Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:22 AM EST

PDB ID	:	3J7B
EMDB ID	:	EMD-6314
Title	:	Catalase solved at 3.2 Angstrom resolution by MicroED
Authors	:	Nannenga, B.L.; Shi, D.; Hattne, J.; Reyes, F.E.; Gonen, T.
Deposited on	:	2014-06-09
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

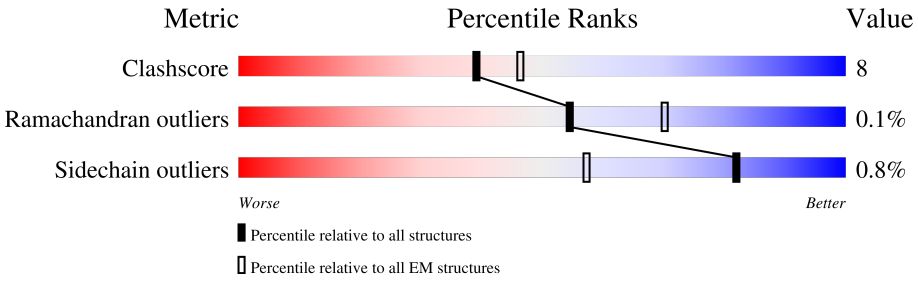
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	19% 77% 17% • 5%
1	B	527	23% 76% 19% 5%
1	C	527	77% 77% 17% 5%
1	D	527	61% 76% 18% • 5%

2 Entry composition

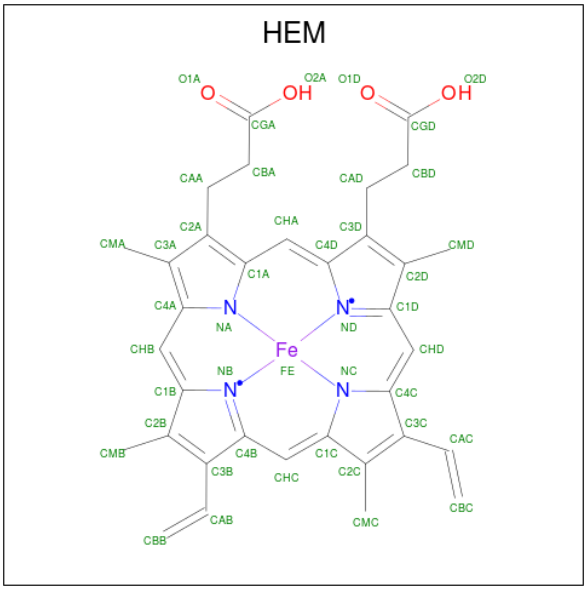
There are 3 unique types of molecules in this entry. The entry contains 16432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Catalase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	B	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	C	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	D	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		

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



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

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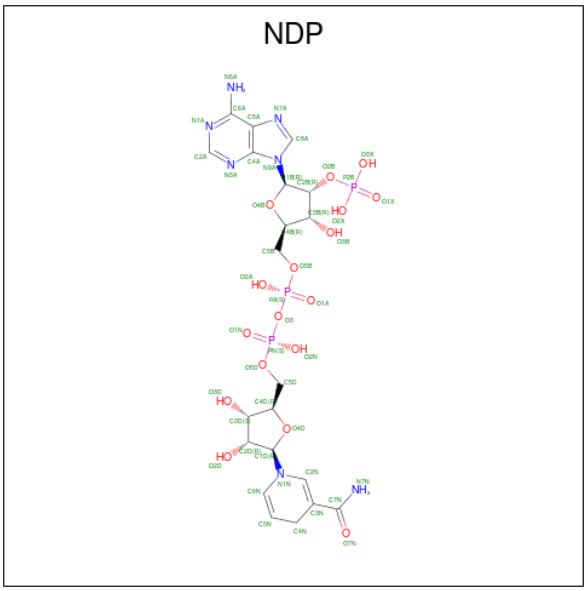
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



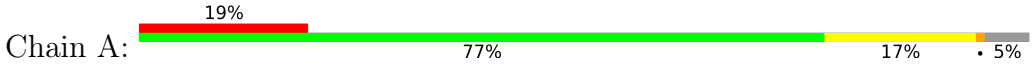
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	B	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	C	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	D	1	Total	C	N	O	P	0
			48	21	7	17	3	

