



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:58 pm BST

PDB ID : 6UNM
Title : CYP3A4 bound to an inhibitor
Authors : Sevrioukova, I.
Deposited on : 2019-10-12
Resolution : 2.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

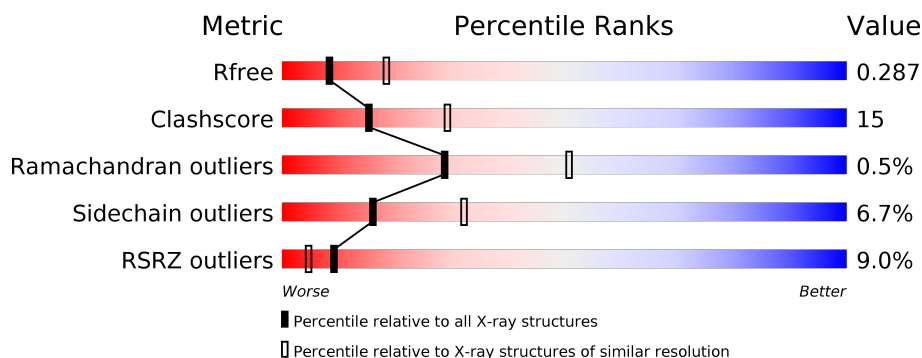
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 on 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	487	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	487	<div> <div>13%</div> <div> <div></div> <div>57%</div> <div>28%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7051 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	438	Total	C	N	O	S	0	0	0
			3512	2289	574	625	24			
1	B	426	Total	C	N	O	S	0	0	0
			3408	2225	551	609	23			

There are 12 discrepancies between the modelled and reference sequences:

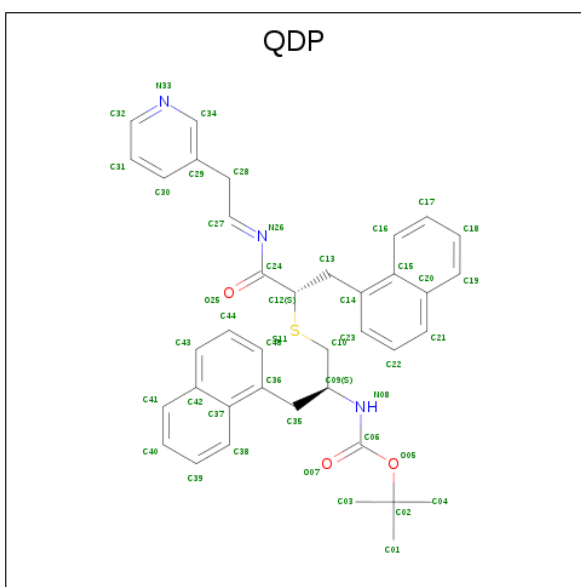
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP P08684
A	22	ALA	-	expression tag	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684
B	21	MET	-	initiating methionine	UNP P08684
B	22	ALA	-	expression tag	UNP P08684
B	504	HIS	-	expression tag	UNP P08684
B	505	HIS	-	expression tag	UNP P08684
B	506	HIS	-	expression tag	UNP P08684
B	507	HIS	-	expression tag	UNP P08684

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



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

- Molecule 3 is tert-butyl [(2S)-1-(naphthalen-1-yl)-3-[[[(2S)-3-(naphthalen-1-yl)-1-oxo-1-[(E)-[2-(pyridin-3-yl)ethylidene]amino}propan-2-yl]sulfanyl}propan-2-yl]carbamate (three-letter code: QDP) (formula: C₃₈H₃₉N₃O₃S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			45	38	3	3	1		

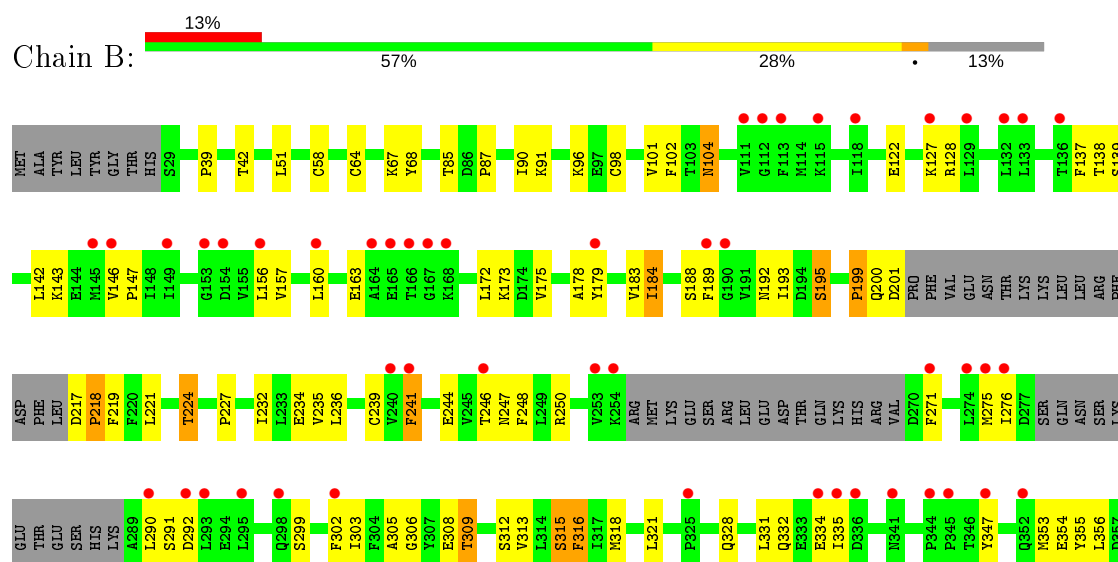
3 Residue-property plots

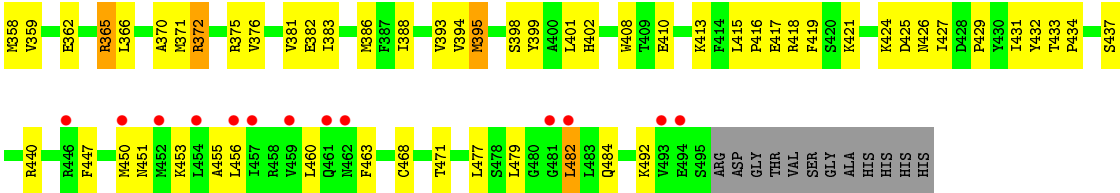
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



• Molecule 1: Cytochrome P450 3A4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.53Å 97.91Å 92.30Å 90.00° 123.57° 90.00°	Depositor
Resolution (Å)	62.30 – 2.83 62.30 – 2.83	Depositor EDS
% Data completeness (in resolution range)	96.5 (62.30-2.83) 96.5 (62.30-2.83)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.231 , 0.282 0.237 , 0.287	Depositor DCC
R_{free} test set	1191 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	105.4	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 97.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7051	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, QDP

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	0.35	0/3598	0.55	0/4867
1	B	0.31	0/3491	0.51	0/4726
All	All	0.34	0/7089	0.53	0/9593

There are no bond length outliers.

