



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 08:21 PM UTC

PDB ID : 1W0G / pdb_00001w0g
Title : Crystal structure of human cytochrome P450 3A4
Authors : Williams, P.A.; Cosme, J.; Vinkovic, D.M.; Ward, A.; Angove, H.C.; Day, P.J.;
Vonnrhein, C.; Tickle, I.J.; Jhoti, H.
Deposited on : 2004-06-03
Resolution : 2.73 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

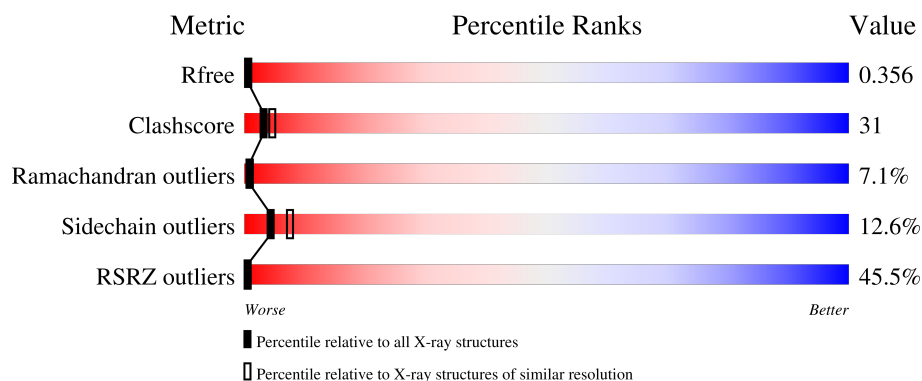
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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 4 unique types of molecules in this entry. The entry contains 3741 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.

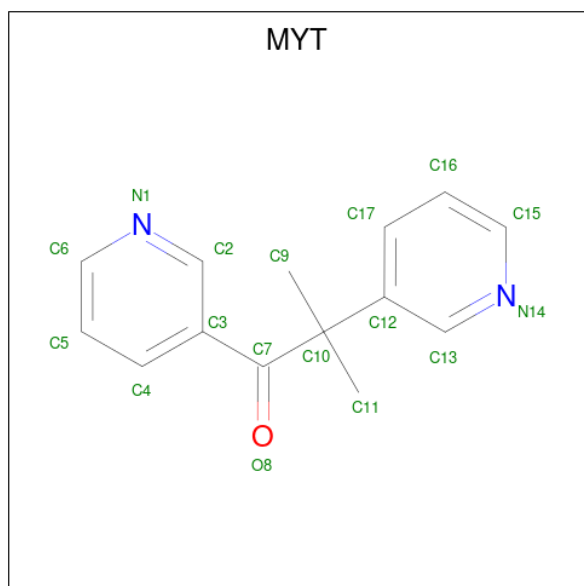
- Molecule 1 is a protein called CYTOCHROME P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	455	3652	2382	597	649	24	0	0	0

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 METYRAPONE (CCD ID: MYT) (formula: $C_{14}H_{14}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	17	14	2	1	0	0

- Molecule 3 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 43	C 34	Fe 1	N 4	O 4	0	0

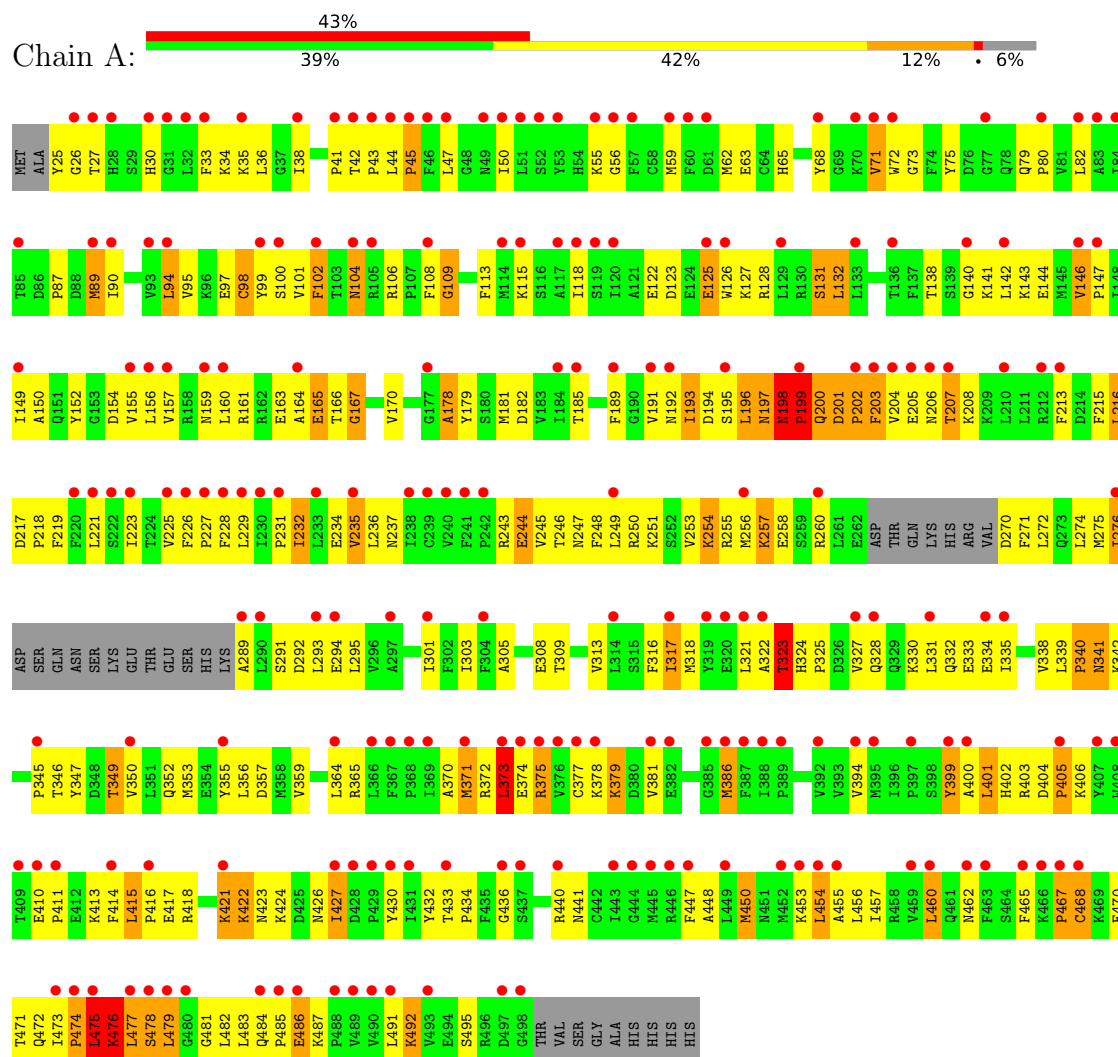
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0