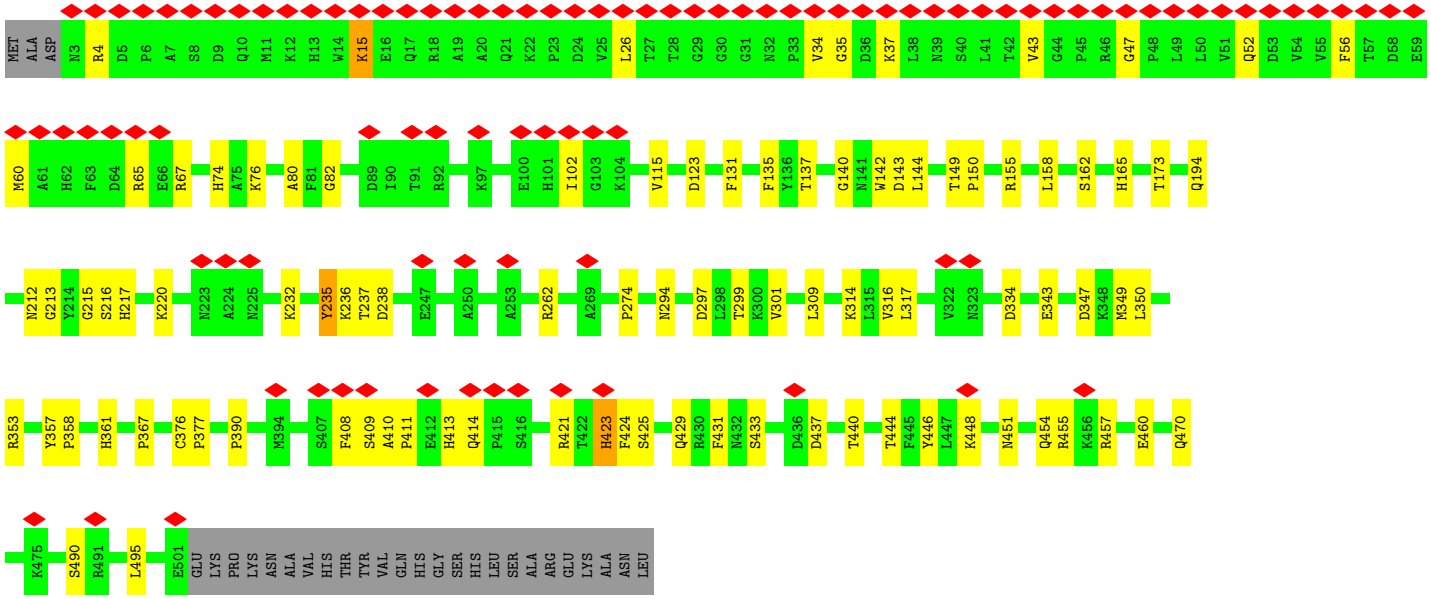
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Catalase

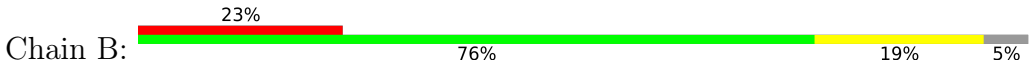
Chain A:

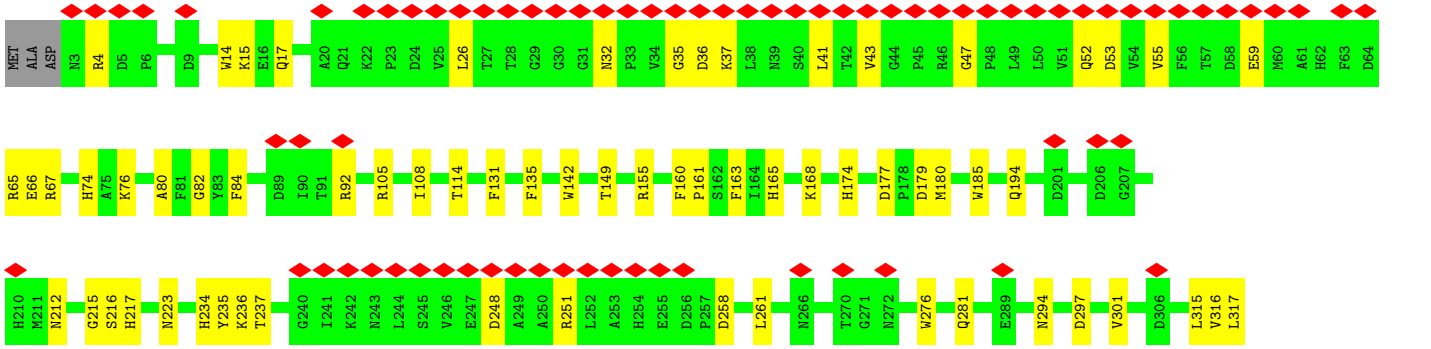


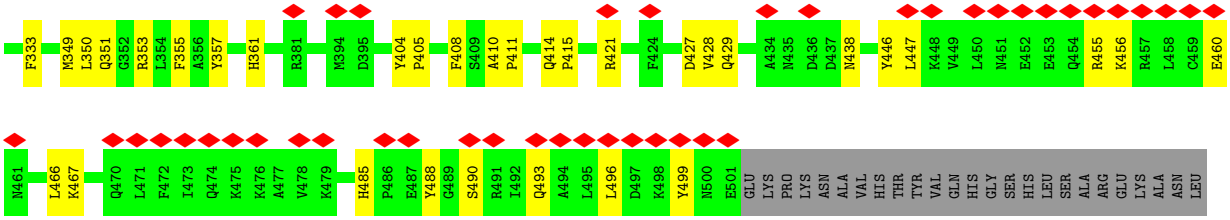


• Molecule 1: Catalase

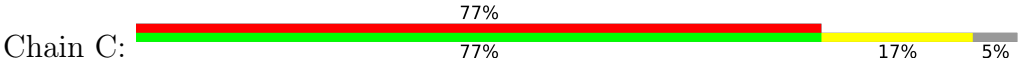
Chain B:



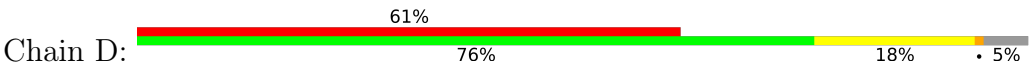


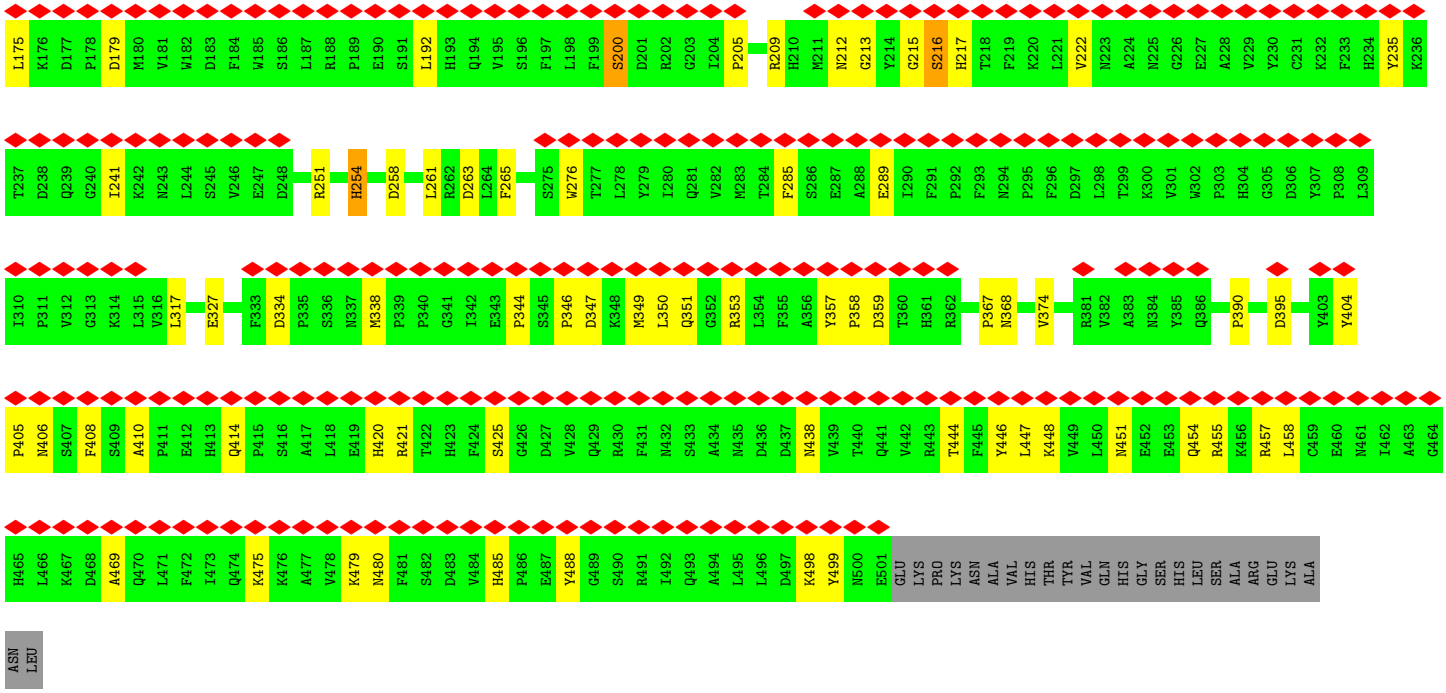


• Molecule 1: Catalase



• Molecule 1: Catalase




L175 K176 D177 P178 D179 M180 V181 W182 D183 F184 W185 S186 L187 R188 P189 E190 S191 L192 H193 Q194 V195 S196 F197 L198 F199 S200 D201 R202 G203 I204 P205 R209 H210 M211 N212 G213 Y214 G215 S216 H217 T218 F219 K220 L221 V222 N223 A224 N225 G226 E227 A228 V229 Y230 C231 K232 F233 H234 Y235 K236
T237 D238 Q239 C240 I241 K242 N243 L244 S245 V246 E247 D248 R251 H254 D258 L261 R262 D263 L264 F265 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 A288 E289 I290 F291 P292 F293 N294 P295 F296 D297 L298 T299 K300 V301 W302 P303 H304 G305 D306 Y307 P308 L309
I310 P311 V312 G313 K314 L315 V316 L317 E327 F333 D334 P335 S336 N337 M338 P339 P340 G341 I342 E343 P344 S345 P346 D347 K348 M349 L350 Q351 G352 R353 L354 F355 A356 Y357 P358 D359 T360 H361 R362 P367 N368 V374 R381 V382 A383 N384 Y385 Q386 P390 D395 Y403 Y404
P405 N406 S407 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 L418 E419 H420 R421 T422 H423 F424 S425 G426 D427 V428 Q429 R430 F431 N432 S433 A434 N435 D436 D437 N438 V439 T440 Q441 V442 R443 T444 F445 Y446 L447 K448 V449 L450 N451 E452 E453 Q454 R455 K456 R457 L458 C459 E460 M461 I462 A463 G464
H465 L466 K467 D468 A469 Q470 L471 F472 I473 Q474 K475 K476 A477 V478 K479 N480 F481 S482 D483 V484 H485 P486 E487 Y488 G489 S490 R491 I492 Q493 A494 L495 L496 D497 K498 Y499 N500 E501 GLU LYS PRO LYS ASN ALA VAL HIS THR TYR VAL GLN HIS GLY SER HIS LEU SER ALA ARG GLU LYS ALA
ASN LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a=Not provided Å, b=Not provided Å, c=Not provided Å, α=Not provided°, β=Not provided°, γ=Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose (e^-/Å^2)	0.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	5.384	Depositor
Minimum map value	-3.715	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	67.64004, 172.08072, 182.0712	wwPDB
Map dimensions	240, 216, 90	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.751556, 0.79667, 0.75863	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 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	0.32	0/4137	0.53	0/5619
1	B	0.34	0/4137	0.54	0/5619
1	C	0.32	0/4137	0.53	2/5619 (0.0%)
1	D	0.31	0/4137	0.51	0/5619
All	All	0.32	0/16548	0.53	2/22476 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	427	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	C	427	ASP	CB-CG-OD1	5.37	123.13	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	200	SER	Peptide

5.2 Too-close contacts (i)

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	4017	0	3844	66	0
1	B	4017	0	3844	84	0
1	C	4017	0	3844	71	0
1	D	4017	0	3844	71	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	48	0	26	2	0
3	B	48	0	26	3	0
3	C	48	0	26	3	0
3	D	48	0	26	1	0
All	All	16432	0	15600	250	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 8.

