



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1W0E / pdb_00001w0e
Title : Crystal structure of human cytochrome P450 3A4
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Deposited on : 2004-06-03
Resolution : 2.80 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

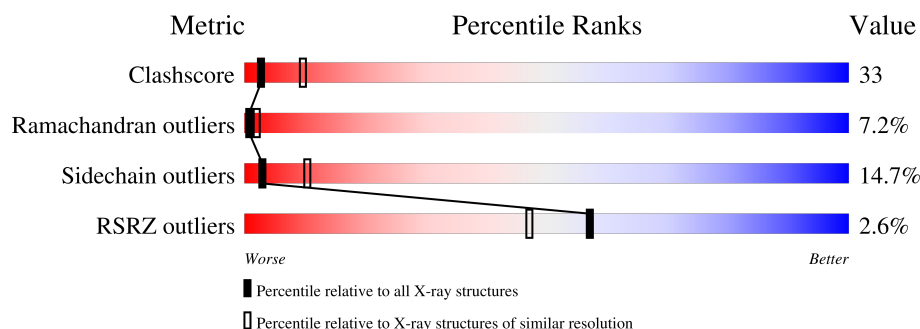
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	485	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3688 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.

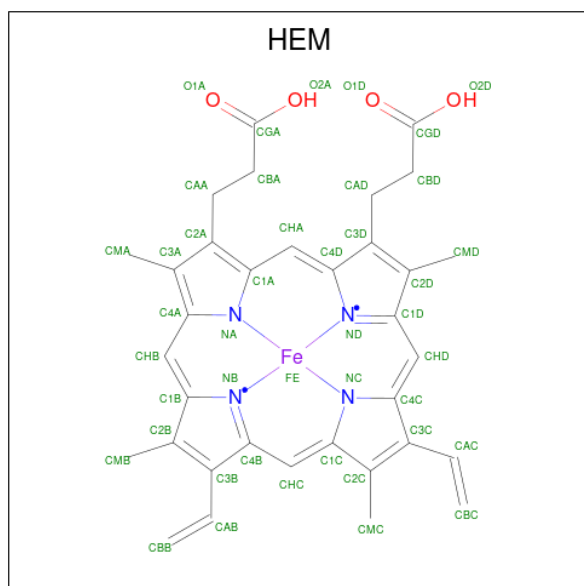
- Molecule 1 is a protein called CYTOCHROME P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	3
			3617	2358	595	640	24			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	VAL	TRP	conflict	UNP P08684