There are no bond angle outliers.

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	3512	0	3591	112	0
1	B	3408	0	3485	96	0
2	A	43	0	30	9	0
2	B	43	0	30	6	0
3	A	45	0	0	0	0
All	All	7051	0	7136	212	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 15.

All (212) 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:185:THR:O	1:A:189:PHE:HB2	1.36	1.25
1:A:257:LYS:HB3	1:A:258:GLU:HA	1.25	1.12
1:A:257:LYS:H	1:A:258:GLU:HB2	1.10	1.08
1:A:188:SER:HB3	1:A:271:PHE:HB3	1.39	1.04
1:A:482:LEU:H	1:A:482:LEU:HD23	1.31	0.94
1:A:133:LEU:HD22	1:A:271:PHE:HE1	1.35	0.91
1:A:257:LYS:N	1:A:258:GLU:HB2	1.87	0.88
1:A:185:THR:O	1:A:189:PHE:CB	2.26	0.80
1:A:236:LEU:HB2	1:A:238:ILE:HG13	1.68	0.75
1:B:104:ASN:OD1	1:B:122:GLU:HB3	1.85	0.75
1:A:257:LYS:HB3	1:A:258:GLU:CA	2.13	0.72
1:B:160:LEU:HG	1:B:175:VAL:HG21	1.71	0.72
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.70	0.71
1:A:369:ILE:HA	1:A:483:LEU:HD22	1.71	0.71
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.03	0.71
2:A:601:HEM:HBC2	2:A:601:HEM:HHD	1.73	0.71
1:A:446:ARG:HE	1:B:425:ASP:HB3	1.54	0.70
1:B:477:LEU:O	1:B:479:LEU:HD12	1.90	0.70
1:A:421:LYS:HA	1:A:424:LYS:HG2	1.72	0.70
1:A:257:LYS:CB	1:A:258:GLU:HA	2.09	0.69
1:A:133:LEU:HD22	1:A:271:PHE:CE1	2.25	0.69
1:A:467:PRO:HB3	1:A:471:THR:HG21	1.74	0.69
1:B:87:PRO:HG3	1:B:431:ILE:HD11	1.76	0.67
1:A:156:LEU:HD13	1:A:179:TYR:HB2	1.77	0.67
1:B:101:VAL:HG21	1:B:381:VAL:HG11	1.77	0.66
1:B:365:ARG:O	1:B:402:HIS:HB3	1.95	0.66
1:B:371:MET:O	1:B:398:SER:HB2	1.96	0.65
1:A:249:LEU:HA	1:A:252:SER:HB2	1.79	0.65
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.79	0.65
1:B:302:PHE:CG	2:B:601:HEM:HBC1	2.32	0.64
1:A:371:MET:CG	1:A:483:LEU:HD13	2.28	0.63
1:B:305:ALA:O	1:B:309:THR:HG23	1.97	0.62
1:B:302:PHE:CD2	2:B:601:HEM:HBC1	2.35	0.62
1:A:477:LEU:O	1:A:479:LEU:HD12	2.00	0.62
1:A:186:SER:HA	1:A:190:GLY:H	1.64	0.61
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.81	0.61
1:A:257:LYS:H	1:A:258:GLU:CB	1.99	0.61
1:A:28:HIS:HB2	1:A:30:HIS:HB2	1.81	0.61
1:B:356:LEU:HG	1:B:453:LYS:HE2	1.81	0.61
1:A:128:ARG:HH21	1:A:290:LEU:HA	1.65	0.60
1:A:421:LYS:HG3	1:A:424:LYS:HE3	1.82	0.60
1:B:305:ALA:HA	1:B:309:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ALA:O	1:B:372:ARG:N	2.33	0.59
1:A:128:ARG:NH2	1:A:290:LEU:HA	2.19	0.58
1:B:156:LEU:HD13	1:B:179:TYR:HB2	1.86	0.58
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.86	0.58
1:B:200:GLN:O	1:B:201:ASP:O	2.22	0.58
1:A:133:LEU:CD2	1:A:271:PHE:HE1	2.12	0.57
1:B:313:VAL:HA	1:B:316:PHE:HB2	1.85	0.57
1:A:436:GLY:HA3	2:A:601:HEM:HBA1	1.86	0.57
1:A:188:SER:HB3	1:A:271:PHE:CB	2.26	0.57
1:A:275:MET:HE2	1:A:290:LEU:HD21	1.87	0.56
1:A:256:MET:HA	1:A:257:LYS:HB2	1.88	0.56
1:A:47:LEU:O	1:A:50:ILE:HG23	2.05	0.55
1:A:87:PRO:HG3	1:A:431:ILE:HD11	1.87	0.55
1:B:482:LEU:HD23	1:B:482:LEU:H	1.72	0.55
1:B:184:ILE:CG1	1:B:306:GLY:HA3	2.37	0.55
1:A:369:ILE:CA	1:A:483:LEU:HD22	2.37	0.54
1:B:246:THR:O	1:B:250:ARG:N	2.39	0.54
1:A:226:PHE:HA	1:A:228:PHE:CE2	2.43	0.54
1:A:156:LEU:HD12	1:A:175:VAL:HG22	1.91	0.53
1:B:421:LYS:HA	1:B:424:LYS:HG2	1.90	0.53
1:B:477:LEU:O	1:B:479:LEU:CD1	2.56	0.53
1:A:229:LEU:HD22	1:A:232:ILE:HD12	1.91	0.53
1:A:375:ARG:NH2	2:A:601:HEM:O1A	2.38	0.53
1:A:105:ARG:HH22	2:A:601:HEM:HBD1	1.73	0.52
1:B:365:ARG:HD2	1:B:402:HIS:O	2.09	0.52
1:B:356:LEU:HD21	1:B:453:LYS:HB3	1.90	0.52
1:B:408:TRP:HE3	1:B:418:ARG:HD3	1.74	0.52
1:B:355:TYR:HA	1:B:358:MET:HB2	1.91	0.52
1:A:59:MET:O	1:A:63:GLU:HG2	2.10	0.52
1:A:369:ILE:HA	1:A:483:LEU:CD2	2.38	0.52
1:A:321:LEU:HB3	1:A:328:GLN:HB2	1.91	0.52
1:A:308:GLU:OE2	1:A:484:GLN:NE2	2.43	0.51
1:B:291:SER:OG	1:B:292:ASP:N	2.43	0.51
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.93	0.51
1:A:403:ARG:NH1	1:A:412:GLU:OE1	2.43	0.51
1:A:471:THR:HG23	1:A:471:THR:O	2.10	0.51
1:B:179:TYR:CZ	1:B:455:ALA:HB2	2.46	0.51
1:A:101:VAL:HG22	1:A:379:LYS:HG2	1.93	0.51
1:B:64:CYS:HA	1:B:67:LYS:HB2	1.94	0.50
1:A:243:ARG:NH1	1:A:247:ASN:OD1	2.45	0.50
1:A:101:VAL:HA	1:A:378:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLN:CD	1:B:248:PHE:HZ	2.14	0.50
1:B:358:MET:HB3	1:B:416:PRO:O	2.12	0.50
1:A:133:LEU:CD2	1:A:271:PHE:CE1	2.91	0.50
1:A:368:PRO:C	1:A:483:LEU:HD22	2.33	0.49
1:B:415:LEU:O	1:B:417:GLU:N	2.46	0.49
1:B:359:VAL:O	1:B:362:GLU:N	2.45	0.49
1:B:305:ALA:HA	1:B:309:THR:CG2	2.43	0.49
1:A:357:ASP:OD1	1:A:453:LYS:NZ	2.31	0.49
1:A:81:VAL:HG22	1:A:393:VAL:HB	1.94	0.49
1:A:193:ILE:HG21	1:A:199:PRO:HB3	1.95	0.49
1:A:256:MET:O	1:A:272:LEU:HD21	2.13	0.49
1:A:170:VAL:O	1:A:490:VAL:HA	2.13	0.49
1:B:188:SER:HA	1:B:271:PHE:HB3	1.96	0.48
1:A:58:CYS:HB3	1:A:399:TYR:CD2	2.48	0.48
1:A:28:HIS:HA	1:A:29:SER:HB3	1.95	0.48
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.96	0.48
1:A:371:MET:O	1:A:398:SER:HB2	2.13	0.48
1:B:87:PRO:HA	1:B:90:ILE:HD12	1.95	0.48
1:A:435:PHE:HB3	1:A:442:CYS:HB3	1.95	0.48
1:B:184:ILE:HG12	1:B:306:GLY:HA3	1.96	0.47
1:A:258:GLU:O	1:A:259:SER:CB	2.61	0.47
1:B:381:VAL:HG23	1:B:388:ILE:HB	1.95	0.47
1:B:234:GLU:C	1:B:236:LEU:H	2.18	0.47
1:A:442:CYS:HB2	2:A:601:HEM:NA	2.30	0.47
