



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:55 PM UTC

PDB ID : 2CCD / pdb_00002ccd
Title : Crystal structure of the catalase-peroxidase (KatG) and S315T mutant from Mycobacterium tuberculosis
Authors : Yu, H.; Sacchettini, J.C.
Deposited on : 2006-01-16
Resolution : 2.10 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)
Xtrriage (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

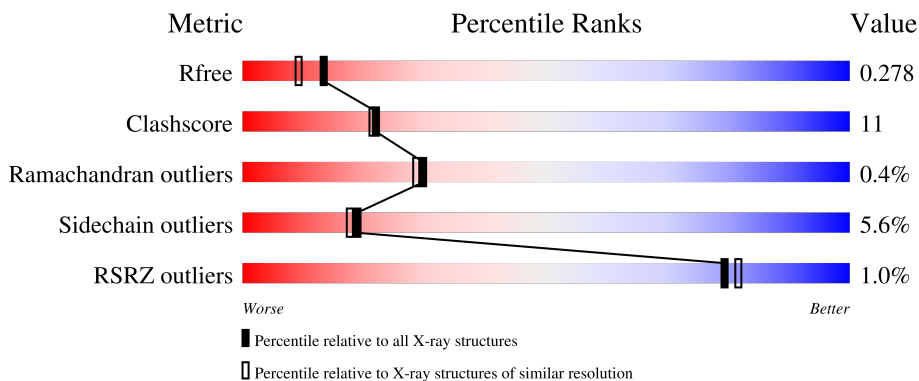
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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.

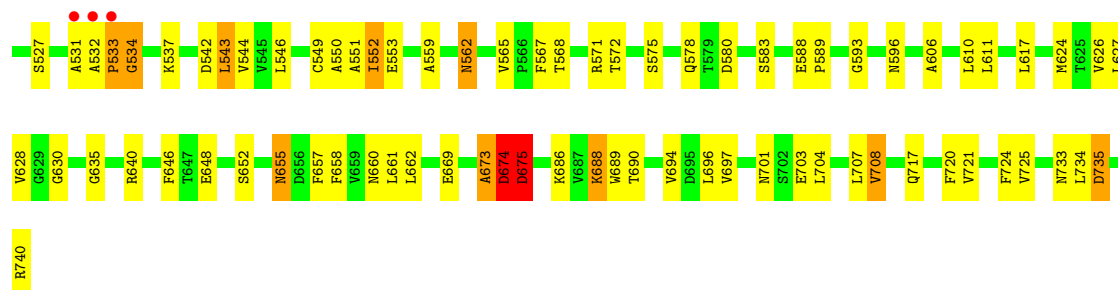
Mol	Chain	Length	Quality of chain
1	A	740	 76% 18% . .
1	B	740	 71% 22% . .

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	340	Total	O	0	0
			340	340		
3	B	255	Total	O	0	0
			255	255		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.81Å 149.81Å 154.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	78.5 (20.00-2.10) 78.3 (20.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.230 , 0.276 0.237 , 0.278	Depositor DCC
R_{free} test set	3987 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k 0.026 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11715	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 i

5.1 Standard geometry i

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	0.76	3/5667 (0.1%)	0.96	6/7714 (0.1%)
1	B	0.68	0/5667	1.02	17/7714 (0.2%)
All	All	0.72	3/11334 (0.0%)	0.99	23/15428 (0.1%)

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
1	B	0	6
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	ASP	CA-C	18.79	1.76	1.52
1	A	440	ASP	C-N	16.10	1.71	1.33
1	A	440	ASP	C-O	6.50	1.32	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	674	ASP	CA-CB-CG	9.08	121.68	112.60
1	B	675	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	440	ASP	O-C-N	-8.07	112.03	121.32
1	B	673	ALA	O-C-N	-7.70	113.85	122.55
1	B	532	ALA	CA-C-N	7.24	128.89	119.84
1	B	532	ALA	C-N-CA	7.24	128.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	GLY	CA-C-N	6.88	127.76	120.12
1	B	428	GLY	C-N-CA	6.88	127.76	120.12
1	B	660	ASN	N-CA-C	5.99	118.77	111.82
1	A	400	HIS	CA-C-N	5.94	125.62	119.56
1	A	400	HIS	C-N-CA	5.94	125.62	119.56
1	B	735	ASP	CB-CA-C	-5.88	99.37	110.67
1	B	215	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	387	ASP	CA-C-N	5.37	126.55	119.84
1	A	387	ASP	C-N-CA	5.37	126.55	119.84
1	B	39	TRP	CA-C-N	5.36	125.00	119.05
1	B	39	TRP	C-N-CA	5.36	125.00	119.05
1	B	734	LEU	CA-C-N	5.33	128.41	120.31
1	B	734	LEU	C-N-CA	5.33	128.41	120.31
1	B	675	ASP	O-C-N	-5.32	115.81	122.35
1	B	71	ILE	N-CA-C	5.23	116.32	109.21
1	B	71	ILE	N-CA-CB	5.15	117.31	110.26
1	A	509	ASP	O-C-N	5.02	127.09	121.32

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	SER	Mainchain
1	B	140	SER	Mainchain
1	B	673	ALA	Peptide,Mainchain
1	B	674	ASP	Mainchain
1	B	675	ASP	Mainchain
1	B	735	ASP	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	5517	0	5347	101	0
1	B	5517	0	5347	139	0
2	A	43	0	30	0	0
2	B	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	340	0	0	9	0
3	B	255	0	0	14	0
All	All	11715	0	10754	233	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 11.

