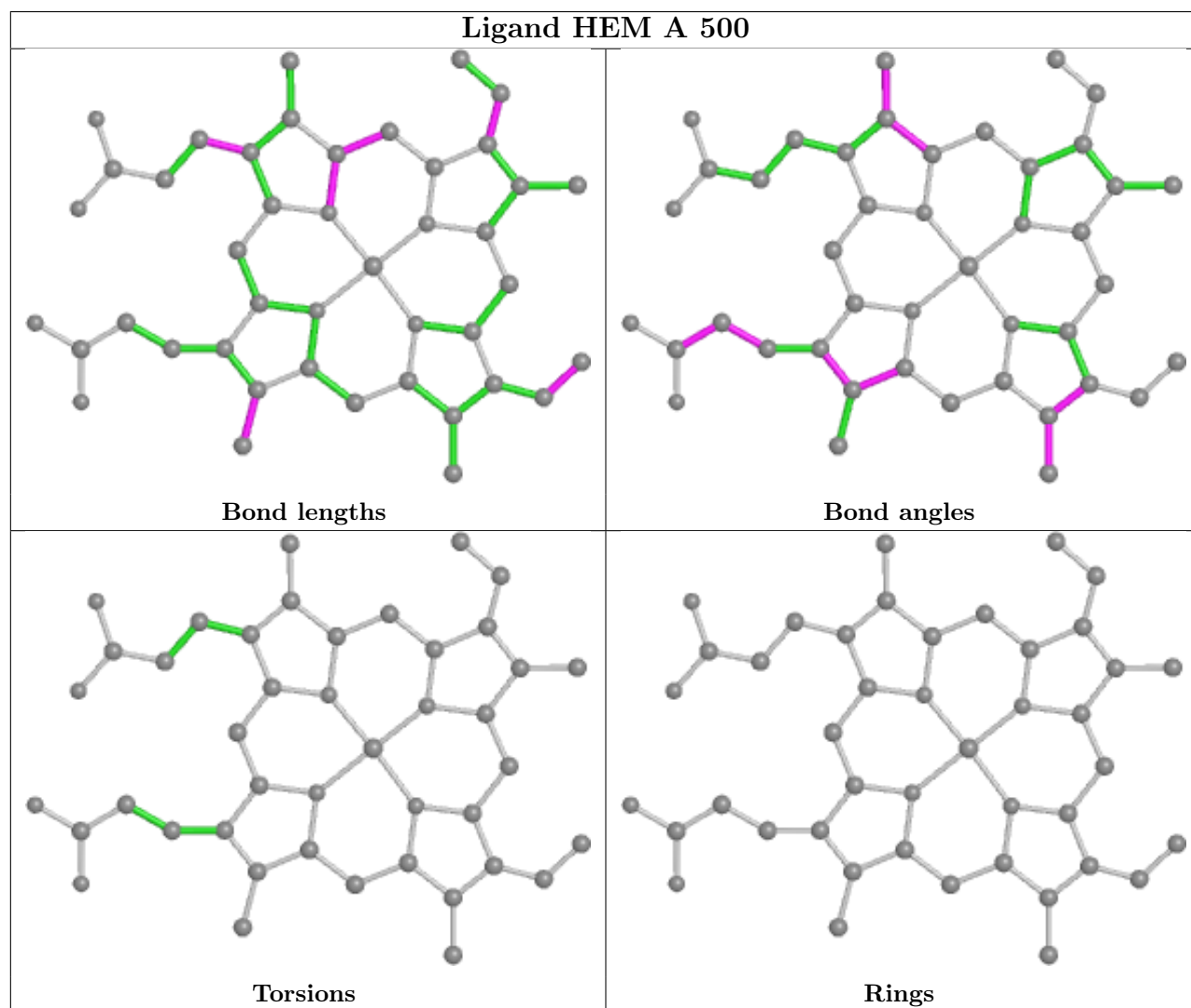
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/476 (97%)	0.65	64 (13%) 2 2	10, 25, 77, 136	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ALA	16.3
1	A	114	ILE	12.2
1	A	115	PHE	11.5
1	A	117	ASN	9.0
1	A	113	VAL	8.8
1	A	111	TYR	8.5
1	A	137	MET	8.4
1	A	476	GLY	8.0
1	A	39	VAL	6.4
1	A	474	GLU	6.3
1	A	475	SER	5.9
1	A	118	GLY	5.7
1	A	283	PHE	5.7
1	A	136	GLY	5.6
1	A	477	VAL	5.3
1	A	473	ARG	5.3
1	A	109	GLN	5.2
1	A	108	PHE	5.1
1	A	104	VAL	4.6
1	A	103	VAL	4.6
1	A	480	VAL	4.5
1	A	48	ARG	4.3
1	A	478	GLY	4.2
1	A	135	PHE	4.1
1	A	101	ILE	4.1
1	A	134	ASP	3.8
1	A	388	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	3.6
1	A	49	LYS	3.5
1	A	335	HIS	3.5
1	A	334	SER	3.5
1	A	206	PHE	3.4
1	A	212	PHE	3.3
1	A	139	LYS	3.3
1	A	472	PRO	3.2
1	A	47	ASP	3.0
1	A	209	ILE	3.0