- 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		

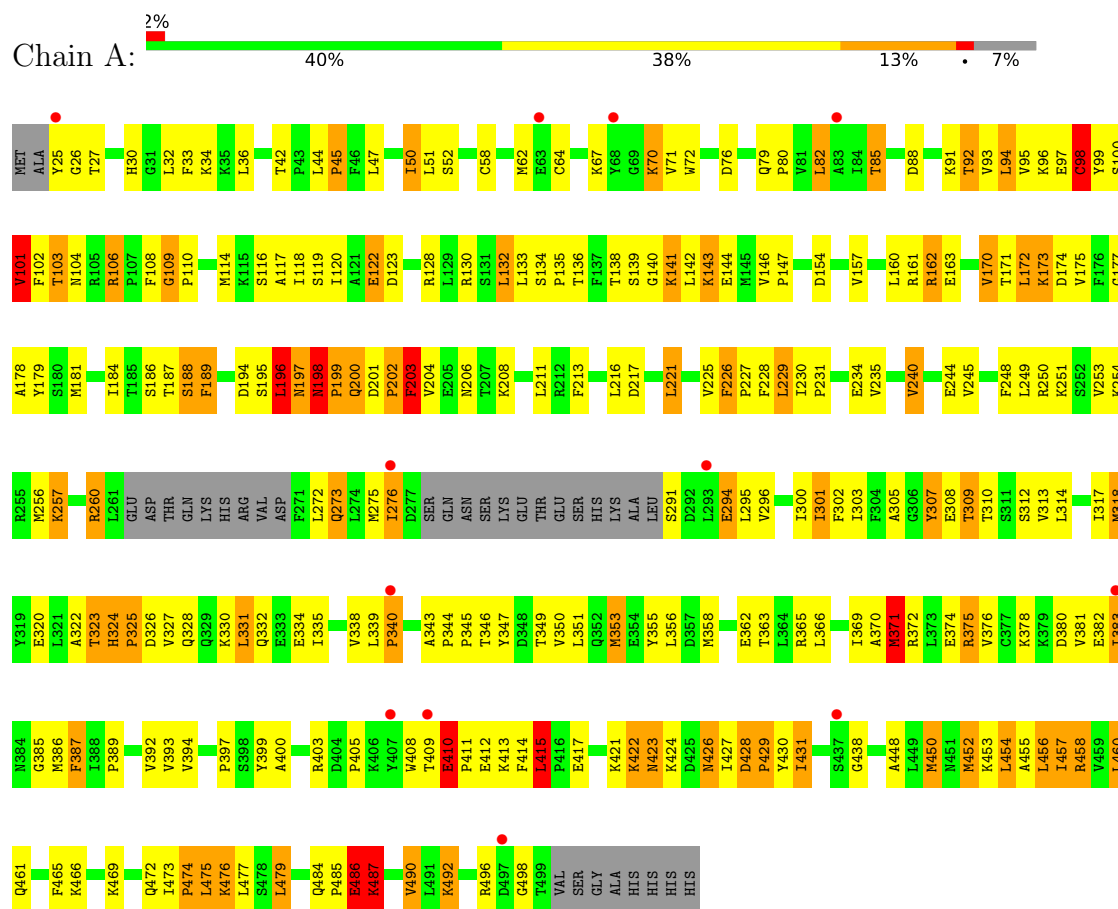
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	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 3A4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.94Å 100.91Å 131.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 2.80 79.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (200.00-2.80) 95.2 (79.94-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.82Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.244 , 0.274 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3688	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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	0.52	2/3707 (0.1%)	1.29	39/5017 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	GLY	C-N	-5.32	1.25	1.33
1	A	260	ARG	C-N	-5.20	1.26	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ILE	CA-C-O	23.93	161.48	120.80
1	A	276	ILE	CA-C-N	-23.17	69.86	116.20
1	A	276	ILE	O-C-N	-18.23	93.83	123.00
1	A	423	ASN	N-CA-C	-11.17	100.14	113.88
1	A	426	ASN	N-CA-C	-10.07	97.97	113.89
1	A	50	ILE	N-CA-C	9.16	119.22	110.42
1	A	415	LEU	CA-C-N	8.79	130.83	119.84
1	A	415	LEU	C-N-CA	8.79	130.83	119.84
1	A	410	GLU	CA-C-N	8.64	128.38	119.56
1	A	410	GLU	C-N-CA	8.64	128.38	119.56
1	A	141	LYS	N-CA-C	-8.44	102.98	113.28
1	A	294	GLU	N-CA-C	-8.37	101.93	112.90
1	A	429	PRO	N-CA-C	-7.89	96.22	112.47
1	A	431	ILE	N-CA-C	-6.99	104.91	111.48
1	A	67	LYS	N-CA-C	6.97	118.56	110.97
1	A	123	ASP	CB-CA-C	-6.77	108.75	116.54
1	A	42	THR	CA-C-N	6.54	127.08	120.14
1	A	42	THR	C-N-CA	6.54	127.08	120.14
1	A	200	GLN	N-CA-C	6.54	120.72	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	GLU	N-CA-C	-6.53	96.90	110.80
1	A	123	ASP	N-CA-C	6.29	117.88	108.31
1	A	199	PRO	N-CA-C	-6.29	103.99	112.48
1	A	257	LYS	N-CA-C	-6.24	104.59	111.82
1	A	226	PHE	CA-C-N	6.07	125.77	119.82
1	A	226	PHE	C-N-CA	6.07	125.77	119.82
1	A	428	ASP	N-CA-C	6.03	117.24	109.65
1	A	275	MET	N-CA-C	-6.01	104.81	111.36
1	A	203	PHE	N-CA-C	-5.95	103.79	113.19
1	A	170	VAL	N-CA-C	5.85	118.36	109.12
1	A	139	SER	N-CA-C	-5.84	101.19	109.96
1	A	198	ASN	CA-C-N	-5.79	110.92	120.88
1	A	198	ASN	C-N-CA	-5.79	110.92	120.88
1	A	34	LYS	N-CA-C	-5.77	105.01	112.68
1	A	186	SER	N-CA-C	5.67	118.23	111.71
1	A	487	LYS	N-CA-C	-5.34	98.00	109.81
1	A	44	LEU	CA-C-N	5.32	126.49	119.84
1	A	44	LEU	C-N-CA	5.32	126.49	119.84
1	A	122	GLU	N-CA-C	5.25	117.67	109.52
1	A	325	PRO	N-CA-C	-5.14	107.16	113.84

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	3617	0	3691	246	0
2	A	43	0	30	2	0
3	A	28	0	0	1	0
All	All	3688	0	3721	246	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 33.