3 Residue-property plots

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

• Molecule 1: CYTOCHROME P450 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)	81.65 – 2.73 79.94 – 2.73	Depositor EDS
% Data completeness (in resolution range)	93.9 (81.65-2.73) 93.1 (79.94-2.73)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0003A	Depositor
R, R_{free}	0.234 , 0.318 0.372 , 0.356	Depositor DCC
R_{free} test set	652 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	3741	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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, MYT

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	0.98	5/3742 (0.1%)	1.15	10/5063 (0.2%)

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	1	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	THR	CA-CB	6.60	1.61	1.53
1	A	313	VAL	CA-CB	-5.59	1.48	1.54
1	A	427	ILE	CA-CB	5.49	1.61	1.54
1	A	232	ILE	CA-CB	-5.30	1.48	1.54
1	A	178	ALA	CA-CB	-5.22	1.44	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	LEU	N-CA-C	-8.19	96.92	109.95
1	A	421	LYS	N-CA-C	7.20	121.10	110.30
1	A	146	VAL	CB-CA-C	-6.96	106.98	114.35
1	A	95	VAL	CB-CA-C	-6.66	105.11	111.44
1	A	421	LYS	CB-CA-C	6.23	118.73	110.06
1	A	421	LYS	N-CA-CB	5.82	118.83	109.28
1	A	56	GLY	N-CA-C	-5.76	104.10	112.17
1	A	118	ILE	N-CA-C	5.29	116.06	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	CYS	N-CA-C	5.15	121.76	110.80
1	A	42	THR	CB-CA-C	5.08	115.99	110.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	421	LYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	PRO	Peptide
1	A	322	ALA	Peptide
1	A	323	THR	Peptide
1	A	33	PHE	Peptide

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	3652	0	3728	230	5
2	A	17	0	14	5	0
3	A	43	0	30	4	0
4	A	29	0	0	5	0
All	All	3741	0	3772	233	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 31.