1:A:434:PRO:O	2:A:601:HEM:HMA1	2.14	0.47
1:B:354:GLU:O	1:B:358:MET:N	2.38	0.47
1:B:408:TRP:CE3	1:B:418:ARG:HD3	2.49	0.47
1:A:258:GLU:O	1:A:259:SER:HB2	2.15	0.47
1:B:104:ASN:HA	1:B:440:ARG:NH1	2.30	0.47
1:B:146:VAL:HG21	1:B:347:TYR:HB2	1.96	0.47
1:B:156:LEU:HD12	1:B:175:VAL:HG22	1.97	0.47
1:A:152:TYR:CD1	1:A:182:ASP:HB3	2.50	0.46
1:A:218:PRO:HG2	1:A:219:PHE:H	1.81	0.46
1:B:184:ILE:HG21	1:B:303:ILE:HA	1.97	0.46
1:B:173:LYS:HE3	1:B:312:SER:HA	1.97	0.46
1:B:429:PRO:O	1:B:433:THR:HG22	2.16	0.46
1:B:91:LYS:HE2	1:B:96:LYS:HE3	1.97	0.46
1:A:101:VAL:HG21	1:A:381:VAL:HG11	1.97	0.46
1:A:257:LYS:N	1:A:258:GLU:CB	2.70	0.46
1:B:172:LEU:HB2	1:B:315:SER:HB3	1.97	0.46
1:A:302:PHE:CG	2:A:601:HEM:HBC1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:HA	1:A:190:GLY:N	2.29	0.46
1:A:256:MET:N	1:A:257:LYS:HA	2.31	0.46
1:B:401:LEU:HB3	1:B:431:ILE:HG23	1.96	0.45
1:B:224:THR:O	1:B:227:PRO:HD3	2.15	0.45
1:A:371:MET:HG3	1:A:483:LEU:HD13	1.98	0.45
1:B:217:ASP:N	1:B:218:PRO:HD3	2.32	0.45
1:A:249:LEU:HD23	1:A:252:SER:HB2	1.98	0.45
1:A:276:ILE:HA	1:A:279:GLN:HB3	1.98	0.45
1:B:332:GLN:HG2	1:B:460:LEU:O	2.16	0.45
1:B:432:TYR:CZ	1:B:434:PRO:HG3	2.51	0.45
1:B:157:VAL:HG13	1:B:463:PHE:CE2	2.51	0.45
1:A:255:ARG:C	1:A:256:MET:HG3	2.36	0.45
1:B:178:ALA:HB1	1:B:195:SER:HB3	1.99	0.45
1:A:251:LYS:O	1:A:255:ARG:HB2	2.17	0.44
1:B:468:CYS:SG	1:B:492:LYS:N	2.91	0.44
1:A:202:PRO:O	1:A:203:PHE:CG	2.71	0.44
1:A:202:PRO:O	1:A:203:PHE:CD2	2.71	0.44
1:A:478:SER:C	1:A:480:GLY:H	2.20	0.44
1:A:219:PHE:HZ	1:A:240:VAL:HG12	1.82	0.44
1:A:395:MET:HE2	1:A:395:MET:HB3	1.88	0.44
1:A:358:MET:HG2	1:A:419:PHE:O	2.18	0.44
1:A:62:MET:HB3	1:A:62:MET:HE2	1.93	0.44
1:B:271:PHE:O	1:B:275:MET:HG3	2.18	0.44
1:B:183:VAL:HG11	1:B:451:ASN:OD1	2.18	0.44
1:A:101:VAL:HG21	1:A:381:VAL:CG1	2.48	0.44
1:B:382:GLU:HA	1:B:386:MET:O	2.18	0.44
1:A:410:GLU:HB3	1:A:413:LYS:HG3	2.01	0.43
1:B:321:LEU:O	1:B:328:GLN:HB2	2.17	0.43
1:B:58:CYS:HB3	1:B:399:TYR:CD2	2.53	0.43
1:A:188:SER:CB	1:A:271:PHE:HB3	2.28	0.43
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.82	0.43
1:B:39:PRO:HG2	1:B:68:TYR:HB3	2.01	0.43
1:A:111:VAL:HG12	1:A:241:PHE:HE1	1.84	0.43
1:B:247:ASN:OD1	1:B:250:ARG:HD3	2.18	0.43
1:A:67:LYS:HD2	1:A:68:TYR:CZ	2.54	0.43
1:A:408:TRP:CE3	1:A:418:ARG:HD3	2.54	0.43
1:A:305:ALA:O	1:A:309:THR:HG23	2.19	0.42
1:B:365:ARG:HD3	1:B:408:TRP:CE3	2.54	0.42
1:B:410:GLU:HB3	1:B:413:LYS:HG3	2.01	0.42
1:B:375:ARG:NH2	2:B:601:HEM:O1A	2.24	0.42
1:B:365:ARG:HB3	1:B:365:ARG:HE	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:O	1:B:335:ILE:HG13	2.18	0.42
1:B:143:LYS:HD3	1:B:347:TYR:CD2	2.54	0.42
1:B:334:GLU:OE2	1:B:353:MET:HB3	2.20	0.42
1:B:383:ILE:HG13	1:B:383:ILE:O	2.18	0.42
1:B:67:LYS:HB3	1:B:68:TYR:CD1	2.55	0.42
1:B:85:THR:O	1:B:85:THR:HG22	2.19	0.42
1:A:482:LEU:H	1:A:482:LEU:CD2	2.07	0.42
1:B:376:VAL:HG22	1:B:393:VAL:HG22	2.01	0.42
1:B:402:HIS:HE1	1:B:434:PRO:HB3	1.85	0.42
1:A:117:ALA:HB1	1:A:301:ILE:CG1	2.46	0.42
1:A:93:VAL:HG13	1:A:102:PHE:CG	2.54	0.42
1:B:232:ILE:O	1:B:235:VAL:HG12	2.20	0.42
1:B:492:LYS:HB3	1:B:492:LYS:HE2	1.78	0.42
1:A:226:PHE:HB3	1:A:229:LEU:HG	2.00	0.42
1:B:102:PHE:HB3	1:B:375:ARG:HB3	2.01	0.42
1:B:189:PHE:CZ	1:B:299:SER:HB3	2.55	0.42
1:A:291:SER:HB3	1:A:294:GLU:HB2	2.02	0.42
1:A:299:SER:O	1:A:303:ILE:HG13	2.20	0.41
1:B:358:MET:HG2	1:B:419:PHE:C	2.41	0.41
1:B:468:CYS:H	1:B:471:THR:HG21	1.85	0.41
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.80	0.41
1:A:226:PHE:O	1:A:229:LEU:HB2	2.20	0.41
1:A:405:PRO:HG3	1:A:411:PRO:HG3	2.00	0.41
1:A:41:PRO:HG2	1:A:49:ASN:ND2	2.35	0.41
2:B:601:HEM:CMB	2:B:601:HEM:HBB2	2.50	0.41
1:B:199:PRO:C	1:B:200:GLN:HG3	2.41	0.41
1:B:468:CYS:H	1:B:471:THR:CG2	2.34	0.41
1:B:173:LYS:NZ	1:B:484:GLN:HG2	2.36	0.41
1:A:328:GLN:HE22	1:A:465:PHE:N	2.19	0.41
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.77	0.41
1:B:365:ARG:HH21	1:B:366:LEU:HG	1.85	0.41
1:A:143:LYS:HD3	1:A:347:TYR:CG	2.56	0.41
1:A:476:LYS:HD2	1:A:486:GLU:OE1	2.20	0.41
1:A:371:MET:SD	1:A:483:LEU:HD13	2.61	0.41
1:B:146:VAL:HB	1:B:147:PRO:HD3	2.03	0.41
1:A:186:SER:HA	1:A:190:GLY:CA	2.51	0.40
1:B:104:ASN:HB3	1:B:122:GLU:HG2	2.03	0.40
1:B:193:ILE:HG21	1:B:199:PRO:HB3	2.03	0.40
1:B:239:CYS:HB3	1:B:241:PHE:O	2.20	0.40
1:B:362:GLU:HA	1:B:419:PHE:HE2	1.86	0.40
1:A:184:ILE:HA	1:A:184:ILE:HD12	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ILE:HA	1:A:474:PRO:HA	1.96	0.40
1:B:137:PHE:CD2	1:B:447:PHE:HB2	2.56	0.40
1:A:413:LYS:HB3	1:A:413:LYS:HE2	1.89	0.40
1:B:395:MET:HE3	1:B:395:MET:HB3	1.86	0.40
1:B:138:THR:O	1:B:142:LEU:HB2	2.22	0.40
1:B:275:MET:HE2	1:B:290:LEU:HD21	2.04	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	430/487 (88%)	382 (89%)	47 (11%)	1 (0%)	47	69
1	B	418/487 (86%)	367 (88%)	48 (12%)	3 (1%)	22	42
All	All	848/974 (87%)	749 (88%)	95 (11%)	4 (0%)	29	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	PRO
1	B	195	SER
1	B	199	PRO
1	A	43	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	399/443 (90%)	377 (94%)	22 (6%)	21	41
1	B	387/443 (87%)	356 (92%)	31 (8%)	12	25
All	All	786/886 (89%)	733 (93%)	53 (7%)	16	32