All (246) 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:339:LEU:HB3	1:A:343:ALA:HB3	1.44	0.97
1:A:382:GLU:HA	1:A:387:PHE:HA	1.55	0.88
1:A:97:GLU:HA	1:A:100:SER:HB3	1.57	0.87
1:A:355:TYR:HA	1:A:358:MET:HE3	1.56	0.87
1:A:421:LYS:HA	1:A:424:LYS:HB3	1.56	0.85
1:A:162:ARG:HG3	1:A:163:GLU:N	1.91	0.84
1:A:154:ASP:O	1:A:157:VAL:HG22	1.77	0.83
1:A:479:LEU:H	1:A:479:LEU:HD23	1.43	0.83
1:A:485:PRO:O	1:A:486:GLU:HB3	1.79	0.81
1:A:162:ARG:HG3	1:A:163:GLU:H	1.46	0.80
1:A:202:PRO:HG2	1:A:203:PHE:H	1.47	0.79
1:A:339:LEU:HD21	1:A:349:THR:HG21	1.63	0.78
1:A:221:LEU:O	1:A:225:VAL:HG23	1.85	0.77
1:A:317:ILE:HG13	1:A:363:THR:HG21	1.69	0.75
1:A:323:THR:O	1:A:323:THR:HG23	1.85	0.74
1:A:345:PRO:HG3	1:A:457:ILE:HG21	1.69	0.74
1:A:226:PHE:HB2	1:A:229:LEU:HD22	1.69	0.73
1:A:250:ARG:HG3	1:A:296:VAL:HG11	1.70	0.73
1:A:324:HIS:N	1:A:325:PRO:CD	2.52	0.72
1:A:228:PHE:O	1:A:231:PRO:HD2	1.92	0.70
1:A:324:HIS:H	1:A:325:PRO:CD	2.03	0.69
1:A:339:LEU:CD2	1:A:349:THR:HG21	2.21	0.69
1:A:291:SER:HB3	1:A:294:GLU:HG3	1.74	0.68
1:A:62:MET:SD	1:A:400:ALA:HA	2.33	0.68
1:A:479:LEU:HD23	1:A:479:LEU:N	2.09	0.68
1:A:410:GLU:N	1:A:411:PRO:HD3	2.10	0.67
1:A:320:GLU:O	1:A:324:HIS:HB2	1.95	0.67
1:A:273:GLN:O	1:A:276:ILE:HG22	1.96	0.66
1:A:102:PHE:HB3	1:A:375:ARG:HG2	1.78	0.65
1:A:76:ASP:OD2	1:A:106:ARG:NH1	2.30	0.64
1:A:226:PHE:O	1:A:229:LEU:HD22	1.98	0.63
1:A:429:PRO:O	1:A:430:TYR:HB2	1.98	0.63
1:A:97:GLU:O	1:A:99:TYR:N	2.32	0.63
1:A:178:ALA:HB1	1:A:196:LEU:HG	1.79	0.63
1:A:62:MET:HE1	1:A:403:ARG:HB2	1.80	0.62
1:A:249:LEU:O	1:A:253:VAL:HG23	2.01	0.61
1:A:64:CYS:HB3	1:A:72:TRP:CE2	2.36	0.61
1:A:188:SER:HB3	1:A:189:PHE:CE1	2.36	0.61
1:A:370:ALA:O	1:A:372:ARG:N	2.34	0.61
1:A:225:VAL:HG12	1:A:226:PHE:CE2	2.36	0.61
1:A:101:VAL:O	1:A:378:LYS:HB2	2.02	0.60
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:CYS:SG	1:A:371:MET:HG2	2.42	0.59
1:A:108:PHE:O	1:A:109:GLY:O	2.21	0.59
1:A:140:GLY:HA2	1:A:143:LYS:HG2	1.85	0.58
1:A:198:ASN:HB2	1:A:199:PRO:HD2	1.85	0.58
1:A:320:GLU:OE2	1:A:320:GLU:HA	2.04	0.57
1:A:301:ILE:HG22	1:A:302:PHE:N	2.18	0.57
1:A:330:LYS:HB3	1:A:355:TYR:CE1	2.39	0.57
1:A:181:MET:HE1	1:A:208:LYS:CB	2.34	0.57
1:A:422:LYS:HG3	1:A:423:ASN:OD1	2.05	0.56
1:A:473:ILE:HA	1:A:474:PRO:O	2.05	0.56
1:A:50:ILE:O	1:A:52:SER:N	2.38	0.56
1:A:355:TYR:CA	1:A:358:MET:HE3	2.33	0.56
1:A:476:LYS:O	1:A:485:PRO:O	2.22	0.56
1:A:114:MET:C	1:A:116:SER:H	2.14	0.56
1:A:194:ASP:HB3	1:A:199:PRO:HD2	1.87	0.56
1:A:328:GLN:O	1:A:332:GLN:HG3	2.05	0.56
1:A:70:LYS:O	1:A:85:THR:HB	2.05	0.56
1:A:475:LEU:O	1:A:476:LYS:HB2	2.06	0.56
1:A:181:MET:HE1	1:A:208:LYS:HB2	1.88	0.56
1:A:429:PRO:C	1:A:431:ILE:H	2.11	0.56
1:A:200:GLN:HG3	1:A:201:ASP:OD2	2.06	0.55
1:A:318:MET:HE2	1:A:465:PHE:CE2	2.41	0.55
1:A:102:PHE:CE2	1:A:394:VAL:HG21	2.41	0.55
1:A:339:LEU:O	1:A:340:PRO:O	2.23	0.55
1:A:202:PRO:CG	1:A:203:PHE:H	2.18	0.55
1:A:204:VAL:HG12	1:A:208:LYS:HE3	1.89	0.55
1:A:485:PRO:O	1:A:486:GLU:CB	2.52	0.55
1:A:356:LEU:HD22	1:A:457:ILE:HD11	1.89	0.54
1:A:486:GLU:O	1:A:487:LYS:CB	2.54	0.54
1:A:119:SER:HB3	2:A:1501:HEM:HAD1	1.89	0.54
1:A:146:VAL:HB	1:A:147:PRO:HD3	1.89	0.54
1:A:226:PHE:HB2	1:A:229:LEU:CD2	2.38	0.54
1:A:181:MET:HE1	1:A:208:LYS:CA	2.38	0.53
1:A:196:LEU:O	1:A:198:ASN:N	2.40	0.53
1:A:317:ILE:CG1	1:A:363:THR:HG21	2.35	0.53
1:A:97:GLU:OE2	1:A:97:GLU:C	2.52	0.53
1:A:458:ARG:NH2	1:A:461:GLN:HE21	2.07	0.53
1:A:225:VAL:C	1:A:226:PHE:CD2	2.87	0.53
1:A:408:TRP:O	1:A:411:PRO:HG3	2.09	0.53
1:A:181:MET:HE1	1:A:208:LYS:HA	1.91	0.52