All (233) 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:178:ALA:HB3	1:A:196:LEU:HD12	1.55	0.88
1:A:104:ASN:ND2	1:A:123:ASP:OD1	2.09	0.86
1:A:178:ALA:HB1	1:A:196:LEU:HA	1.60	0.84
1:A:472:GLN:HE22	1:A:487:LYS:NZ	1.78	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TYR:HB3	4:A:2001:HOH:O	1.82	0.79
1:A:472:GLN:HB2	1:A:476:LYS:HZ1	1.46	0.79
1:A:472:GLN:HE22	1:A:487:LYS:HZ3	1.30	0.77
1:A:332:GLN:HA	1:A:335:ILE:HD12	1.69	0.74
1:A:373:LEU:HD21	1:A:436:GLY:HA2	1.69	0.74
1:A:413:LYS:HB2	1:A:415:LEU:HD11	1.70	0.73
1:A:198:ASN:O	1:A:200:GLN:N	2.22	0.72
1:A:276:ILE:HD12	1:A:276:ILE:N	2.05	0.71
1:A:101:VAL:HA	1:A:378:LYS:HG3	1.72	0.71
1:A:146:VAL:HG13	1:A:454:LEU:HD21	1.73	0.70
1:A:178:ALA:CB	1:A:196:LEU:HA	2.21	0.70
1:A:472:GLN:HB2	1:A:476:LYS:NZ	2.05	0.70
1:A:101:VAL:HG22	1:A:102:PHE:CD1	2.26	0.70
1:A:323:THR:O	1:A:324:HIS:CD2	2.47	0.68
1:A:330:LYS:HB3	1:A:355:TYR:CE1	2.30	0.67
1:A:477:LEU:N	1:A:485:PRO:O	2.24	0.67
1:A:345:PRO:HG3	1:A:457:ILE:HG21	1.75	0.67
1:A:479:LEU:H	1:A:479:LEU:HD23	1.60	0.66
1:A:201:ASP:H	1:A:202:PRO:HD3	1.59	0.66
1:A:201:ASP:N	1:A:202:PRO:HD3	2.11	0.66
1:A:55:LYS:HB3	1:A:59:MET:HB2	1.76	0.66
1:A:377:CYS:SG	1:A:379:LYS:O	2.53	0.65
1:A:181:MET:O	1:A:185:THR:HG23	1.97	0.65
1:A:357:ASP:HA	1:A:453:LYS:HZ1	1.61	0.64
1:A:179:TYR:CE1	1:A:455:ALA:HB2	2.31	0.64
1:A:251:LYS:O	1:A:254:LYS:HB3	1.97	0.63
1:A:309:THR:HG21	2:A:1499:MYT:H16	1.79	0.63
1:A:370:ALA:O	1:A:372:ARG:N	2.32	0.63
1:A:185:THR:HG21	1:A:193:ILE:HD11	1.81	0.63
1:A:155:VAL:HG12	1:A:196:LEU:HD22	1.82	0.62
1:A:101:VAL:HG23	1:A:378:LYS:HB2	1.81	0.62
1:A:99:TYR:HD2	1:A:127:LYS:CE	2.13	0.62
1:A:194:ASP:OD2	1:A:198:ASN:ND2	2.27	0.60
1:A:123:ASP:OD1	1:A:378:LYS:NZ	2.31	0.60
1:A:423:ASN:O	1:A:426:ASN:ND2	2.34	0.60
1:A:318:MET:CE	1:A:465:PHE:CD2	2.84	0.60
1:A:62:MET:O	1:A:65:HIS:N	2.35	0.60
1:A:475:LEU:C	1:A:476:LYS:HD3	2.26	0.59
1:A:291:SER:HB3	1:A:294:GLU:CD	2.27	0.59
1:A:140:GLY:O	1:A:144:GLU:HB2	2.03	0.59
1:A:318:MET:HE2	1:A:465:PHE:CE2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:TYR:HD2	1:A:127:LYS:HE2	1.68	0.58
1:A:400:ALA:O	1:A:401:LEU:C	2.46	0.58
1:A:321:LEU:HD21	1:A:359:VAL:HG11	1.86	0.57
1:A:101:VAL:O	1:A:102:PHE:HB2	2.04	0.57
1:A:472:GLN:HB3	1:A:476:LYS:HE3	1.85	0.57
1:A:357:ASP:HA	1:A:453:LYS:NZ	2.20	0.57
1:A:415:LEU:N	1:A:415:LEU:HD12	2.21	0.56
1:A:178:ALA:HB1	1:A:196:LEU:CA	2.32	0.56
1:A:253:VAL:HG13	1:A:272:LEU:HD21	1.88	0.56
1:A:272:LEU:C	1:A:272:LEU:HD13	2.31	0.55
1:A:472:GLN:CB	1:A:476:LYS:HE3	2.37	0.55
1:A:164:ALA:O	1:A:167:GLY:N	2.39	0.54
1:A:195:SER:O	1:A:197:ASN:N	2.40	0.54
1:A:460:LEU:C	1:A:462:ASN:H	2.15	0.54
1:A:228:PHE:O	1:A:231:PRO:HD2	2.08	0.54
1:A:178:ALA:CB	1:A:196:LEU:HD12	2.34	0.54
1:A:482:LEU:HB2	1:A:484:GLN:OE1	2.07	0.54
1:A:25:TYR:CB	4:A:2001:HOH:O	2.49	0.54
1:A:25:TYR:CD1	4:A:2001:HOH:O	2.53	0.54
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.90	0.54
1:A:178:ALA:O	1:A:182:ASP:CG	2.51	0.53
1:A:154:ASP:O	1:A:157:VAL:HG22	2.09	0.53
1:A:159:ASN:HD22	1:A:196:LEU:HD23	1.73	0.53
1:A:189:PHE:O	1:A:260:ARG:NH2	2.42	0.52
1:A:26:GLY:O	1:A:45:PRO:O	2.28	0.52
1:A:94:LEU:HD21	1:A:373:LEU:HD23	1.92	0.52
1:A:146:VAL:N	1:A:147:PRO:CD	2.72	0.52
1:A:138:THR:OG1	1:A:141:LYS:HD3	2.09	0.52
1:A:328:GLN:O	1:A:332:GLN:HG3	2.10	0.52
1:A:485:PRO:O	1:A:486:GLU:CB	2.58	0.52
1:A:386:MET:HE3	1:A:386:MET:HA	1.92	0.52
1:A:156:LEU:HA	1:A:196:LEU:HD21	1.90	0.51
1:A:327:VAL:HG22	1:A:355:TYR:OH	2.10	0.51