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:440:ASP:C	1:A:440:ASP:CA	1.76	1.52
1:A:440:ASP:C	1:A:441:PRO:N	1.71	1.45
1:B:107:TRP:CH2	1:B:229:TYR:CE1	2.17	1.31
1:A:229:TYR:CE2	1:A:255:MET:SD	2.25	1.30
1:B:107:TRP:HH2	1:B:229:TYR:CE1	1.50	1.28
1:B:107:TRP:CH2	1:B:229:TYR:HE1	1.50	1.27
1:B:350:ALA:HB1	3:B:2106:HOH:O	1.21	1.25
1:B:229:TYR:CE2	1:B:255:MET:SD	2.39	1.16
1:B:447:HIS:HB2	1:B:537:LYS:HE2	1.34	1.07
1:B:45:LEU:HD23	1:B:611:LEU:HD21	1.40	1.02
1:B:447:HIS:CB	1:B:537:LYS:HE2	1.90	1.01
1:A:229:TYR:HE2	1:A:255:MET:SD	1.76	0.95
1:A:516:LYS:NZ	3:A:2240:HOH:O	1.86	0.92
1:B:552:ILE:HG23	1:B:565:VAL:HG21	1.56	0.86
1:A:609:MET:HE2	1:A:609:MET:HA	1.58	0.85
1:B:229:TYR:CZ	1:B:255:MET:SD	2.70	0.85
1:A:229:TYR:HE2	1:A:255:MET:CG	1.91	0.82
1:B:51:ASN:HD21	1:B:190:GLN:HB3	1.44	0.80
1:B:533:PRO:O	1:B:534:GLY:O	2.00	0.79
1:A:440:ASP:C	1:A:440:ASP:CB	2.56	0.78
1:B:117:ASP:OD1	1:B:119:ARG:NH1	2.18	0.77
1:B:701:ASN:HD22	1:B:704:LEU:H	1.32	0.77
1:B:229:TYR:HE2	1:B:255:MET:SD	2.07	0.77
1:B:542:ASP:HB2	1:B:567:PHE:HZ	1.47	0.77
1:B:107:TRP:HH2	1:B:229:TYR:CD1	2.02	0.77
1:B:107:TRP:CH2	1:B:229:TYR:CD1	2.74	0.75
1:B:258:ASN:C	1:B:258:ASN:HD22	1.93	0.75
1:B:527:SER:O	1:B:531:ALA:HB2	1.86	0.75
1:B:433:LYS:H	1:B:433:LYS:HD2	1.51	0.74
1:A:51:ASN:HD21	1:A:191:TRP:H	1.35	0.72
1:A:505:TRP:HB2	1:A:508:ASN:HD22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:HG12	1:B:455:ILE:HG13	1.72	0.71
1:A:229:TYR:CZ	1:A:255:MET:SD	2.84	0.70
1:A:406:ASP:O	1:A:410:LYS:HG3	1.91	0.70
1:B:210:TYR:HD2	1:B:214:ARG:O	1.75	0.69
1:B:447:HIS:HB2	1:B:537:LYS:CE	2.18	0.69
1:B:395:ARG:NH2	3:B:2166:HOH:O	2.24	0.69
1:B:447:HIS:HB3	1:B:537:LYS:HE2	1.74	0.68
1:B:553:GLU:HG3	1:B:565:VAL:HG23	1.76	0.67
1:B:210:TYR:CD2	1:B:214:ARG:O	2.48	0.67
1:B:357:ASP:HB3	3:B:2153:HOH:O	1.95	0.66
1:B:610:LEU:HD22	1:B:694:VAL:HG13	1.77	0.65
1:A:318:GLU:H	1:A:352:GLN:HE22	1.43	0.64
1:A:440:ASP:C	1:A:441:PRO:CA	2.68	0.64
1:A:45:LEU:HD23	1:A:611:LEU:HD21	1.79	0.63
1:B:107:TRP:CZ3	1:B:229:TYR:HE1	2.14	0.63
1:B:195:GLU:HB2	3:B:2085:HOH:O	1.99	0.62
1:B:170:ASN:HD22	1:B:412:TRP:HE1	1.46	0.62
1:B:655:ASN:ND2	1:B:717:GLN:HE21	1.96	0.62
1:B:239:PRO:HG3	1:B:351:TRP:CG	2.35	0.61
1:A:133:ASN:HD22	1:A:134:SER:N	1.98	0.60
1:A:505:TRP:HB2	1:A:508:ASN:ND2	2.17	0.60
1:B:459:LYS:HD3	1:B:546:LEU:HD11	1.83	0.60
1:A:258:ASN:HD22	1:A:258:ASN:C	2.09	0.60
1:B:26:MET:N	3:B:2002:HOH:O	2.35	0.60
1:A:258:ASN:ND2	1:A:261:GLU:H	2.00	0.59
1:B:542:ASP:HB2	1:B:567:PHE:CZ	2.34	0.58
1:B:125:GLY:O	1:B:128:ARG:HG2	2.02	0.58
1:A:531:ALA:HB2	3:A:2243:HOH:O	2.03	0.58
2:B:1741:HEM:HMB1	2:B:1741:HEM:HBB2	1.84	0.58
1:B:318:GLU:H	1:B:352:GLN:HE22	1.53	0.57
1:B:433:LYS:HD2	1:B:433:LYS:N	2.17	0.57
1:B:239:PRO:O	1:B:241:PRO:HD3	2.05	0.57
1:A:440:ASP:CA	1:A:441:PRO:N	2.68	0.56
1:B:275:THR:HG22	2:B:1741:HEM:CAA	2.35	0.56
1:A:133:ASN:HD22	1:A:133:ASN:C	2.12	0.56
1:A:41:ASN:OD1	1:B:27:LYS:NZ	2.36	0.56
1:A:181:PHE:CE2	1:A:432:PRO:HG3	2.41	0.56
1:B:113:TYR:HB3	1:B:418:ARG:HH11	1.72	0.55
1:B:187:ARG:HA	3:B:2075:HOH:O	2.06	0.55
1:B:257:MET:HE2	1:B:418:ARG:HH21	1.72	0.55
1:B:658:PHE:HD2	1:B:708:VAL:HB	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:LEU:HB2	1:B:551:ALA:HB2	1.90	0.54
1:B:210:TYR:OH	1:B:223:VAL:HG12	2.08	0.54
1:B:357:ASP:CB	3:B:2153:HOH:O	2.54	0.54
1:B:323:ASN:H	1:B:323:ASN:HD22	1.55	0.54
1:B:350:ALA:CB	3:B:2106:HOH:O	2.02	0.53
1:B:733:ASN:O	1:B:740:ARG:NH1	2.41	0.53
1:B:459:LYS:HG3	1:B:550:ALA:HB2	1.90	0.53