1:A:203:PHE:O	1:A:203:PHE:CD1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASN:CB	1:A:199:PRO:CD	2.87	0.52
1:A:110:PRO:HB3	1:A:234:GLU:HG3	1.91	0.52
1:A:27:THR:HG22	1:A:30:HIS:CE1	2.45	0.52
1:A:273:GLN:C	1:A:276:ILE:HG22	2.35	0.52
1:A:324:HIS:H	1:A:325:PRO:HD3	1.72	0.51
1:A:472:GLN:O	1:A:473:ILE:HG13	2.10	0.51
1:A:305:ALA:O	1:A:309:THR:HG21	2.11	0.51
1:A:334:GLU:OE1	1:A:355:TYR:HB2	2.10	0.51
1:A:322:ALA:O	1:A:323:THR:HG22	2.11	0.51
1:A:429:PRO:HG2	1:A:430:TYR:CD1	2.46	0.51
1:A:334:GLU:O	1:A:338:VAL:HG23	2.11	0.51
1:A:94:LEU:O	1:A:438:GLY:HA3	2.11	0.51
1:A:93:VAL:HG23	1:A:94:LEU:HD13	1.92	0.50
1:A:162:ARG:CG	1:A:163:GLU:N	2.70	0.50
1:A:332:GLN:NE2	1:A:496:ARG:HD2	2.25	0.50
1:A:79:GLN:NE2	1:A:80:PRO:HD2	2.26	0.50
1:A:194:ASP:O	1:A:195:SER:C	2.53	0.50
1:A:106:ARG:HG3	1:A:393:VAL:HG21	1.94	0.50
1:A:429:PRO:O	1:A:430:TYR:CB	2.56	0.50
1:A:296:VAL:O	1:A:300:ILE:HG13	2.11	0.50
1:A:492:LYS:NZ	1:A:492:LYS:HB3	2.27	0.50
1:A:198:ASN:HB2	1:A:199:PRO:CD	2.42	0.49
1:A:26:GLY:O	1:A:45:PRO:O	2.30	0.49
1:A:117:ALA:HB3	1:A:120:ILE:HG12	1.94	0.49
1:A:146:VAL:HG21	1:A:347:TYR:HB2	1.92	0.49
1:A:184:ILE:O	1:A:188:SER:HB2	2.11	0.49
1:A:327:VAL:HG13	1:A:355:TYR:OH	2.12	0.49
1:A:330:LYS:HD3	1:A:355:TYR:CZ	2.48	0.49
1:A:194:ASP:O	1:A:199:PRO:HD2	2.12	0.49
1:A:101:VAL:HG22	1:A:102:PHE:N	2.26	0.49
1:A:335:ILE:HG12	1:A:353:MET:CE	2.42	0.49
1:A:27:THR:CG2	1:A:45:PRO:HA	2.42	0.49
1:A:323:THR:O	1:A:323:THR:CG2	2.57	0.49
1:A:323:THR:O	1:A:324:HIS:CG	2.65	0.49
1:A:188:SER:HB3	1:A:189:PHE:CD1	2.47	0.49
1:A:202:PRO:HD2	1:A:204:VAL:HB	1.94	0.48
1:A:350:VAL:HG21	1:A:450:MET:HE1	1.95	0.48
1:A:118:ILE:HD11	1:A:130:ARG:HA	1.95	0.48
1:A:93:VAL:O	1:A:97:GLU:HG2	2.13	0.48
1:A:198:ASN:O	1:A:200:GLN:N	2.43	0.48
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HG2	1:A:203:PHE:N	2.23	0.48
1:A:64:CYS:HB3	1:A:72:TRP:NE1	2.28	0.48
1:A:179:TYR:CE1	1:A:455:ALA:HB2	2.48	0.48
1:A:295:LEU:HD23	1:A:295:LEU:C	2.39	0.48
1:A:199:PRO:O	1:A:202:PRO:HD3	2.14	0.48
1:A:332:GLN:HE22	1:A:496:ARG:HD2	1.78	0.47
1:A:92:THR:HA	1:A:96:LYS:HG2	1.96	0.47
1:A:173:LYS:NZ	1:A:312:SER:HB2	2.29	0.47
1:A:225:VAL:CG1	1:A:226:PHE:CE2	2.97	0.47
1:A:102:PHE:O	1:A:103:THR:OG1	2.28	0.47
1:A:198:ASN:C	1:A:200:GLN:N	2.72	0.47
1:A:323:THR:O	1:A:324:HIS:ND1	2.47	0.47
1:A:146:VAL:O	1:A:147:PRO:C	2.58	0.47
1:A:291:SER:HB3	1:A:294:GLU:CG	2.42	0.47
1:A:350:VAL:HB	1:A:450:MET:HE1	1.97	0.47
1:A:370:ALA:O	1:A:371:MET:C	2.57	0.47
1:A:198:ASN:C	1:A:200:GLN:H	2.21	0.47
1:A:226:PHE:HB3	1:A:228:PHE:CE2	2.50	0.47
1:A:475:LEU:CG	1:A:476:LYS:H	2.28	0.47
1:A:162:ARG:NH1	1:A:162:ARG:HG2	2.28	0.47
1:A:486:GLU:O	1:A:487:LYS:HB3	2.14	0.47
1:A:308:GLU:O	1:A:312:SER:HB2	2.15	0.47
1:A:250:ARG:CG	1:A:296:VAL:HG11	2.40	0.47
1:A:163:GLU:HB3	1:A:170:VAL:HG22	1.97	0.47
1:A:135:PRO:O	1:A:141:LYS:HD2	2.15	0.46
1:A:58:CYS:HB3	1:A:399:TYR:CD1	2.49	0.46
1:A:62:MET:HE1	1:A:403:ARG:CB	2.45	0.46
1:A:213:PHE:CZ	1:A:240:VAL:HG13	2.50	0.46
1:A:365:ARG:NH2	1:A:366:LEU:HD21	2.30	0.46
1:A:428:ASP:C	1:A:429:PRO:O	2.53	0.46
1:A:135:PRO:O	1:A:138:THR:HG23	2.14	0.46
1:A:428:ASP:OD2	1:A:429:PRO:HD2	2.16	0.46
1:A:50:ILE:C	1:A:52:SER:N	2.74	0.46
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.81	0.46
1:A:225:VAL:C	1:A:227:PRO:HD3	2.41	0.46
1:A:173:LYS:HZ1	1:A:308:GLU:HG2	1.81	0.46
1:A:197:ASN:HA	1:A:200:GLN:HB3	1.97	0.46
1:A:71:VAL:HG13	1:A:82:LEU:HD21	1.98	0.45
1:A:170:VAL:HG12	1:A:171:THR:N	2.31	0.45
1:A:184:ILE:CG2	1:A:303:ILE:HG12	2.47	0.45