1:A:206:ASN:ND2	1:A:248:PHE:CD1	2.78	0.51
1:A:170:VAL:N	1:A:491:LEU:O	2.43	0.51
1:A:338:VAL:HG12	1:A:349:THR:HG22	1.92	0.51
1:A:467:PRO:O	1:A:468:CYS:HB3	2.10	0.51
1:A:201:ASP:N	1:A:202:PRO:CD	2.74	0.51
1:A:181:MET:SD	1:A:207:THR:HB	2.51	0.50
1:A:243:ARG:HD2	4:A:2017:HOH:O	2.11	0.50
1:A:256:MET:HE2	1:A:260:ARG:NH1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:C	1:A:257:LYS:HD2	2.36	0.50
1:A:346:THR:HB	1:A:349:THR:OG1	2.10	0.50
1:A:25:TYR:HD1	4:A:2001:HOH:O	1.94	0.50
1:A:97:GLU:O	1:A:99:TYR:N	2.45	0.50
1:A:97:GLU:HB3	1:A:101:VAL:CG1	2.42	0.50
1:A:404:ASP:O	1:A:406:LYS:N	2.45	0.50
1:A:185:THR:HG21	1:A:193:ILE:CD1	2.42	0.50
1:A:106:ARG:HD2	1:A:374:GLU:OE2	2.12	0.49
1:A:126:TRP:CZ2	1:A:440:ARG:HG2	2.47	0.49
1:A:189:PHE:O	1:A:256:MET:HE1	2.12	0.49
1:A:243:ARG:HA	1:A:246:THR:OG1	2.12	0.49
1:A:340:PRO:O	1:A:341:ASN:C	2.55	0.49
1:A:216:LEU:HD22	1:A:481:GLY:CA	2.42	0.49
1:A:226:PHE:HB2	1:A:229:LEU:HD22	1.94	0.49
1:A:339:LEU:O	1:A:340:PRO:C	2.55	0.49
1:A:316:PHE:O	1:A:317:ILE:C	2.54	0.49
1:A:318:MET:HE2	1:A:465:PHE:CD2	2.47	0.49
1:A:357:ASP:CA	1:A:453:LYS:HZ1	2.25	0.49
1:A:62:MET:O	1:A:63:GLU:C	2.56	0.49
1:A:128:ARG:NH1	1:A:289:ALA:O	2.46	0.49
1:A:353:MET:O	1:A:356:LEU:HB3	2.13	0.49
1:A:472:GLN:CB	1:A:476:LYS:CE	2.90	0.49
1:A:108:PHE:O	1:A:109:GLY:O	2.30	0.49
1:A:198:ASN:CB	1:A:199:PRO:HD2	2.43	0.49
2:A:1499:MYT:C17	2:A:1499:MYT:H4	2.43	0.49
1:A:160:LEU:HD12	1:A:163:GLU:HB2	1.95	0.49
1:A:101:VAL:HG11	1:A:381:VAL:HG21	1.95	0.49
1:A:159:ASN:ND2	1:A:196:LEU:HD23	2.27	0.49
1:A:359:VAL:HG13	1:A:414:PHE:HZ	1.78	0.49
1:A:441:ASN:HA	3:A:1501:HEM:HBA2	1.95	0.48
1:A:194:ASP:OD1	1:A:196:LEU:HB3	2.13	0.48
1:A:356:LEU:O	1:A:357:ASP:C	2.54	0.48
1:A:340:PRO:O	1:A:341:ASN:O	2.30	0.48
1:A:471:THR:HG21	1:A:491:LEU:HD23	1.96	0.48
1:A:181:MET:HE1	1:A:208:LYS:N	2.29	0.48
1:A:346:THR:O	1:A:350:VAL:HG23	2.14	0.48
1:A:403:ARG:O	1:A:405:PRO:HD3	2.14	0.48
1:A:475:LEU:O	1:A:476:LYS:HB2	2.14	0.48
1:A:101:VAL:HG22	1:A:102:PHE:HD1	1.78	0.47
1:A:113:PHE:C	1:A:115:LYS:N	2.71	0.47
1:A:450:MET:SD	1:A:454:LEU:HD22	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG12	1:A:353:MET:HE1	1.97	0.47
1:A:472:GLN:HB2	1:A:476:LYS:CE	2.44	0.47
1:A:71:VAL:HG13	1:A:82:LEU:HD21	1.96	0.47
1:A:97:GLU:HB3	1:A:101:VAL:HG12	1.96	0.47
1:A:102:PHE:CE2	1:A:394:VAL:HG21	2.50	0.47
1:A:347:TYR:CD1	1:A:347:TYR:C	2.93	0.47
1:A:243:ARG:O	1:A:244:GLU:C	2.55	0.47
1:A:217:ASP:HB2	1:A:218:PRO:CD	2.45	0.47
1:A:415:LEU:CD1	1:A:418:ARG:NH1	2.78	0.46
1:A:338:VAL:HG12	1:A:349:THR:CG2	2.45	0.46
1:A:125:GLU:OE1	1:A:125:GLU:HA	2.15	0.46
1:A:142:LEU:HD11	1:A:450:MET:HG3	1.98	0.46
2:A:1499:MYT:H13	3:A:1501:HEM:C4D	2.50	0.46
1:A:276:ILE:N	1:A:276:ILE:CD1	2.72	0.46
1:A:202:PRO:HB2	1:A:203:PHE:CB	2.46	0.46
1:A:271:PHE:O	1:A:275:MET:HE2	2.15	0.46
1:A:113:PHE:C	1:A:115:LYS:H	2.23	0.46
1:A:323:THR:O	1:A:324:HIS:CG	2.69	0.46
1:A:334:GLU:OE1	1:A:355:TYR:HB3	2.16	0.46
1:A:478:SER:HB2	1:A:484:GLN:HG2	1.97	0.46
1:A:62:MET:HE2	1:A:399:TYR:HE1	1.81	0.46
1:A:166:THR:O	1:A:167:GLY:C	2.58	0.46
1:A:350:VAL:HB	1:A:450:MET:HE1	1.98	0.46
1:A:213:PHE:HB2	1:A:215:PHE:CE1	2.50	0.45
1:A:213:PHE:O	1:A:482:LEU:HD21	2.16	0.45
1:A:275:MET:C	1:A:276:ILE:HD12	2.41	0.45
1:A:356:LEU:HD21	1:A:453:LYS:HB3	1.98	0.45
1:A:41:PRO:HD2	1:A:73:GLY:O	2.17	0.45
1:A:321:LEU:O	1:A:328:GLN:NE2	2.49	0.45
1:A:364:LEU:O	1:A:365:ARG:C	2.56	0.45
1:A:476:LYS:N	1:A:476:LYS:CD	2.79	0.45
1:A:198:ASN:O	1:A:199:PRO:C	2.58	0.45