1:A:159:LEU:HD21	1:A:164:LEU:HD13	1.91	0.52
1:A:84:MET:HE2	1:A:102:PHE:HD2	1.74	0.52
1:A:143:LYS:NZ	3:A:2058:HOH:O	2.42	0.52
1:A:731:VAL:HA	1:A:734:LEU:HG	1.92	0.52
1:A:620:SER:HB2	1:A:622:PRO:HD2	1.92	0.52
1:B:107:TRP:CD1	1:B:108:HIS:HD2	2.28	0.51
1:B:470:SER:OG	1:B:635:GLY:HA3	2.10	0.51
1:A:125:GLY:O	1:A:128:ARG:HG2	2.09	0.51
1:B:626:VAL:HG23	1:B:720:PHE:CD1	2.46	0.51
1:A:143:LYS:H	1:A:143:LYS:HD2	1.76	0.51
1:B:284:VAL:HG22	1:B:302:SER:HB2	1.93	0.51
1:A:341:TRP:HB2	1:A:382:LEU:HD21	1.92	0.50
1:B:170:ASN:ND2	1:B:412:TRP:HE1	2.08	0.50
1:A:263:ALA:O	1:A:267:VAL:CG1	2.59	0.50
1:B:493:ASN:HD21	1:B:572:THR:H	1.59	0.50
1:B:36:GLN:H	1:B:36:GLN:NE2	2.09	0.50
1:A:26:MET:HA	1:B:200:LYS:O	2.12	0.50
1:B:113:TYR:HB3	1:B:418:ARG:NH1	2.27	0.50
1:A:107:TRP:CD1	1:A:108:HIS:HD2	2.30	0.49
1:A:694:VAL:O	1:A:697:VAL:HG12	2.11	0.49
1:A:263:ALA:O	1:A:267:VAL:HG13	2.13	0.49
1:B:416:ILE:HG22	1:B:416:ILE:O	2.13	0.49
1:A:128:ARG:NH1	3:B:2240:HOH:O	2.45	0.49
1:A:195:GLU:HB3	1:B:29:PRO:HB3	1.95	0.49
1:A:459:LYS:NZ	3:A:2210:HOH:O	2.43	0.49
1:B:134:SER:HB3	1:B:287:GLU:HG3	1.94	0.49
1:B:67:GLU:HB3	1:B:158:LYS:HA	1.94	0.49
1:B:662:LEU:HD21	1:B:708:VAL:HG22	1.94	0.49
1:B:701:ASN:ND2	1:B:703:GLU:H	2.10	0.49
1:B:181:PHE:CE2	1:B:432:PRO:HG2	2.48	0.48
1:B:542:ASP:HB3	1:B:571:ARG:HH11	1.78	0.48
1:B:694:VAL:O	1:B:697:VAL:HG12	2.13	0.48
1:B:137:ASP:HB2	1:B:226:GLY:O	2.13	0.48
1:A:136:PRO:HD2	1:A:226:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:SER:HB3	1:B:54:VAL:HG22	1.95	0.48
1:A:662:LEU:HD13	1:B:149:TRP:CZ2	2.48	0.48
1:A:129:PHE:HB3	1:A:193:PRO:HG3	1.95	0.48
1:B:552:ILE:HG13	1:B:724:PHE:HE2	1.78	0.48
1:B:701:ASN:ND2	1:B:704:LEU:H	2.05	0.48
1:B:265:LEU:O	2:B:1741:HEM:HBC2	2.13	0.47
1:A:310:LYS:HB2	3:A:2151:HOH:O	2.13	0.47
1:A:696:LEU:HD13	1:B:296:MET:HE3	1.95	0.47
1:B:565:VAL:HG13	1:B:725:VAL:HG13	1.96	0.47
1:B:721:VAL:O	1:B:725:VAL:HG23	2.15	0.47
1:A:462:ILE:HG21	1:A:547:GLY:HA2	1.96	0.47
1:A:590:LYS:HB2	1:A:602:ASN:HD21	1.80	0.47
1:A:701:ASN:HD22	1:A:704:LEU:H	1.63	0.47
1:A:385:ARG:O	1:A:391:GLU:HG2	2.15	0.47
1:A:68:VAL:O	1:A:71:ILE:HG22	2.15	0.47
1:A:262:THR:O	1:A:266:ILE:HG13	2.15	0.47
1:A:423:VAL:HA	1:A:426:TYR:CD2	2.50	0.47
1:B:450:VAL:HG13	1:B:454:GLU:HB2	1.97	0.47
1:B:214:ARG:O	1:B:215:ASP:C	2.56	0.47
1:A:36:GLN:O	1:A:40:PRO:HA	2.15	0.46
1:A:134:SER:HB3	1:A:287:GLU:HG3	1.96	0.46
1:A:229:TYR:HE2	1:A:255:MET:HG3	1.75	0.46
1:A:455:ILE:HG22	1:A:459:LYS:HE2	1.98	0.46
1:B:201:GLU:OE2	1:B:208:GLU:N	2.46	0.46
1:A:239:PRO:HG2	1:A:343:LEU:HD11	1.98	0.46
1:A:504:GLY:HA2	1:A:510:PRO:HB3	1.97	0.46
1:B:462:ILE:HA	1:B:465:SER:OG	2.15	0.46
1:A:139:ALA:O	1:A:314:THR:HG23	2.15	0.46
1:A:95:TYR:CZ	1:A:325:PRO:HG2	2.51	0.46
1:A:26:MET:N	3:A:2001:HOH:O	2.50	0.45
3:A:2014:HOH:O	1:B:707:LEU:HD11	2.15	0.45
1:B:229:TYR:OH	1:B:255:MET:SD	2.74	0.45
1:B:630:GLY:HA3	1:B:724:PHE:CE1	2.52	0.45
1:B:575:SER:OG	1:B:578:GLN:HG3	2.16	0.45
1:B:593:GLY:HA3	1:B:610:LEU:HD13	1.97	0.45
1:B:229:TYR:HE2	1:B:255:MET:CG	2.30	0.45
1:A:276:HIS:HB2	1:A:314:THR:HB	1.99	0.45
1:A:207:ASP:OD2	1:A:207:ASP:C	2.60	0.44
1:B:471:GLN:HE21	1:B:513:ASP:CG	2.25	0.44
1:A:321:TRP:NE1	1:A:381:ASP:OD2	2.50	0.44
1:A:119:ARG:HH21	1:A:615:ASN:ND2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:HD21	1:A:289:GLU:HG2	1.83	0.44
1:B:501:PRO:HB2	1:B:505:TRP:CZ3	2.52	0.44
1:B:258:ASN:HB2	3:B:2119:HOH:O	2.18	0.44
1:B:107:TRP:CZ3	1:B:229:TYR:CE1	2.94	0.44
1:B:414:LYS:O	1:B:418:ARG:HG2	2.18	0.44
1:B:559:ALA:HB2	1:B:652:SER:OG	2.18	0.43