1:A:323:THR:H	1:A:325:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TRP:CH2	1:A:427:ILE:HG21	2.52	0.45
1:A:475:LEU:HD12	1:A:476:LYS:N	2.32	0.45
1:A:184:ILE:HG23	1:A:303:ILE:HG12	1.99	0.45
1:A:181:MET:CE	1:A:208:LYS:HB2	2.46	0.45
1:A:389:PRO:HG2	1:A:392:VAL:CG2	2.47	0.45
1:A:101:VAL:O	1:A:378:LYS:HE2	2.16	0.45
1:A:409:THR:O	1:A:410:GLU:C	2.60	0.45
1:A:206:ASN:HB3	1:A:245:VAL:HG13	1.99	0.45
1:A:383:ILE:O	1:A:383:ILE:HG22	2.17	0.44
1:A:170:VAL:O	1:A:490:VAL:HA	2.18	0.44
1:A:429:PRO:C	1:A:431:ILE:N	2.74	0.44
1:A:324:HIS:CD2	1:A:414:PHE:HD2	2.36	0.44
1:A:140:GLY:CA	1:A:143:LYS:HG2	2.46	0.44
1:A:50:ILE:C	1:A:52:SER:H	2.26	0.44
1:A:350:VAL:CB	1:A:450:MET:HE1	2.47	0.44
1:A:453:LYS:O	1:A:454:LEU:C	2.60	0.44
1:A:452:MET:O	1:A:456:LEU:HD22	2.18	0.44
1:A:143:LYS:HB2	1:A:143:LYS:NZ	2.32	0.43
1:A:320:GLU:C	1:A:322:ALA:H	2.26	0.43
1:A:344:PRO:HA	1:A:345:PRO:HD3	1.91	0.43
1:A:350:VAL:CG2	1:A:450:MET:HE1	2.49	0.43
1:A:134:SER:N	1:A:135:PRO:CD	2.81	0.43
1:A:136:THR:O	1:A:136:THR:HG22	2.18	0.43
1:A:108:PHE:N	1:A:108:PHE:CD2	2.86	0.43
1:A:260:ARG:HE	1:A:273:GLN:HG2	1.84	0.43
1:A:475:LEU:HG	1:A:476:LYS:H	1.83	0.43
1:A:114:MET:C	1:A:116:SER:N	2.73	0.43
1:A:117:ALA:HB1	1:A:301:ILE:CG1	2.49	0.43
1:A:189:PHE:CD1	1:A:189:PHE:N	2.86	0.43
1:A:410:GLU:N	1:A:411:PRO:CD	2.81	0.42
1:A:309:THR:CG2	1:A:310:THR:N	2.80	0.42
1:A:428:ASP:O	1:A:431:ILE:HB	2.19	0.42
1:A:347:TYR:CD1	1:A:347:TYR:C	2.97	0.42
1:A:350:VAL:HG11	1:A:450:MET:HE2	1.99	0.42
1:A:313:VAL:HG21	2:A:1501:HEM:HBB2	2.00	0.42
1:A:314:LEU:HG	1:A:452:MET:HG2	2.00	0.42
1:A:27:THR:HG22	1:A:45:PRO:HA	2.01	0.42
1:A:101:VAL:O	1:A:378:LYS:CB	2.67	0.42
1:A:217:ASP:OD2	1:A:217:ASP:C	2.62	0.42
1:A:173:LYS:HZ1	1:A:312:SER:HB2	1.84	0.42
1:A:134:SER:HB2	1:A:135:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PHE:CD1	1:A:203:PHE:C	2.98	0.42
1:A:382:GLU:O	1:A:383:ILE:HB	2.19	0.42
1:A:162:ARG:HG2	1:A:162:ARG:HH11	1.84	0.42
1:A:177:GLY:O	1:A:307:TYR:HE2	2.03	0.42
1:A:98:CYS:C	1:A:100:SER:H	2.27	0.41
1:A:128:ARG:O	1:A:132:LEU:HB2	2.20	0.41
1:A:203:PHE:O	1:A:203:PHE:CG	2.73	0.41
1:A:25:TYR:C	1:A:27:THR:H	2.27	0.41
1:A:421:LYS:O	1:A:422:LYS:HB3	2.21	0.41
1:A:324:HIS:C	1:A:326:ASP:N	2.77	0.41
1:A:346:THR:HG22	1:A:347:TYR:N	2.34	0.41
1:A:474:PRO:HB2	1:A:475:LEU:H	1.72	0.41
1:A:172:LEU:O	1:A:174:ASP:N	2.54	0.41
1:A:230:ILE:N	1:A:231:PRO:CD	2.84	0.41
1:A:228:PHE:CE1	1:A:229:LEU:HD13	2.55	0.41
1:A:318:MET:HE2	1:A:465:PHE:CD2	2.55	0.41
1:A:171:THR:CG2	1:A:174:ASP:OD2	2.69	0.41
1:A:142:LEU:C	1:A:144:GLU:N	2.75	0.41
1:A:254:LYS:HD2	1:A:254:LYS:HA	1.90	0.41
1:A:104:ASN:HB3	1:A:122:GLU:HG2	2.02	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.85	0.41
1:A:228:PHE:CE1	1:A:229:LEU:CD1	3.04	0.41
1:A:351:LEU:N	1:A:351:LEU:HD23	2.33	0.41
1:A:371:MET:HE3	1:A:371:MET:HB2	1.90	0.41
1:A:362:GLU:HG3	1:A:414:PHE:CD1	2.56	0.41
1:A:448:ALA:O	1:A:452:MET:HE3	2.20	0.41
1:A:382:GLU:HG3	1:A:387:PHE:N	2.36	0.40
1:A:91:LYS:O	1:A:95:VAL:HB	2.20	0.40
1:A:272:LEU:CD2	1:A:295:LEU:HD21	2.50	0.40
1:A:331:LEU:HD13	1:A:460:LEU:HG	2.02	0.40
1:A:133:LEU:O	1:A:136:THR:HB	2.21	0.40
1:A:170:VAL:CG1	1:A:171:THR:N	2.84	0.40
1:A:221:LEU:HD12	1:A:221:LEU:HA	1.80	0.40
1:A:413:LYS:HB3	1:A:415:LEU:HD23	2.03	0.40
1:A:70:LYS:HG3	1:A:71:VAL:N	2.35	0.40
1:A:82:LEU:C	1:A:82:LEU:CD2	2.94	0.40
1:A:203:PHE:CD2	1:A:248:PHE:HE1	2.39	0.40
1:A:244:GLU:HB2	3:A:2017:HOH:O	2.21	0.40
1:A:251:LYS:N	1:A:251:LYS:HD2	2.36	0.40
1:A:307:TYR:C	1:A:309:THR:N	2.80	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	447/485 (92%)	370 (83%)	45 (10%)	32 (7%)	1 2