1:A:305:ALA:HB1	2:A:1499:MYT:N14	2.32	0.45
1:A:421:LYS:O	1:A:422:LYS:CB	2.65	0.45
1:A:204:VAL:O	1:A:208:LYS:HB2	2.17	0.45
1:A:460:LEU:C	1:A:462:ASN:N	2.73	0.45
1:A:59:MET:O	1:A:63:GLU:HG3	2.16	0.44
1:A:75:TYR:HA	1:A:79:GLN:O	2.17	0.44
1:A:87:PRO:HA	1:A:90:ILE:HB	1.99	0.44
1:A:131:SER:O	1:A:132:LEU:HB2	2.17	0.44
1:A:226:PHE:O	1:A:229:LEU:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:HH12	1:A:272:LEU:HD12	1.83	0.44
1:A:203:PHE:HD1	1:A:203:PHE:O	2.01	0.44
1:A:123:ASP:CG	1:A:378:LYS:NZ	2.76	0.44
1:A:89:MET:O	1:A:90:ILE:C	2.61	0.44
1:A:460:LEU:O	1:A:462:ASN:N	2.51	0.44
1:A:235:VAL:HG12	1:A:236:LEU:HD22	2.00	0.43
1:A:432:TYR:CZ	1:A:434:PRO:HG3	2.53	0.43
1:A:295:LEU:HD23	1:A:295:LEU:C	2.43	0.43
1:A:483:LEU:C	1:A:483:LEU:HD23	2.43	0.43
1:A:472:GLN:NE2	1:A:487:LYS:NZ	2.56	0.43
1:A:75:TYR:CE2	1:A:80:PRO:HB3	2.54	0.43
1:A:223:ILE:O	1:A:223:ILE:HG22	2.17	0.43
1:A:470:GLU:O	1:A:472:GLN:HG3	2.19	0.43
1:A:27:THR:HG22	1:A:45:PRO:HA	1.99	0.43
1:A:291:SER:HB3	1:A:294:GLU:CG	2.48	0.43
1:A:415:LEU:HD11	1:A:418:ARG:NH1	2.33	0.43
1:A:470:GLU:O	1:A:472:GLN:N	2.52	0.43
1:A:30:HIS:CE1	1:A:43:PRO:HB2	2.54	0.43
1:A:225:VAL:C	1:A:227:PRO:HD3	2.44	0.43
1:A:333:GLU:O	1:A:334:GLU:C	2.62	0.43
1:A:198:ASN:CB	1:A:199:PRO:CD	2.97	0.43
1:A:317:ILE:HG21	1:A:456:LEU:HD11	2.01	0.43
1:A:399:TYR:CD1	1:A:399:TYR:C	2.96	0.43
1:A:415:LEU:CD1	1:A:418:ARG:HH11	2.32	0.43
1:A:207:THR:O	1:A:208:LYS:C	2.60	0.42
1:A:90:ILE:HG21	1:A:430:TYR:HB3	2.01	0.42
1:A:375:ARG:NH1	3:A:1501:HEM:O2A	2.52	0.42
1:A:479:LEU:H	1:A:479:LEU:CD2	2.31	0.42
1:A:251:LYS:HD2	1:A:251:LYS:N	2.34	0.42
1:A:492:LYS:CB	1:A:492:LYS:NZ	2.82	0.42
1:A:152:TYR:OH	1:A:192:ASN:ND2	2.22	0.42
1:A:472:GLN:HB3	1:A:476:LYS:CE	2.47	0.42
1:A:79:GLN:NE2	1:A:80:PRO:HD2	2.34	0.42
1:A:143:LYS:HA	1:A:146:VAL:HG23	2.02	0.42
1:A:179:TYR:CZ	1:A:455:ALA:HB2	2.55	0.42
1:A:330:LYS:HD3	1:A:355:TYR:CE2	2.55	0.42
1:A:423:ASN:O	1:A:424:LYS:C	2.62	0.42
1:A:189:PHE:CE1	1:A:303:ILE:HD11	2.55	0.42
1:A:219:PHE:CE1	1:A:223:ILE:HD11	2.55	0.42
1:A:476:LYS:HD3	1:A:476:LYS:N	2.35	0.42
1:A:476:LYS:HZ3	1:A:476:LYS:HG2	1.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:PHE:O	1:A:448:ALA:C	2.62	0.41
1:A:36:LEU:HG	1:A:38:ILE:HD12	2.02	0.41
1:A:68:TYR:HB2	1:A:72:TRP:HB3	2.02	0.41
1:A:339:LEU:HD21	1:A:349:THR:HG21	2.02	0.41
1:A:219:PHE:CZ	1:A:223:ILE:HD11	2.56	0.41
1:A:206:ASN:HB3	1:A:245:VAL:HG13	2.01	0.41
2:A:1499:MYT:H13	3:A:1501:HEM:ND	2.35	0.41
1:A:217:ASP:OD2	1:A:217:ASP:C	2.64	0.41
1:A:243:ARG:HG2	1:A:247:ASN:HD21	1.85	0.41
1:A:404:ASP:C	1:A:406:LYS:N	2.79	0.41
1:A:410:GLU:N	1:A:411:PRO:HD3	2.35	0.41
1:A:198:ASN:HB3	1:A:199:PRO:HD2	2.01	0.41
1:A:104:ASN:HD22	1:A:122:GLU:HB3	1.86	0.41
1:A:161:ARG:O	1:A:165:GLU:N	2.48	0.41
1:A:191:VAL:HG12	1:A:193:ILE:HG23	2.02	0.41
1:A:327:VAL:HG22	1:A:355:TYR:HH	1.86	0.40
1:A:334:GLU:O	1:A:338:VAL:HG23	2.21	0.40
1:A:102:PHE:H	1:A:378:LYS:CG	2.34	0.40
1:A:149:ILE:O	1:A:150:ALA:C	2.63	0.40
1:A:292:ASP:HB3	1:A:293:LEU:HD22	2.03	0.40
1:A:473:ILE:N	1:A:474:PRO:CD	2.85	0.40
1:A:485:PRO:O	1:A:486:GLU:HB2	2.21	0.40
1:A:324:HIS:N	1:A:325:PRO:HD3	2.37	0.40
1:A:416:PRO:O	1:A:418:ARG:N	2.55	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)
1:A:226:PHE:CE2	1:A:226:PHE:CZ[2_775]	1.36	0.84
1:A:232:ILE:CD1	1:A:232:ILE:CD1[4_575]	1.73	0.47
1:A:226:PHE:CE2	1:A:226:PHE:CE2[2_775]	1.85	0.35
1:A:226:PHE:CZ	1:A:226:PHE:CZ[2_775]	2.06	0.14
1:A:228:PHE:CB	1:A:231:PRO:O[4_575]	2.10	0.10