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	50	ILE
1	A	62	MET
1	A	66	LYS
1	A	100	SER
1	A	111	VAL
1	A	158	ARG
1	A	163	GLU
1	A	187	THR
1	A	197	ASN
1	A	200	GLN
1	A	219	PHE
1	A	221	LEU
1	A	222	SER
1	A	259	SER
1	A	377	CYS
1	A	381	VAL
1	A	425	ASP
1	A	426	ASN
1	A	440	ARG
1	A	475	LEU
1	A	482	LEU
1	B	42	THR
1	B	51	LEU
1	B	98	CYS
1	B	104	ASN
1	B	127	LYS
1	B	128	ARG
1	B	139	SER
1	B	163	GLU
1	B	184	ILE
1	B	192	ASN
1	B	219	PHE
1	B	221	LEU

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Mol	Chain	Res	Type
1	B	224	THR
1	B	241	PHE
1	B	244	GLU
1	B	276	ILE
1	B	308	GLU
1	B	309	THR
1	B	315	SER
1	B	316	PHE
1	B	318	MET
1	B	365	ARG
1	B	372	ARG
1	B	394	VAL
1	B	395	MET
1	B	426	ASN
1	B	427	ILE
1	B	437	SER
1	B	450	MET
1	B	456	LEU
1	B	482	LEU