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	109	GLY
1	A	196	LEU
1	A	197	ASN
1	A	198	ASN
1	A	202	PRO
1	A	307	TYR
1	A	323	THR
1	A	340	PRO
1	A	371	MET
1	A	422	LYS
1	A	474	PRO
1	A	51	LEU
1	A	101	VAL
1	A	103	THR
1	A	132	LEU
1	A	385	GLY
1	A	386	MET
1	A	457	ILE
1	A	469	LYS
1	A	32	LEU
1	A	173	LYS
1	A	324	HIS
1	A	387	PHE
1	A	417	GLU
1	A	33	PHE
1	A	397	PRO
1	A	486	GLU

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Mol	Chain	Res	Type
1	A	172	LEU
1	A	383	ILE
1	A	487	LYS
1	A	369	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	408/441 (92%)	348 (85%)	60 (15%)	3 10

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	45	PRO
1	A	70	LYS
1	A	82	LEU
1	A	85	THR
1	A	88	ASP
1	A	92	THR
1	A	94	LEU
1	A	98	CYS
1	A	101	VAL
1	A	106	ARG
1	A	143	LYS
1	A	160	LEU
1	A	162	ARG
1	A	175	VAL
1	A	187	THR
1	A	188	SER
1	A	189	PHE
1	A	196	LEU
1	A	203	PHE
1	A	211	LEU
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	221	LEU
1	A	229	LEU
1	A	235	VAL
1	A	240	VAL
1	A	256	MET
1	A	257	LYS
1	A	273	GLN
1	A	301	ILE
1	A	309	THR
1	A	318	MET
1	A	331	LEU
1	A	353	MET
1	A	371	MET
1	A	374	GLU
1	A	375	ARG
1	A	376	VAL
1	A	380	ASP
1	A	381	VAL
1	A	405	PRO
1	A	410	GLU
1	A	412	GLU
1	A	415	LEU
1	A	426	ASN
1	A	450	MET
1	A	452	MET
1	A	454	LEU
1	A	456	LEU
1	A	458	ARG
1	A	460	LEU
1	A	466	LYS
1	A	475	LEU
1	A	476	LYS
1	A	477	LEU
1	A	479	LEU
1	A	484	GLN
1	A	486	GLU
1	A	490	VAL
1	A	492	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	65	HIS
1	A	192	ASN
1	A	197	ASN
1	A	200	GLN
1	A	206	ASN
1	A	332	GLN
1	A	384	ASN
1	A	451	ASN
1	A	461	GLN
1	A	472	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1501	1	50,50,50	1.42	8 (16%)	67,82,82	0.99	4 (5%)