1	A	44	LEU	2.9
1	A	46	MET	2.8
1	A	121	TRP	2.8
1	A	389	PHE	2.8
1	A	37	LEU	2.8
1	A	282	GLU	2.7
1	A	100	LYS	2.7
1	A	479	ASN	2.7
1	A	123	ALA	2.6
1	A	112	GLY	2.6
1	A	38	PRO	2.6
1	A	106	PRO	2.6
1	A	72	SER	2.5
1	A	53	ARG	2.5
1	A	43	LEU	2.5
1	A	208	LEU	2.4
1	A	492	HIS	2.4
1	A	292	VAL	2.4
1	A	133	ARG	2.4
1	A	217	PHE	2.3
1	A	126	ARG	2.3
1	A	140	ARG	2.3
1	A	276	LYS	2.2
1	A	280	SER	2.2
1	A	78	LEU	2.1
1	A	379	GLY	2.0
1	A	50	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

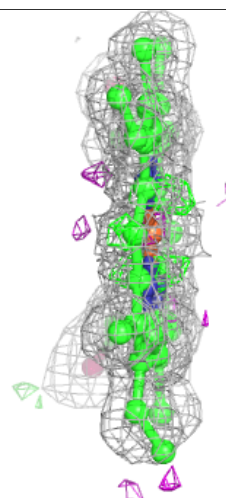
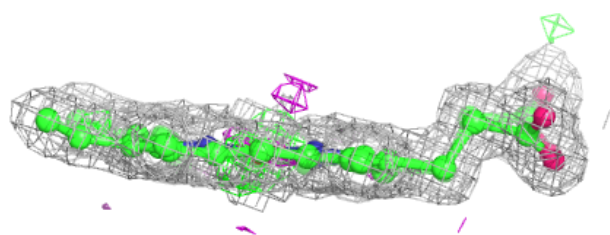
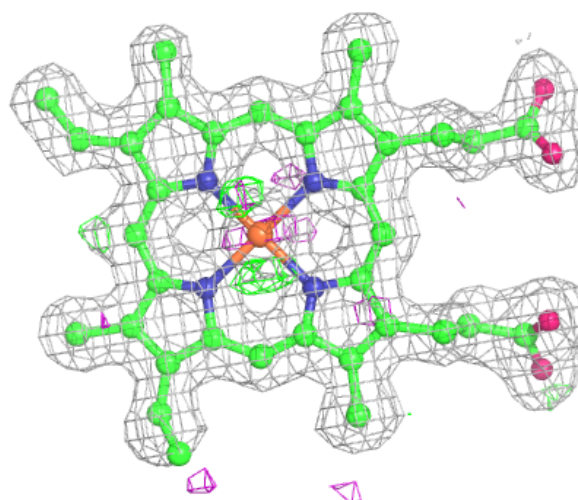
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	500	43/43	0.98	0.08	8,13,24,35	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 500:

$2mF_o-DF_c$ (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.