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

Mol	Chain	Res	Type
1	A	30	HIS
1	B	159	ASN
1	B	402	HIS
1	B	441	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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	B	601	-	27,50,50	1.94	5 (18%)	17,82,82	1.53	5 (29%)
2	HEM	A	601	1,3	27,50,50	1.90	4 (14%)	17,82,82	2.33	6 (35%)
3	QDP	A	602	2	47,49,49	2.16	6 (12%)	55,67,67	1.59	9 (16%)

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	B	601	-	-	0/6/54/54	-
2	HEM	A	601	1,3	-	0/6/54/54	-
3	QDP	A	602	2	-	12/27/32/32	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	QDP	C12-S11	7.69	1.91	1.83
3	A	602	QDP	C10-S11	6.71	1.89	1.82
3	A	602	QDP	C27-N26	5.92	1.48	1.26
3	A	602	QDP	C35-C09	4.69	1.63	1.53
2	B	601	HEM	C3C-C2C	-4.49	1.34	1.40
2	B	601	HEM	C3B-C2B	-4.13	1.34	1.40
2	A	601	HEM	C3C-C2C	-4.11	1.34	1.40
2	B	601	HEM	C3B-CAB	3.99	1.56	1.47
2	B	601	HEM	C3C-CAC	3.92	1.55	1.47
2	A	601	HEM	C3C-CAC	3.81	1.55	1.47
2	A	601	HEM	C3B-CAB	3.72	1.55	1.47
2	A	601	HEM	C3B-C2B	-3.66	1.35	1.40
3	A	602	QDP	O05-C06	3.63	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	QDP	C06-N08	3.43	1.43	1.34
2	B	601	HEM	CAA-C2A	2.06	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	QDP	C14-C13-C12	5.87	121.54	113.27
2	A	601	HEM	CAD-CBD-CGD	-5.10	104.12	112.67
2	A	601	HEM	CAA-CBA-CGA	-4.37	105.34	112.67
3	A	602	QDP	O05-C06-N08	4.14	116.97	110.02
3	A	602	QDP	O05-C06-O07	-3.71	118.86	125.62
2	A	601	HEM	CBA-CAA-C2A	-3.30	106.40	112.49
2	B	601	HEM	CAD-CBD-CGD	-2.90	107.80	112.67
2	A	601	HEM	CMA-C3A-C4A	-2.86	124.07	128.46
2	A	601	HEM	CMD-C2D-C1D	-2.70	124.32	128.46
3	A	602	QDP	C09-N08-C06	2.65	126.39	122.30
2	B	601	HEM	CMA-C3A-C4A	-2.50	124.63	128.46
3	A	602	QDP	C38-C37-C42	-2.49	114.67	117.89
3	A	602	QDP	C10-C09-C35	2.43	116.59	111.76
3	A	602	QDP	C35-C36-C37	2.40	124.55	120.76
2	B	601	HEM	CMB-C2B-C3B	2.31	128.99	124.68
2	B	601	HEM	CMD-C2D-C1D	-2.18	125.12	128.46
3	A	602	QDP	C39-C38-C37	2.15	123.88	120.89
3	A	602	QDP	O25-C24-N26	-2.06	117.18	123.88
2	B	601	HEM	CAA-CBA-CGA	-2.02	109.28	112.67
2	A	601	HEM	CMA-C3A-C2A	2.02	128.74	124.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	QDP	C24-C12-S11-C10
3	A	602	QDP	C12-C13-C14-C15
3	A	602	QDP	C12-C13-C14-C23
3	A	602	QDP	C09-C35-C36-C45
3	A	602	QDP	O07-C06-O05-C02
3	A	602	QDP	N08-C06-O05-C02
3	A	602	QDP	O07-C06-N08-C09
3	A	602	QDP	O05-C06-N08-C09
3	A	602	QDP	N08-C09-C35-C36
3	A	602	QDP	C10-C09-C35-C36
3	A	602	QDP	C13-C12-C24-O25

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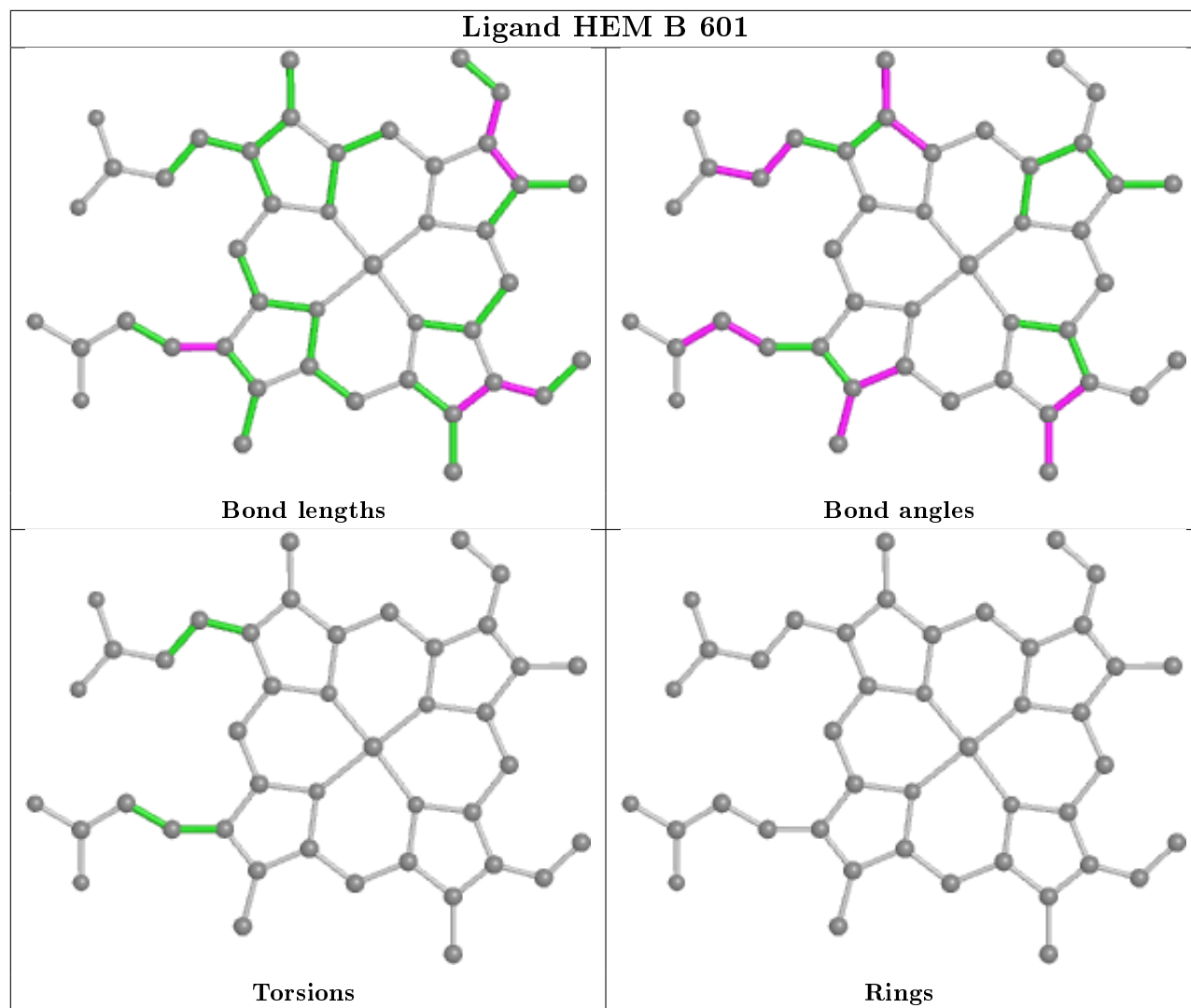
Mol	Chain	Res	Type	Atoms
3	A	602	QDP	C13-C12-S11-C10