1:B:688:LYS:HG3	1:B:689:TRP:CE2	2.53	0.43
1:A:80:ILE:HG22	1:A:84:MET:HE3	2.00	0.43
1:A:319:VAL:HG22	1:A:376:THR:HB	2.00	0.43
1:B:324:THR:O	3:B:2142:HOH:O	2.20	0.43
1:A:258:ASN:C	1:A:258:ASN:ND2	2.75	0.43
1:B:105:MET:HE1	1:B:148:LEU:HD11	2.01	0.43
1:B:275:THR:HG22	2:B:1741:HEM:HAA2	2.01	0.43
1:A:181:PHE:CE2	1:A:432:PRO:CG	3.01	0.43
1:A:502:GLN:HG2	1:A:505:TRP:CZ3	2.54	0.43
1:A:46:LYS:HG2	1:A:49:HIS:CE1	2.53	0.43
1:A:418:ARG:HE	1:A:418:ARG:CA	2.32	0.43
1:B:280:PRO:HB2	1:B:282:ASP:OD2	2.19	0.43
1:B:258:ASN:C	1:B:258:ASN:ND2	2.65	0.43
1:A:388:PRO:O	1:A:392:ARG:HG3	2.18	0.43
1:A:274:LYS:HE3	1:A:367:PRO:HG3	2.01	0.43
1:A:279:GLY:O	1:A:348:ALA:HB2	2.18	0.43
1:B:341:TRP:HB2	1:B:382:LEU:HD21	2.01	0.43
1:B:493:ASN:ND2	1:B:572:THR:H	2.16	0.43
1:A:604:LEU:HB2	1:A:609:MET:HE3	2.01	0.42
1:B:235:PRO:HB3	3:B:2094:HOH:O	2.19	0.42
1:A:119:ARG:HH21	1:A:615:ASN:HD22	1.66	0.42
1:A:528:PHE:O	1:A:532:ALA:HB2	2.19	0.42
1:B:624:MET:O	1:B:628:VAL:HG23	2.19	0.42
1:B:387:ASP:O	1:B:391:GLU:HB2	2.19	0.42
1:B:505:TRP:HA	1:B:505:TRP:CE3	2.54	0.42
1:B:505:TRP:HA	1:B:505:TRP:HE3	1.85	0.42
1:A:207:ASP:HB2	1:A:224:GLN:HG2	2.02	0.42
1:A:552:ILE:HD13	1:A:724:PHE:HE2	1.85	0.42
1:B:263:ALA:O	1:B:267:VAL:HG23	2.20	0.42
1:B:343:LEU:HD11	1:B:351:TRP:CE3	2.54	0.42
1:B:317:ILE:HG23	1:B:352:GLN:HE21	1.84	0.42
1:B:431:VAL:HA	1:B:432:PRO:HD3	1.91	0.42
1:A:210:TYR:HH	1:A:223:VAL:HG12	1.85	0.41
1:B:458:LEU:HD22	1:B:543:LEU:HD11	2.01	0.41
1:A:257:MET:HE3	1:A:265:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLY:HA3	1:A:610:LEU:HD13	2.00	0.41
1:A:610:LEU:HD22	1:A:694:VAL:HG13	2.02	0.41
1:B:606:ALA:HB1	1:B:694:VAL:HG23	2.02	0.41
1:A:387:ASP:HA	1:A:388:PRO:HD2	1.82	0.41
1:B:646:PHE:HE2	1:B:661:LEU:HD13	1.85	0.41
1:A:139:ALA:HA	1:A:300:TRP:CZ3	2.55	0.41
1:B:201:GLU:HG2	1:B:206:GLY:C	2.46	0.41
1:A:133:ASN:C	1:A:133:ASN:ND2	2.77	0.41
1:A:505:TRP:CE2	1:A:588:GLU:HB2	2.56	0.41
1:B:126:MET:HE2	1:B:126:MET:HA	2.03	0.41
1:A:123:GLY:O	1:A:187:ARG:HB3	2.21	0.41
1:A:296:MET:HE1	1:B:696:LEU:HB3	2.02	0.41
1:A:422:PRO:HG3	3:A:2220:HOH:O	2.20	0.41
1:A:726:ALA:HB1	3:A:2324:HOH:O	2.20	0.41
1:A:447:HIS:CD2	1:A:537:LYS:HG3	2.55	0.41
1:A:346:SER:HB3	1:A:352:GLN:NE2	2.35	0.41
1:B:475:THR:HG22	1:B:544:VAL:HG13	2.02	0.41
1:B:580:ASP:HB3	1:B:583:SER:HB3	2.03	0.41
1:A:131:PRO:HD3	1:B:35:ASN:HD21	1.86	0.41
1:B:61:ALA:HB3	3:B:2019:HOH:O	2.21	0.41
1:B:322:THR:HB	1:B:331:SER:OG	2.21	0.41
1:B:360:GLY:O	1:B:375:PRO:HD3	2.21	0.41
1:B:588:GLU:HA	1:B:589:PRO:HD3	1.94	0.41
1:B:646:PHE:HB2	1:B:657:PHE:HA	2.02	0.41
1:A:119:ARG:HD3	1:A:196:VAL:HG22	2.02	0.41
1:B:239:PRO:HG3	1:B:351:TRP:CD1	2.56	0.41
1:B:346:SER:OG	1:B:350:ALA:HB3	2.20	0.41
1:B:549:CYS:HA	1:B:552:ILE:HG22	2.02	0.41
1:B:562:ASN:HD22	1:B:562:ASN:HA	1.66	0.41
1:B:38:TRP:HB2	1:B:39:TRP:CE3	2.56	0.40
1:B:46:LYS:HG2	1:B:49:HIS:CE1	2.56	0.40
1:B:388:PRO:HG2	3:B:2161:HOH:O	2.20	0.40
1:B:626:VAL:HG23	1:B:720:PHE:HD1	1.86	0.40
1:A:174:GLU:OE2	1:A:180:THR:OG1	2.38	0.40
1:B:71:ILE:HD13	1:B:71:ILE:HG21	1.88	0.40
1:A:39:TRP:HB2	1:A:42:ARG:HD2	2.04	0.40
1:A:93:ALA:HB2	1:A:98:TYR:CZ	2.57	0.40
1:B:481:SER:HA	1:B:617:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	713/740 (96%)	681 (96%)	30 (4%)	2 (0%)	36	36
1	B	713/740 (96%)	684 (96%)	25 (4%)	4 (1%)	21	18
All	All	1426/1480 (96%)	1365 (96%)	55 (4%)	6 (0%)	30	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	534	GLY
1	A	674	ASP
1	B	370	GLY
1	A	424	ALA
1	B	674	ASP
1	B	533	PRO