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	449/485 (93%)	351 (78%)	66 (15%)	32 (7%)	1 1

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	196	LEU
1	A	198	ASN
1	A	199	PRO
1	A	203	PHE
1	A	237	ASN
1	A	255	ARG
1	A	323	THR
1	A	341	ASN
1	A	342	LYS
1	A	467	PRO
1	A	468	CYS
1	A	476	LYS
1	A	486	GLU
1	A	109	GLY
1	A	132	LEU
1	A	167	GLY
1	A	340	PRO
1	A	401	LEU
1	A	422	LYS
1	A	475	LEU
1	A	477	LEU
1	A	371	MET
1	A	402	HIS
1	A	474	PRO
1	A	100	SER
1	A	254	LYS
1	A	417	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	PHE
1	A	201	ASP
1	A	405	PRO
1	A	165	GLU

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	412/441 (93%)	360 (87%)	52 (13%)	4 7

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

Mol	Chain	Res	Type
1	A	34	LYS
1	A	35	LYS
1	A	44	LEU
1	A	45	PRO
1	A	71	VAL
1	A	89	MET
1	A	94	LEU
1	A	104	ASN
1	A	125	GLU
1	A	131	SER
1	A	193	ILE
1	A	197	ASN
1	A	198	ASN
1	A	199	PRO
1	A	200	GLN
1	A	205	GLU
1	A	207	THR
1	A	216	LEU
1	A	221	LEU
1	A	234	GLU
1	A	235	VAL
1	A	244	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	249	LEU
1	A	250	ARG
1	A	257	LYS
1	A	258	GLU
1	A	270	ASP
1	A	274	LEU
1	A	276	ILE
1	A	301	ILE
1	A	308	GLU
1	A	317	ILE
1	A	331	LEU
1	A	349	THR
1	A	352	GLN
1	A	371	MET
1	A	373	LEU
1	A	375	ARG
1	A	379	LYS
1	A	386	MET
1	A	399	TYR
1	A	415	LEU
1	A	427	ILE
1	A	450	MET
1	A	454	LEU
1	A	460	LEU
1	A	475	LEU
1	A	476	LYS
1	A	478	SER
1	A	479	LEU
1	A	492	LYS
1	A	495	SER

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	65	HIS
1	A	104	ASN
1	A	192	ASN
1	A	197	ASN
1	A	206	ASN
1	A	247	ASN
1	A	324	HIS
1	A	328	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	329	GLN
1	A	451	ASN
1	A	472	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 ⓘ

2 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	$\# Z > 2$
3	HEM	A	1501	2,1	50,50,50	1.80	9 (18%)	67,82,82	1.34	10 (14%)
2	MYT	A	1499	3	18,18,18	1.39	2 (11%)	23,25,25	1.83	4 (17%)

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
3	HEM	A	1501	2,1	-	4/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYT	A	1499	3	-	0/16/16/16	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	HEM	C3D-C2D	6.60	1.51	1.36
3	A	1501	HEM	FE-ND	5.05	2.10	1.94
2	A	1499	MYT	C10-C12	-3.77	1.50	1.53
2	A	1499	MYT	C10-C7	-3.31	1.51	1.54
3	A	1501	HEM	FE-NB	-3.21	1.85	1.94
3	A	1501	HEM	C2A-C3A	-3.12	1.30	1.38
3	A	1501	HEM	CAC-C3C	2.92	1.55	1.47
3	A	1501	HEM	CMD-C2D	2.44	1.55	1.50
3	A	1501	HEM	CAB-C3B	2.43	1.53	1.47
3	A	1501	HEM	C3C-C2C	-2.39	1.32	1.37
3	A	1501	HEM	C3B-C2B	-2.13	1.32	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1499	MYT	O8-C7-C10	-4.87	115.92	120.04
3	A	1501	HEM	C4D-ND-C1D	3.59	109.46	105.21
2	A	1499	MYT	C12-C13-N14	-3.48	121.22	124.06
3	A	1501	HEM	CMD-C2D-C1D	3.41	130.36	125.03
3	A	1501	HEM	CHB-C1B-NB	3.17	128.28	124.37
3	A	1501	HEM	CHA-C4D-ND	2.95	128.01	124.37
2	A	1499	MYT	C16-C17-C12	-2.64	118.07	120.75
2	A	1499	MYT	C6-N1-C2	2.59	121.39	116.85
3	A	1501	HEM	C3B-C2B-C1B	2.26	108.11	106.41
3	A	1501	HEM	C1C-CHC-C4B	-2.20	121.34	126.02
3	A	1501	HEM	CHC-C4B-NB	2.13	126.72	124.42
3	A	1501	HEM	C1A-CHA-C4D	-2.11	121.29	126.25
3	A	1501	HEM	CAD-CBD-CGD	-2.07	108.17	113.67
3	A	1501	HEM	C4C-C3C-C2C	2.07	108.61	106.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	HEM	C2B-C3B-CAB-CBB
3	A	1501	HEM	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