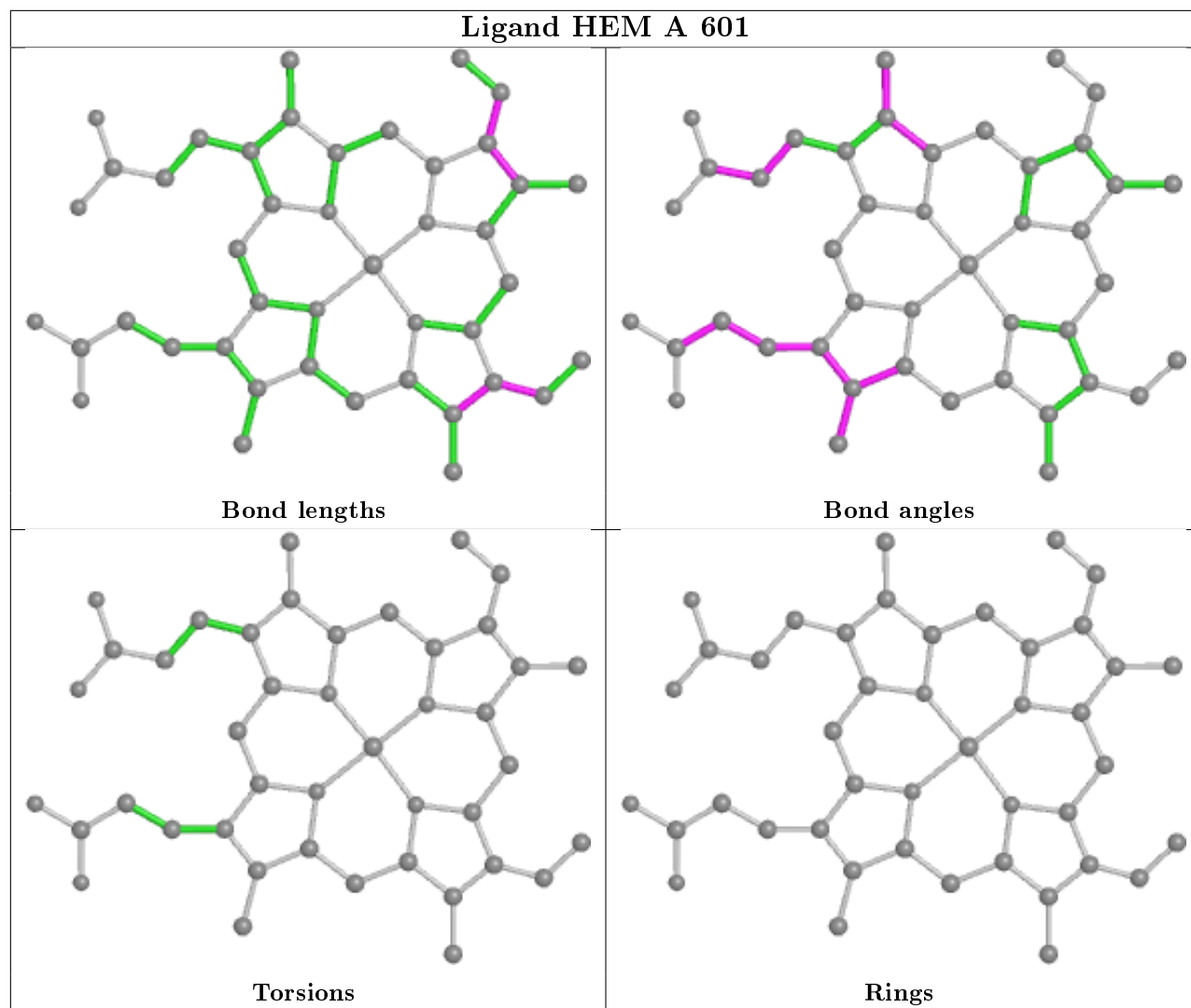
There are no ring outliers.