5.3.2 Protein sidechains [i](#)

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	564/584 (97%)	539 (96%)	25 (4%)	25	26
1	B	564/584 (97%)	526 (93%)	38 (7%)	15	12
All	All	1128/1168 (97%)	1065 (94%)	63 (6%)	19	18

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	51	ASN
1	A	114	ARG
1	A	133	ASN
1	A	157	LYS
1	A	194	ASP
1	A	200	LYS
1	A	213	LYS
1	A	258	ASN
1	A	267	VAL
1	A	293	LEU
1	A	310	LYS
1	A	327	LYS
1	A	376	THR
1	A	391	GLU
1	A	418	ARG
1	A	538	VAL
1	A	543	LEU
1	A	609	MET
1	A	626	VAL
1	A	651	GLU
1	A	666	ILE
1	A	669	GLU
1	A	690	THR
1	A	696	LEU
1	B	36	GLN
1	B	170	ASN
1	B	195	GLU
1	B	203	THR
1	B	258	ASN
1	B	302	SER
1	B	313	ILE
1	B	323	ASN
1	B	329	ASP
1	B	330	ASN
1	B	380	THR
1	B	391	GLU
1	B	418	ARG
1	B	423	VAL
1	B	433	LYS
1	B	435	THR
1	B	446	SER
1	B	447	HIS

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Mol	Chain	Res	Type
1	B	449	LEU
1	B	459	LYS
1	B	460	SER
1	B	469	VAL
1	B	505	TRP
1	B	543	LEU
1	B	552	ILE
1	B	562	ASN
1	B	568	THR
1	B	596	ASN
1	B	627	LEU
1	B	640	ARG
1	B	648	GLU
1	B	655	ASN
1	B	669	GLU
1	B	675	ASP
1	B	686	LYS
1	B	688	LYS
1	B	690	THR
1	B	708	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	50	GLN
1	A	51	ASN
1	A	133	ASN
1	A	190	GLN
1	A	218	ASN
1	A	236	ASN
1	A	238	ASN
1	A	258	ASN
1	A	330	ASN
1	A	352	GLN
1	A	461	GLN
1	A	508	ASN
1	A	561	HIS
1	A	562	ASN
1	A	602	ASN
1	A	615	ASN
1	A	701	ASN

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Mol	Chain	Res	Type
1	B	35	ASN
1	B	36	GLN
1	B	41	ASN
1	B	50	GLN
1	B	51	ASN
1	B	170	ASN
1	B	218	ASN
1	B	236	ASN
1	B	258	ASN
1	B	323	ASN
1	B	330	ASN
1	B	352	GLN
1	B	439	GLN
1	B	493	ASN
1	B	500	GLN
1	B	562	ASN
1	B	655	ASN
1	B	679	GLN
1	B	701	ASN

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](#)

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
2	HEM	A	1741	1	50,50,50	2.14	10 (20%)	67,82,82	1.22	4 (5%)
2	HEM	B	1741	1	50,50,50	2.00	8 (16%)	67,82,82	1.49	9 (13%)