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	1501	1	-	6/14/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	HEM	FE-NC	3.74	2.07	1.95
2	A	1501	HEM	FE-NB	3.24	2.04	1.94
2	A	1501	HEM	C4C-NC	-3.04	1.33	1.39
2	A	1501	HEM	FE-ND	2.90	2.03	1.94
2	A	1501	HEM	CHD-C4C	2.89	1.44	1.38
2	A	1501	HEM	FE-NA	2.88	2.04	1.95
2	A	1501	HEM	C2A-C3A	-2.28	1.33	1.38
2	A	1501	HEM	C4D-ND	-2.22	1.36	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	HEM	O1D-CGD-CBD	-3.30	112.63	123.09
2	A	1501	HEM	O2D-CGD-CBD	2.78	122.77	114.00
2	A	1501	HEM	CAD-C3D-C4D	2.34	128.77	124.70
2	A	1501	HEM	CAD-C3D-C2D	-2.05	124.04	127.87

There are no chirality outliers.

All (6) torsion outliers are listed below:

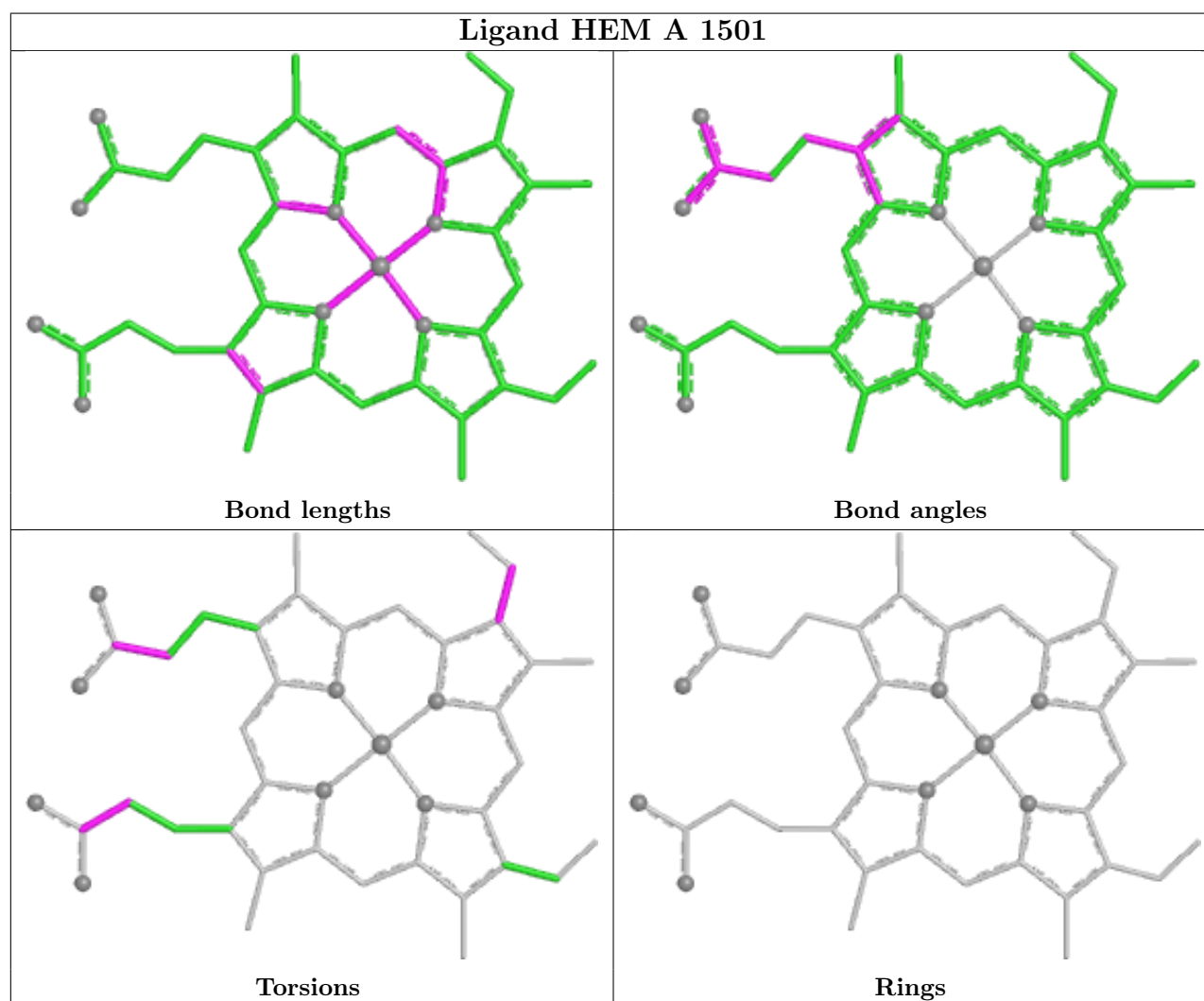
Mol	Chain	Res	Type	Atoms
2	A	1501	HEM	C2C-C3C-CAC-CBC
2	A	1501	HEM	C4C-C3C-CAC-CBC
2	A	1501	HEM	CAA-CBA-CGA-O2A
2	A	1501	HEM	CAA-CBA-CGA-O1A
2	A	1501	HEM	CAD-CBD-CGD-O2D
2	A	1501	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	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 ⓘ