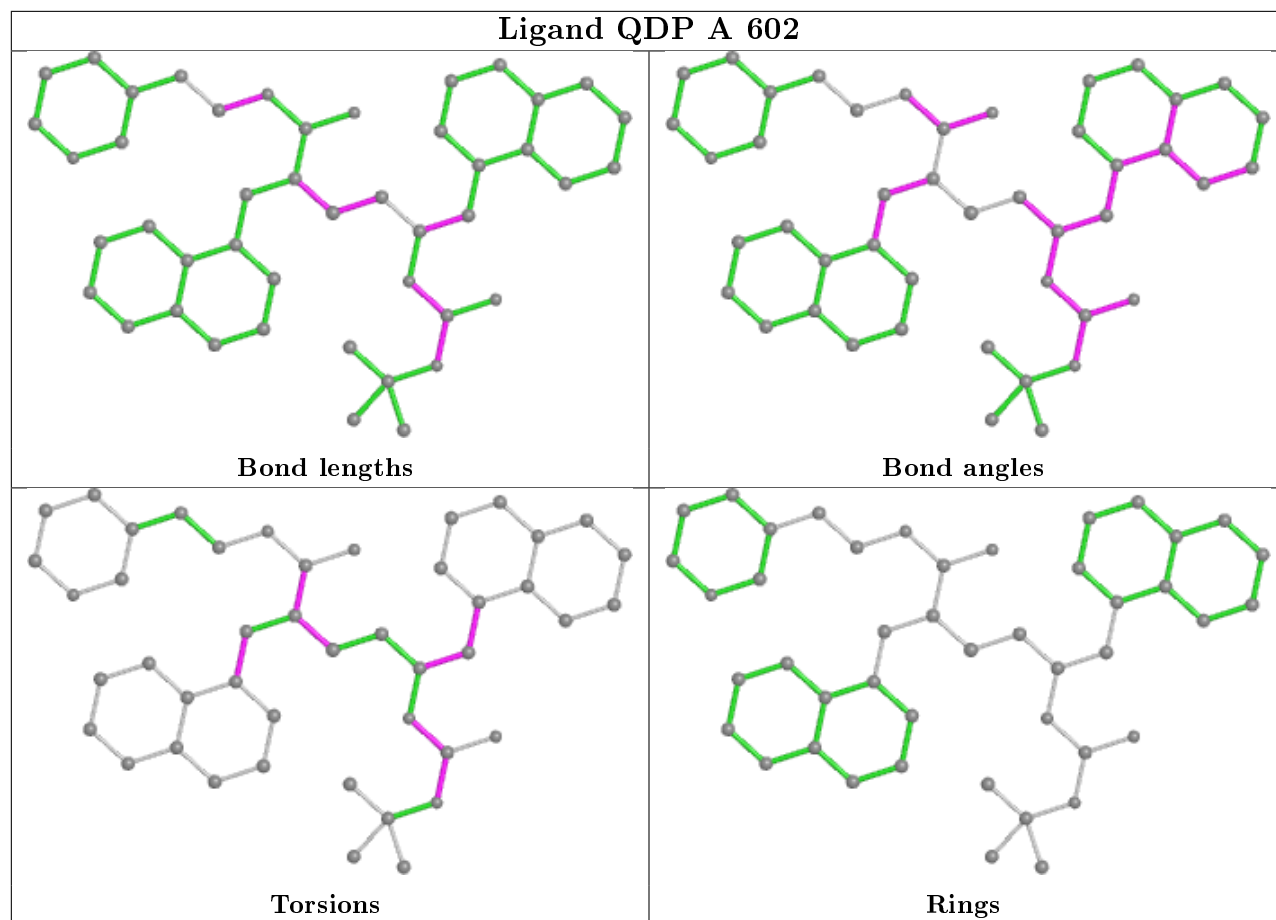
2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	6	0
2	A	601	HEM	9	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	438/487 (89%)	0.09	16 (3%) 41 33	62, 121, 187, 258	0
1	B	426/487 (87%)	0.65	62 (14%) 2 1	81, 175, 283, 369	0
All	All	864/974 (88%)	0.37	78 (9%) 9 5	62, 145, 257, 369	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	PRO	18.3
1	B	156	LEU	9.8
1	B	253	VAL	6.8
1	B	335	ILE	6.6
1	B	457	ILE	6.4
1	B	461	GLN	6.4
1	B	459	VAL	6.1
1	B	165	GLU	5.9
1	B	246	THR	5.2
1	B	133	LEU	5.2
1	B	295	LEU	5.2
1	B	344	PRO	5.2
1	A	167	GLY	5.0
1	B	454	LEU	5.0
1	B	341	ASN	4.9
1	B	189	PHE	4.8
1	B	145	MET	4.8
1	B	271	PHE	4.8
1	B	168	LYS	4.6
1	B	118	ILE	4.6
1	B	494	GLU	4.4
1	B	446	ARG	4.2
1	A	492	LYS	4.2
1	A	164	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	278	SER	4.0
1	B	167	GLY	3.9
1	B	241	PHE	3.9
1	B	302	PHE	3.8
1	B	298	GLN	3.8
1	A	275	MET	3.7
1	B	450	MET	3.7
1	B	493	VAL	3.7
1	B	154	ASP	3.6
1	B	292	ASP	3.4
1	B	127	LYS	3.4
1	B	166	THR	3.4
1	B	153	GLY	3.3
1	B	325	PRO	3.2
1	B	481	GLY	3.2
1	B	347	TYR	3.1
1	B	452	MET	2.9
1	B	254	LYS	2.9
1	B	240	VAL	2.8
1	A	493	VAL	2.8
1	B	132	LEU	2.8
1	B	115	LYS	2.8
1	B	129	LEU	2.7
1	B	190	GLY	2.7
1	A	218	PRO	2.6
1	B	352	GLN	2.6
1	B	112	GLY	2.6
1	A	254	LYS	2.6
1	B	113	PHE	2.5
1	B	275	MET	2.5
1	B	334	GLU	2.5
1	A	168	LYS	2.5
1	B	274	LEU	2.4
1	A	335	ILE	2.4
1	A	163	GLU	2.4
1	A	226	PHE	2.4
1	B	164	ALA	2.4
1	A	191	VAL	2.3
1	B	290	LEU	2.3
1	B	462	ASN	2.3
1	A	460	LEU	2.3
1	B	160	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	271	PHE	2.2
1	B	482	LEU	2.2
1	B	336	ASP	2.1
1	A	192	ASN	2.1
1	B	179	TYR	2.1
1	B	149	ILE	2.1
1	B	146	VAL	2.1
1	B	136	THR	2.1
1	B	276	ILE	2.1
1	B	111	VAL	2.0
1	B	456	LEU	2.0
1	B	293	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

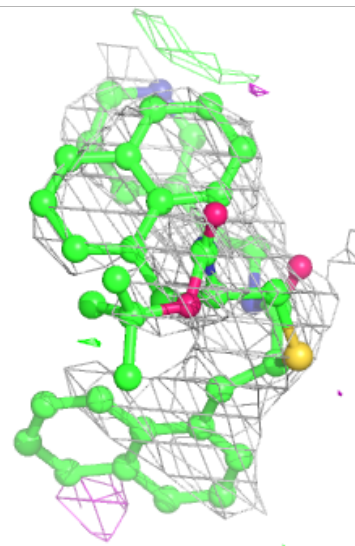
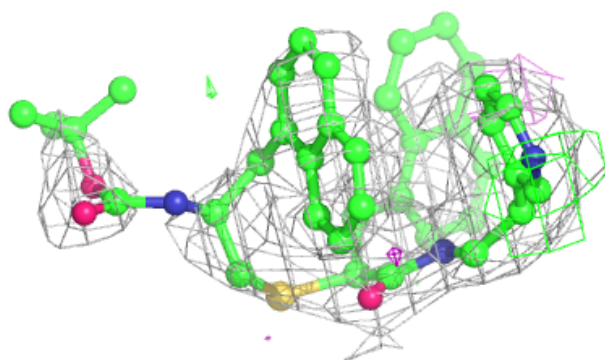
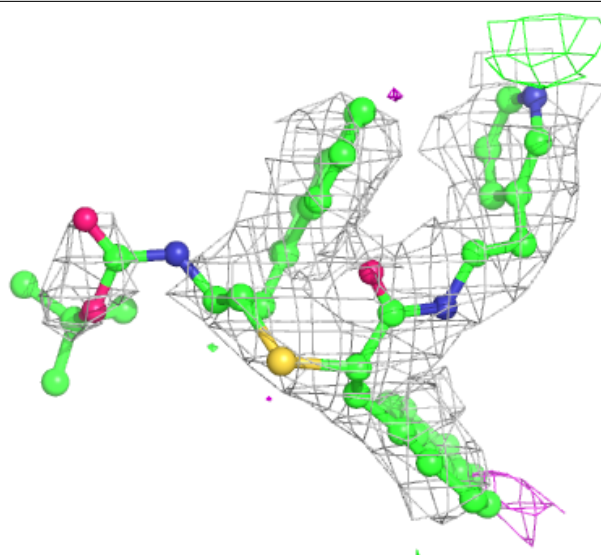
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	QDP	A	602	45/45	0.89	0.30	90,148,179,185	0
2	HEM	A	601	43/43	0.97	0.23	49,70,96,111	0
2	HEM	B	601	43/43	0.98	0.20	67,99,142,145	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.