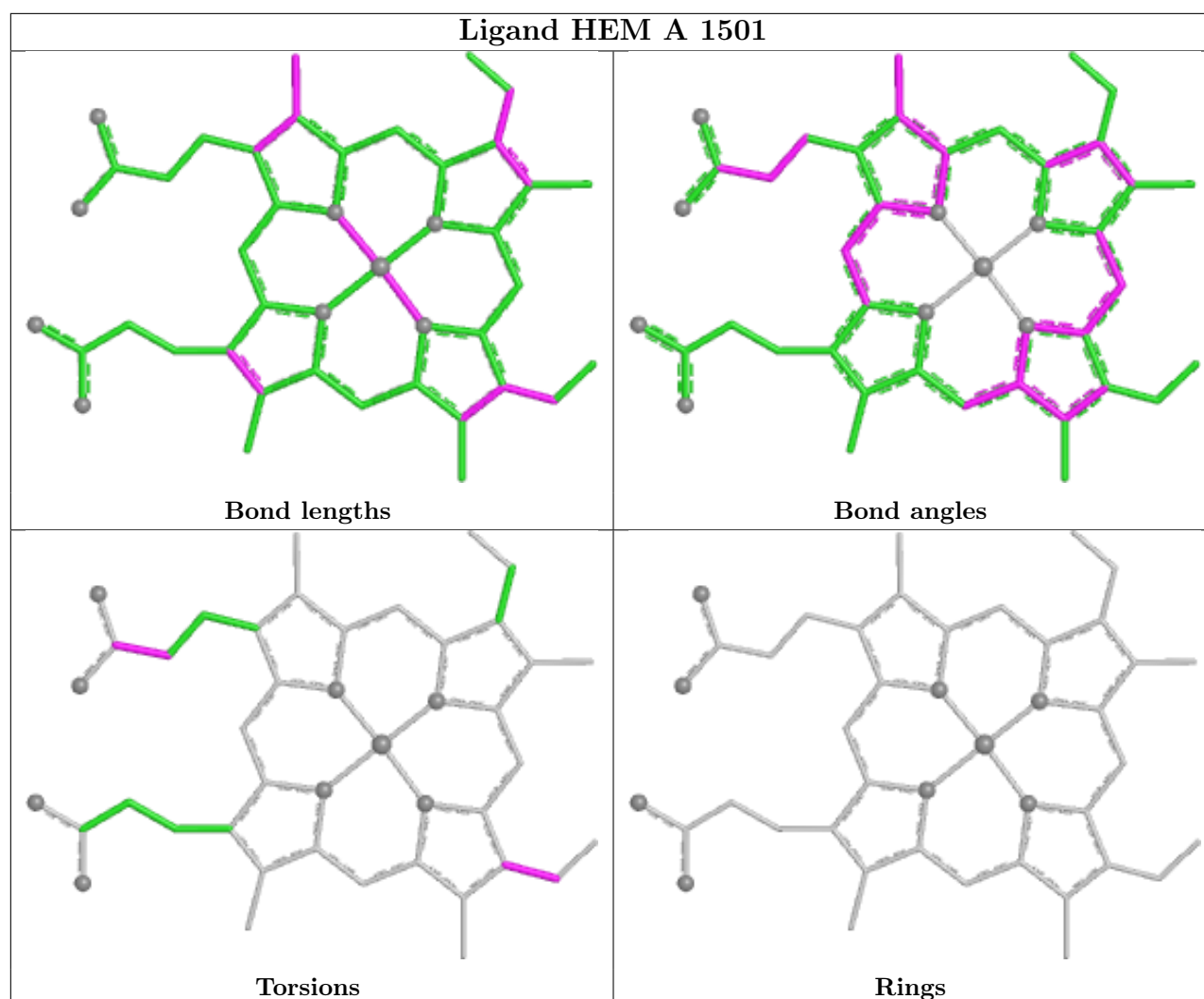
Mol	Chain	Res	Type	Atoms
3	A	1501	HEM	CAD-CBD-CGD-O1D
3	A	1501	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	HEM	4	0
2	A	1499	MYT	5	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 ⓘ