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 [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	453/485 (93%)	0.32	12 (2%) 57 47	30, 64, 89, 100	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	ILE	3.0
1	A	409	THR	2.7
1	A	83	ALA	2.7
1	A	25	TYR	2.6
1	A	497	ASP	2.6
1	A	276	ILE	2.4
1	A	437	SER	2.4
1	A	407	TYR	2.2
1	A	63	GLU	2.1
1	A	293	LEU	2.1
1	A	68	TYR	2.0
1	A	340	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

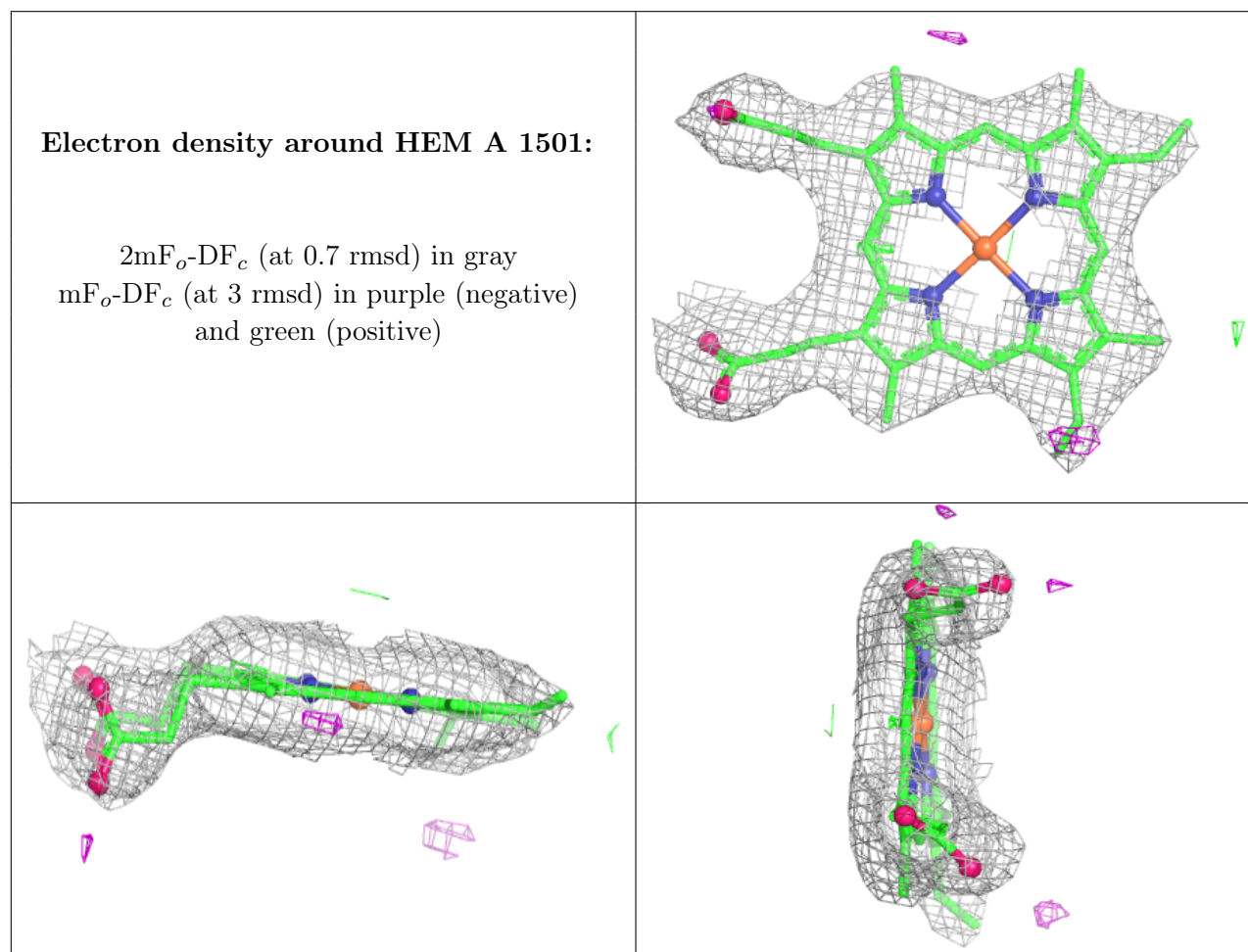
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	1501	43/43	0.95	0.09	27,33,47,52	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.