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	1741	1	-	5/14/54/54	-
2	HEM	B	1741	1	-	4/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1741	HEM	FE-NB	7.92	2.19	1.94
2	B	1741	HEM	C3D-C2D	7.83	1.53	1.36
2	A	1741	HEM	C3D-C2D	7.35	1.52	1.36
2	B	1741	HEM	FE-ND	7.19	2.17	1.94
2	A	1741	HEM	FE-NC	5.49	2.13	1.95
2	B	1741	HEM	FE-NB	3.99	2.07	1.94
2	A	1741	HEM	CAC-C3C	3.43	1.56	1.47
2	B	1741	HEM	CAC-C3C	3.13	1.55	1.47
2	A	1741	HEM	CAB-C3B	3.08	1.55	1.47
2	B	1741	HEM	CAB-C3B	3.00	1.55	1.47
2	A	1741	HEM	CMC-C2C	2.75	1.56	1.50
2	B	1741	HEM	FE-NC	2.59	2.03	1.95
2	A	1741	HEM	FE-ND	2.52	2.02	1.94
2	B	1741	HEM	CMC-C2C	2.47	1.55	1.50
2	A	1741	HEM	CMB-C2B	2.33	1.55	1.50
2	A	1741	HEM	C2A-C3A	-2.10	1.33	1.38
2	B	1741	HEM	CMB-C2B	2.03	1.54	1.50
2	A	1741	HEM	CMD-C2D	2.01	1.54	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1741	HEM	C4D-ND-C1D	5.30	111.48	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1741	HEM	C4D-ND-C1D	4.70	110.78	105.21
2	B	1741	HEM	CHC-C1C-NC	3.46	128.22	124.45
2	B	1741	HEM	CAA-CBA-CGA	-3.21	105.16	113.67
2	B	1741	HEM	CAD-C3D-C4D	2.74	129.48	124.70
2	B	1741	HEM	CHA-C1A-NA	2.68	128.72	123.86
2	B	1741	HEM	C1C-CHC-C4B	2.43	131.19	126.02
2	B	1741	HEM	C4A-CHB-C1B	-2.40	120.60	126.25
2	A	1741	HEM	C2A-C1A-NA	-2.36	107.53	110.15
2	B	1741	HEM	C1A-CHA-C4D	2.17	131.35	126.25
2	A	1741	HEM	C4D-C3D-C2D	-2.17	103.73	106.89
2	A	1741	HEM	CAA-CBA-CGA	-2.09	108.13	113.67
2	B	1741	HEM	C2A-C1A-NA	-2.04	107.89	110.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1741	HEM	C2B-C3B-CAB-CBB
2	A	1741	HEM	C4B-C3B-CAB-CBB
2	B	1741	HEM	C2C-C3C-CAC-CBC
2	B	1741	HEM	CAA-CBA-CGA-O2A
2	A	1741	HEM	CAA-CBA-CGA-O2A
2	B	1741	HEM	CAA-CBA-CGA-O1A
2	A	1741	HEM	CAA-CBA-CGA-O1A
2	B	1741	HEM	C4C-C3C-CAC-CBC
2	A	1741	HEM	C2C-C3C-CAC-CBC

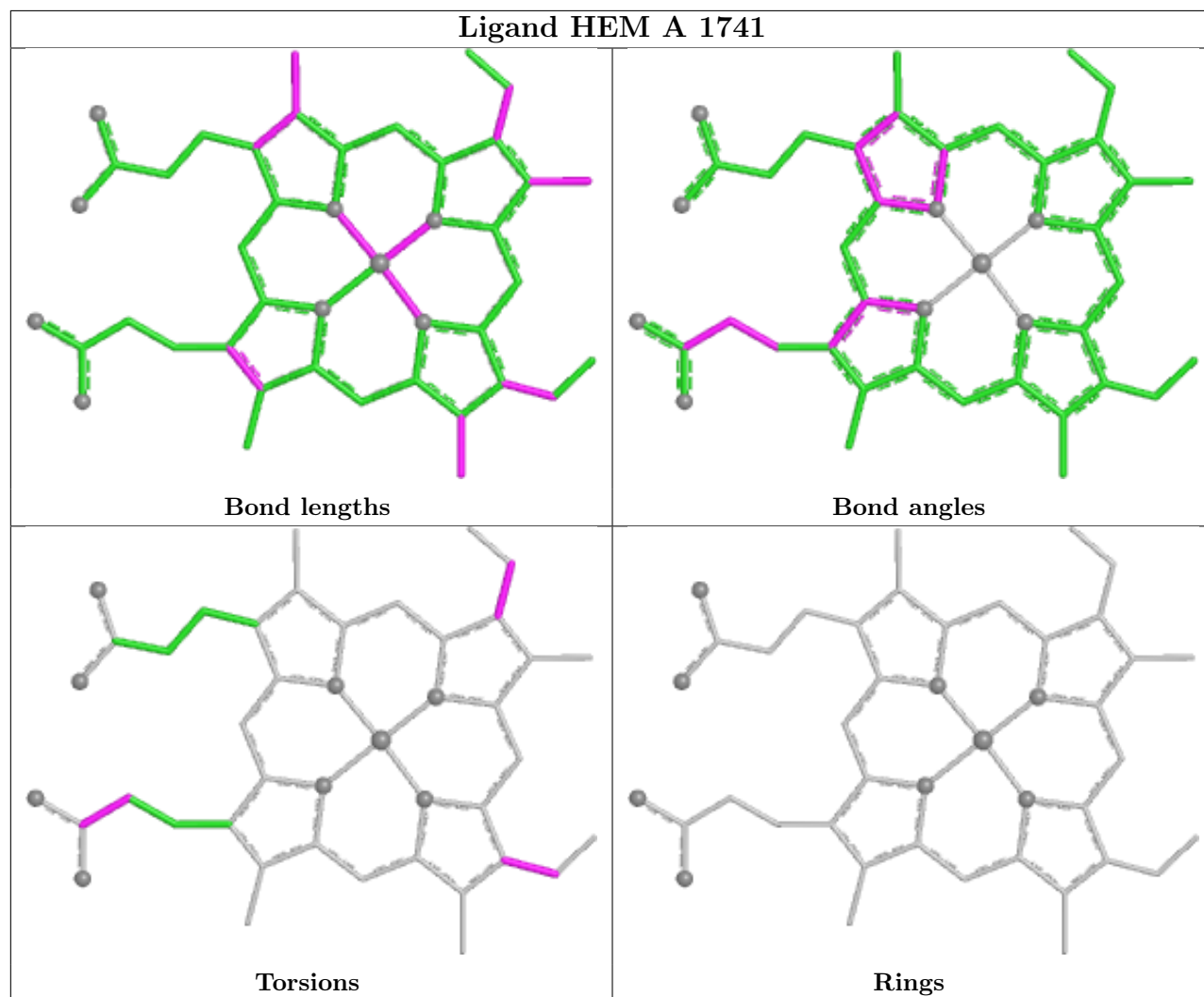
There are no ring outliers.