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	455/485 (93%)	2.10	207 (45%) 0 0	48, 81, 110, 122	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	VAL	7.7
1	A	231	PRO	7.6
1	A	437	SER	6.7
1	A	463	PHE	5.8
1	A	226	PHE	5.7
1	A	411	PRO	5.6
1	A	319	TYR	5.3
1	A	228	PHE	5.1
1	A	222	SER	5.0
1	A	475	LEU	4.9
1	A	449	LEU	4.4
1	A	68	TYR	4.4
1	A	276	ILE	4.3
1	A	373	LEU	4.3
1	A	460	LEU	4.3
1	A	364	LEU	4.2
1	A	241	PHE	4.1
1	A	328	GLN	4.1
1	A	83	ALA	4.1
1	A	84	ILE	4.0
1	A	301	ILE	4.0
1	A	108	PHE	4.0
1	A	206	ASN	4.0
1	A	491	LEU	4.0
1	A	455	ALA	3.9
1	A	474	PRO	3.8
1	A	119	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	71	VAL	3.8
1	A	433	THR	3.8
1	A	203	PHE	3.8
1	A	72	TRP	3.8
1	A	120	ILE	3.8
1	A	160	LEU	3.8
1	A	149	ILE	3.8
1	A	191	VAL	3.8
1	A	235	VAL	3.7
1	A	82	LEU	3.7
1	A	221	LEU	3.7
1	A	35	LYS	3.6
1	A	467	PRO	3.6
1	A	408	TRP	3.6
1	A	375	ARG	3.6
1	A	376	VAL	3.6
1	A	26	GLY	3.5
1	A	31	GLY	3.5
1	A	490	VAL	3.5
1	A	427	ILE	3.5
1	A	159	ASN	3.5
1	A	290	LEU	3.5
1	A	350	VAL	3.5
1	A	85	THR	3.4
1	A	230	ILE	3.4
1	A	177	GLY	3.4
1	A	210	LEU	3.4
1	A	369	ILE	3.4
1	A	480	GLY	3.4
1	A	27	THR	3.3
1	A	486	GLU	3.3
1	A	44	LEU	3.2
1	A	60	PHE	3.2
1	A	57	PHE	3.2
1	A	317	ILE	3.2
1	A	249	LEU	3.2
1	A	233	LEU	3.1
1	A	239	CYS	3.1
1	A	498	GLY	3.1
1	A	184	ILE	3.1
1	A	225	VAL	3.1
1	A	459	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	30	HIS	3.1
1	A	223	ILE	3.1
1	A	289	ALA	3.1
1	A	238	ILE	3.1
1	A	407	TYR	3.0
1	A	397	PRO	3.0
1	A	388	ILE	3.0
1	A	229	LEU	3.0
1	A	80	PRO	3.0
1	A	118	ILE	3.0
1	A	371	MET	3.0
1	A	213	PHE	3.0
1	A	381	VAL	3.0
1	A	331	LEU	3.0
1	A	416	PRO	3.0
1	A	157	VAL	3.0
1	A	367	PHE	2.9
1	A	454	LEU	2.9
1	A	345	PRO	2.9
1	A	462	ASN	2.9
1	A	465	PHE	2.9
1	A	436	GLY	2.9
1	A	314	LEU	2.9
1	A	322	ALA	2.9
1	A	102	PHE	2.9
1	A	473	ILE	2.8
1	A	207	THR	2.8
1	A	46	PHE	2.8
1	A	320	GLU	2.8
1	A	452	MET	2.8
1	A	52	SER	2.8
1	A	185	THR	2.8
1	A	189	PHE	2.8
1	A	51	LEU	2.8
1	A	56	GLY	2.8
1	A	478	SER	2.7
1	A	484	GLN	2.7
1	A	304	PHE	2.7
1	A	431	ILE	2.7
1	A	385	GLY	2.7
1	A	199	PRO	2.7
1	A	104	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	410	GLU	2.7
1	A	297	ALA	2.7
1	A	374	GLU	2.6
1	A	394	VAL	2.6
1	A	493	VAL	2.6
1	A	136	THR	2.6
1	A	497	ASP	2.6
1	A	156	LEU	2.6
1	A	466	LYS	2.6
1	A	327	VAL	2.6
1	A	400	ALA	2.6
1	A	164	ALA	2.6
1	A	142	LEU	2.6
1	A	45	PRO	2.6
1	A	387	PHE	2.6
1	A	205	GLU	2.5
1	A	41	PRO	2.5
1	A	446	ARG	2.5
1	A	55	LYS	2.5
1	A	133	LEU	2.5
1	A	293	LEU	2.5
1	A	382	GLU	2.4
1	A	368	PRO	2.4
1	A	117	ALA	2.4
1	A	115	LYS	2.4
1	A	355	TYR	2.4
1	A	212	ARG	2.4
1	A	334	GLU	2.4
1	A	59	MET	2.4
1	A	395	MET	2.4
1	A	105	ARG	2.4
1	A	155	VAL	2.4
1	A	38	ILE	2.3
1	A	335	ILE	2.3
1	A	294	GLU	2.3
1	A	428	ASP	2.3
1	A	468	CYS	2.3
1	A	414	PHE	2.3
1	A	430	TYR	2.3
1	A	42	THR	2.3
1	A	409	THR	2.3
1	A	114	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	125	GLU	2.3
1	A	220	PHE	2.3
1	A	53	TYR	2.3
1	A	49	ASN	2.3
1	A	202	PRO	2.3
1	A	488	PRO	2.3
1	A	100	SER	2.3
1	A	429	PRO	2.3
1	A	47	LEU	2.3
1	A	129	LEU	2.3
1	A	447	PHE	2.3
1	A	50	ILE	2.2
1	A	240	VAL	2.2
1	A	378	LYS	2.2
1	A	89	MET	2.2
1	A	389	PRO	2.2
1	A	392	VAL	2.2
1	A	489	VAL	2.2
1	A	33	PHE	2.2
1	A	256	MET	2.2
1	A	405	PRO	2.2
1	A	485	PRO	2.2
1	A	477	LEU	2.2
1	A	192	ASN	2.2
1	A	140	GLY	2.2
1	A	204	VAL	2.2
1	A	377	CYS	2.1
1	A	43	PRO	2.1
1	A	99	TYR	2.1
1	A	28	HIS	2.1
1	A	70	LYS	2.1
1	A	147	PRO	2.1
1	A	32	LEU	2.1
1	A	77	GLY	2.1
1	A	443	ILE	2.1
1	A	421	LYS	2.1
1	A	227	PRO	2.1
1	A	386	MET	2.1
1	A	366	LEU	2.1
1	A	479	LEU	2.1
1	A	399	TYR	2.1
1	A	440	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	453	LYS	2.0
1	A	242	PRO	2.0
1	A	146	VAL	2.0
1	A	260	ARG	2.0
1	A	61	ASP	2.0
1	A	195	SER	2.0
1	A	126	TRP	2.0
1	A	445	MET	2.0
1	A	94	LEU	2.0
1	A	321	LEU	2.0
1	A	90	ILE	2.0
1	A	444	GLY	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](#)

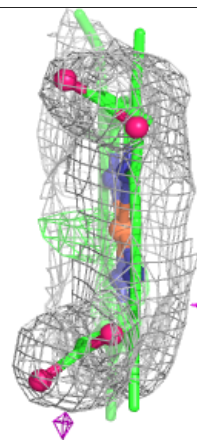
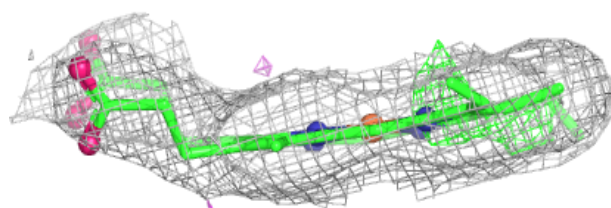
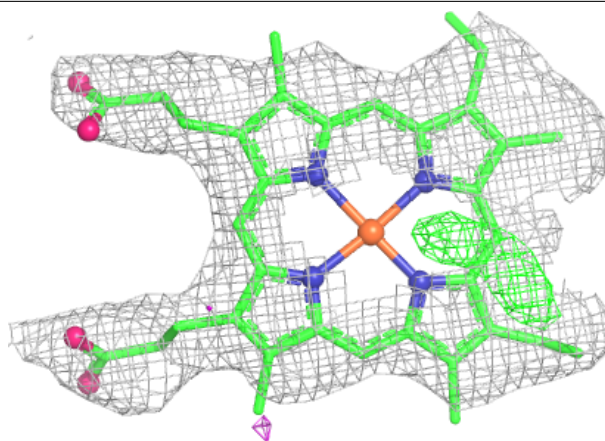
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MYT	A	1499	17/17	0.82	0.20	67,70,75,76	0
3	HEM	A	1501	43/43	0.90	0.15	49,59,70,73	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 1501:

$2mF_o-DF_c$ (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.