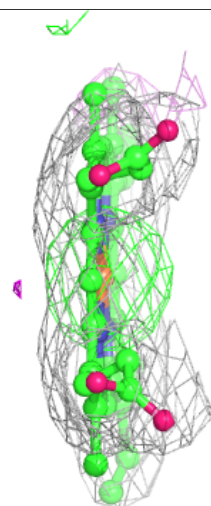
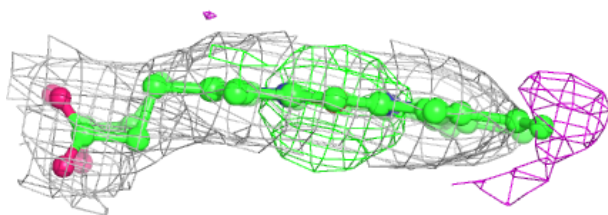
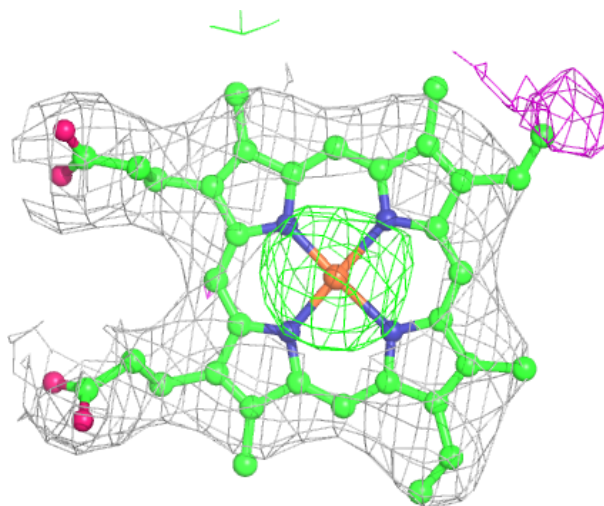
Electron density around QDP A 602:

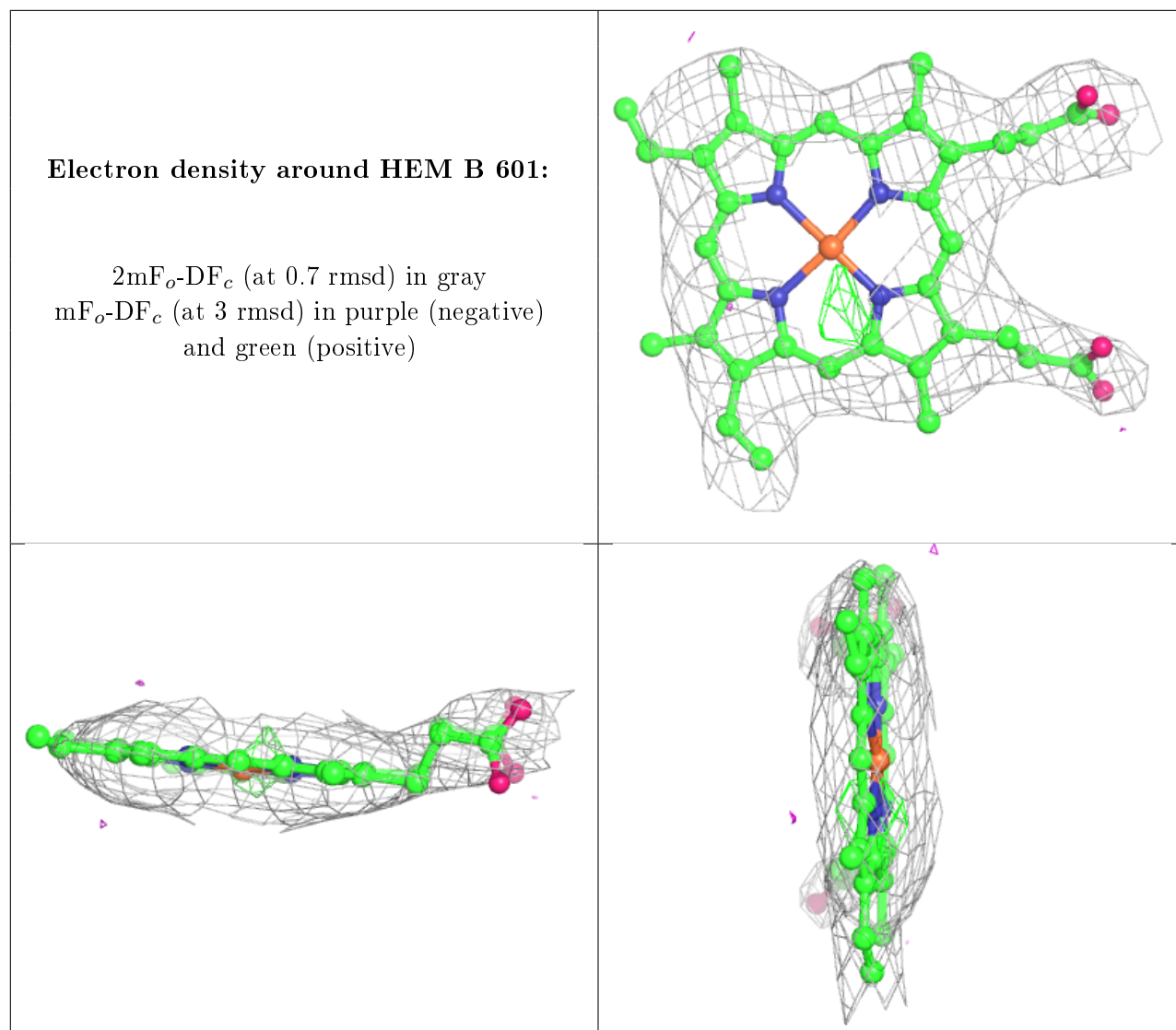
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.