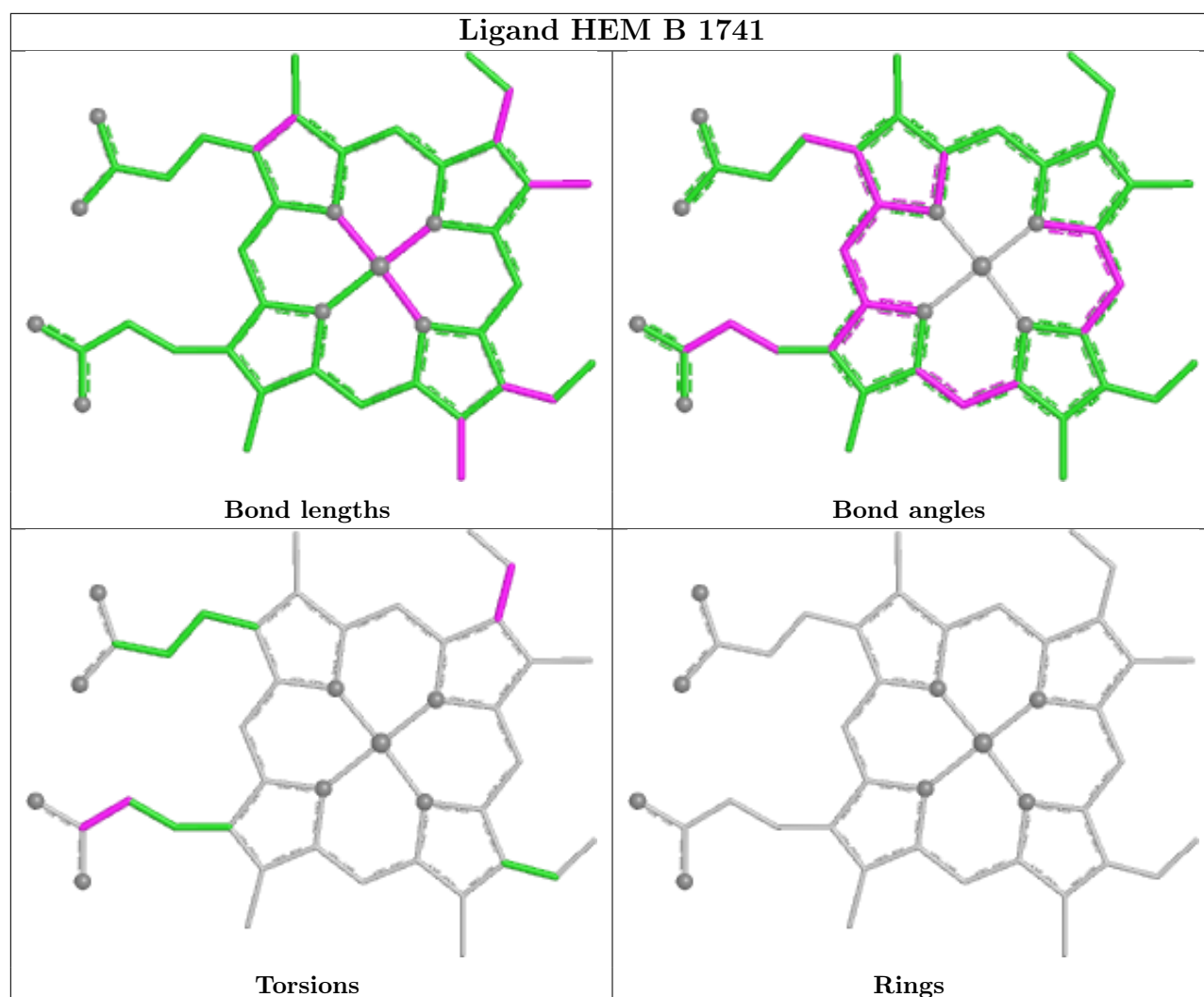
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1741	HEM	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	440:ASP	C	441:PRO	N	1.71

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	715/740 (96%)	0.13	5 (0%) 84 86	7, 19, 31, 38	0
1	B	715/740 (96%)	0.25	10 (1%) 73 75	8, 20, 34, 40	0
All	All	1430/1480 (96%)	0.19	15 (1%) 79 81	7, 20, 33, 40	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	533	PRO	4.7
1	A	79	ASP	3.5
1	B	532	ALA	3.4
1	A	510	PRO	3.3
1	B	531	ALA	2.7
1	B	79	ASP	2.6
1	B	469	VAL	2.6
1	A	369	GLY	2.5
1	B	510	PRO	2.5
1	B	447	HIS	2.5
1	B	505	TRP	2.2
1	B	305	GLY	2.2
1	A	582	GLU	2.2
1	A	54	VAL	2.1
1	B	237	GLY	2.1

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](#)

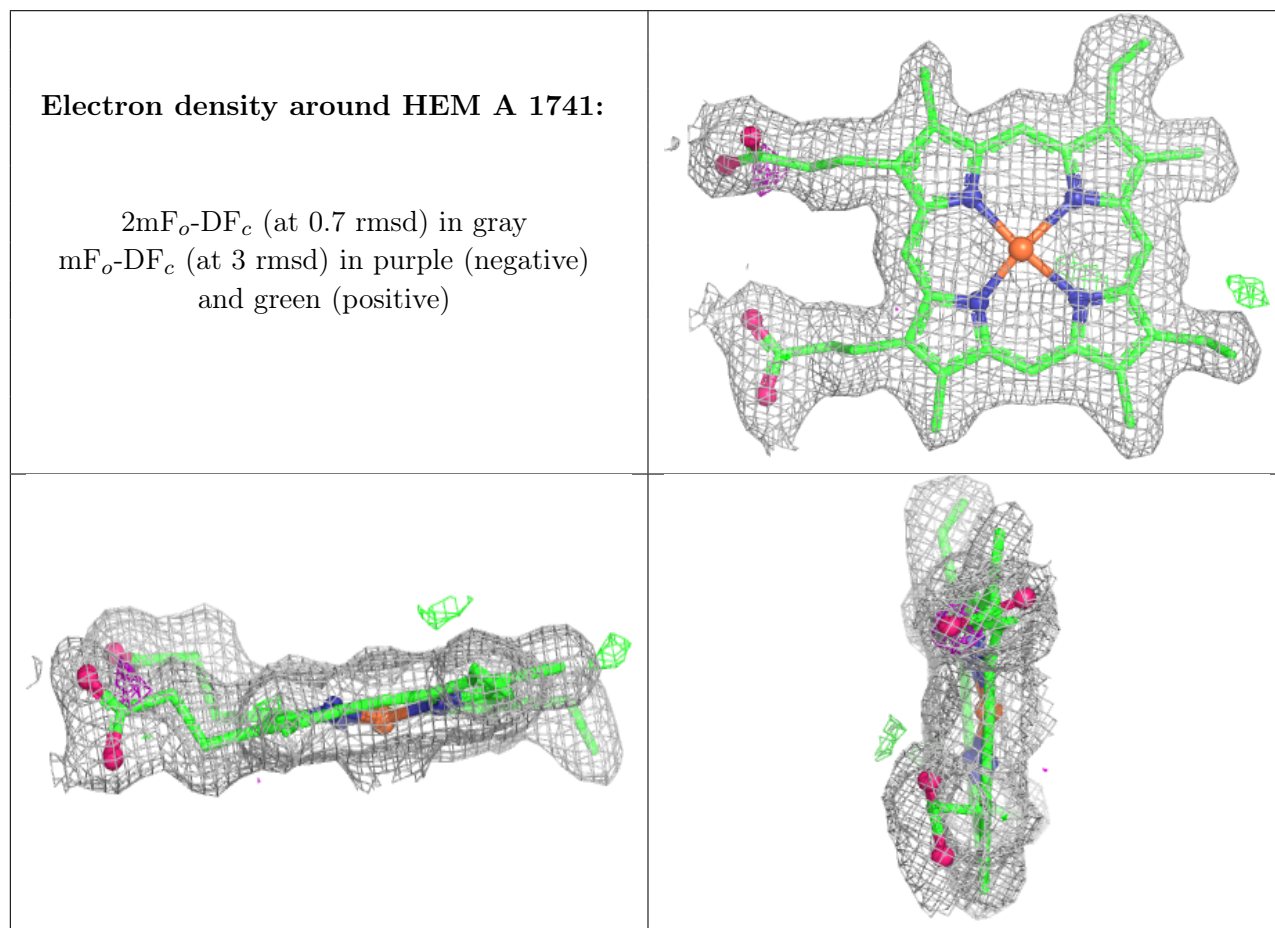
There are no oligosaccharides in this entry.

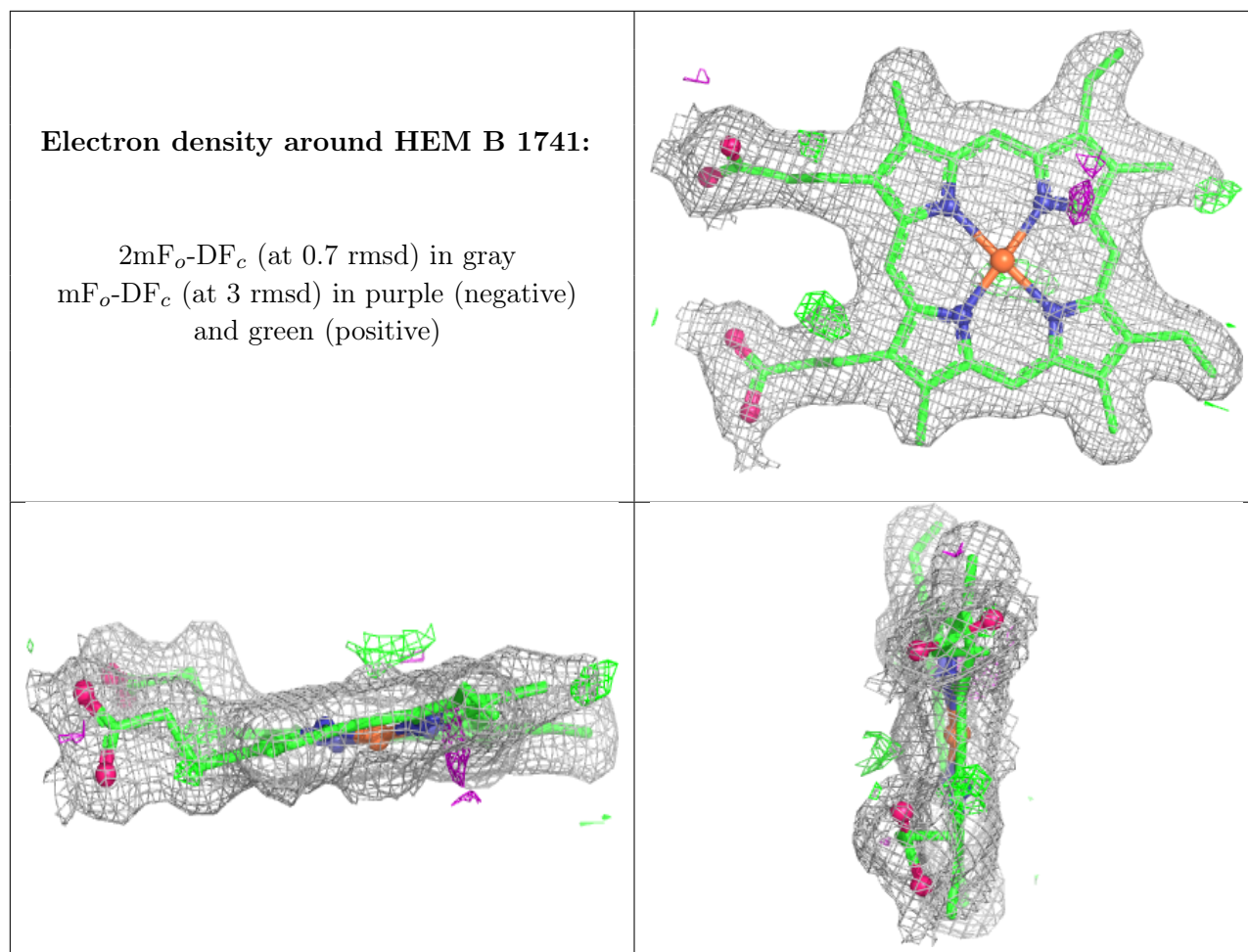
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	HEM	A	1741	43/43	0.96	0.06	2,7,10,12	0
2	HEM	B	1741	43/43	0.96	0.07	3,7,10,15	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.