All (250) 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:150:PRO:HG3	3:A:602:NDP:H41N	1.55	0.87
1:B:235:TYR:CZ	1:B:276:TRP:HB2	2.17	0.79
1:B:174:HIS:HB3	1:C:261:LEU:HD21	1.65	0.78
1:D:251:ARG:O	1:D:254:HIS:CD2	2.38	0.77
1:B:235:TYR:CE1	1:B:315:LEU:HD12	2.20	0.77
1:A:409:SER:OG	1:C:15:LYS:NZ	2.19	0.74
1:D:251:ARG:O	1:D:254:HIS:HD2	1.71	0.72
1:A:149:THR:HG21	1:A:194:GLN:HE22	1.54	0.72
1:A:65:ARG:NH1	1:D:359:ASP:OD2	2.22	0.71
1:D:209:ARG:NH1	1:D:263:ASP:OD2	2.23	0.70
1:B:37:LYS:NZ	1:B:59:GLU:OE2	2.21	0.70
1:B:408:PHE:HA	1:D:15:LYS:HD3	1.74	0.70
1:A:67:ARG:HH21	1:D:168:LYS:HE2	1.58	0.69
1:B:490:SER:HA	1:B:493:GLN:HB3	1.77	0.67
1:C:427:ASP:OD2	1:C:429:GLN:HG2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASP:HB3	1:A:350:LEU:HB3	1.77	0.67
1:B:67:ARG:HH21	1:C:168:LYS:HE2	1.60	0.65
1:C:43:VAL:HG11	1:D:43:VAL:HG11	1.79	0.64
1:C:212:ASN:ND2	1:C:241:ILE:HD11	2.13	0.63
1:D:475:LYS:O	1:D:479:LYS:HG2	1.98	0.63
1:B:131:PHE:CZ	1:B:235:TYR:CE2	2.87	0.63
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.63	0.62
1:D:150:PRO:HG3	3:D:602:NDP:H41N	1.81	0.62
1:B:168:LYS:HE2	1:C:67:ARG:HH21	1.64	0.61
1:C:236:LYS:NZ	3:C:602:NDP:O1X	2.32	0.61
1:C:139:ASP:HB3	1:C:340:PRO:HD2	1.83	0.60
1:A:444:THR:O	1:A:448:LYS:HG2	2.02	0.60
1:C:40:SER:HB3	1:C:49:LEU:HD13	1.83	0.60
1:D:213:GLY:HA3	1:D:235:TYR:CE1	2.36	0.59
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.84	0.59
1:A:451:ASN:O	1:A:455:ARG:HG3	2.02	0.59
1:B:235:TYR:HE1	1:B:315:LEU:HB2	1.66	0.59
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.66	0.59
1:C:213:GLY:HA3	1:C:235:TYR:CE1	2.38	0.59
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.85	0.58
1:B:36:ASP:O	1:C:430:ARG:NH1	2.37	0.58
1:B:258:ASP:OD2	1:C:169:ARG:NH1	2.31	0.58
1:C:150:PRO:HG3	3:C:602:NDP:H41N	1.85	0.57
1:B:53:ASP:OD1	1:C:430:ARG:NH2	2.38	0.57
1:A:76:LYS:NZ	1:A:123:ASP:OD1	2.32	0.57
1:D:258:ASP:HB3	1:D:261:LEU:HB3	1.85	0.57
1:A:216:SER:O	1:A:232:LYS:NZ	2.25	0.57
1:B:52:GLN:HE21	1:D:351:GLN:HE22	1.53	0.57
1:A:15:LYS:NZ	1:C:407:SER:O	2.30	0.57
2:B:601:HEM:HMD2	2:B:601:HEM:HBD2	1.87	0.56
1:C:71:ARG:NH2	1:C:331:LEU:O	2.37	0.56
1:A:423:HIS:HB2	1:B:427:ASP:HA	1.87	0.56
1:B:235:TYR:CE1	1:B:315:LEU:HB2	2.41	0.56
1:A:274:PRO:HG2	1:A:317:LEU:HB2	1.87	0.56
1:B:43:VAL:O	1:B:47:GLY:HA3	2.05	0.56
1:A:361:HIS:NE2	2:A:601:HEM:O1A	2.29	0.55
1:A:408:PHE:HA	1:C:15:LYS:HD2	1.88	0.55
1:C:149:THR:HG21	1:C:194:GLN:HE22	1.73	0.55
1:B:351:GLN:NE2	1:D:52:GLN:OE1	2.40	0.54
1:B:236:LYS:NZ	3:B:602:NDP:O1X	2.39	0.54
1:B:65:ARG:NH1	1:C:359:ASP:OD2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:HEM:HMC1	2:D:601:HEM:HBC2	1.89	0.54
1:D:200:SER:HB2	1:D:458:LEU:HD13	1.90	0.53
1:D:40:SER:HB3	1:D:49:LEU:HD13	1.91	0.53
1:A:236:LYS:HE3	1:A:309:LEU:HD21	1.91	0.53
1:A:82:GLY:HA3	1:A:316:VAL:O	2.08	0.53
1:B:82:GLY:HA3	1:B:316:VAL:O	2.08	0.53
1:B:35:GLY:HA2	1:D:414:GLN:O	2.09	0.53
1:C:429:GLN:HB3	1:D:421:ARG:HG2	1.91	0.52
1:B:80:ALA:HB3	1:B:317:LEU:HD13	1.90	0.52
1:D:347:ASP:O	1:D:351:GLN:HG2	2.08	0.52
1:D:215:GLY:O	1:D:217:HIS:N	2.39	0.52
1:B:4:ARG:NH1	1:C:468:ASP:O	2.42	0.52
1:A:4:ARG:NH2	1:D:179:ASP:OD2	2.42	0.52
1:A:165:HIS:NE2	1:D:66:GLU:OE2	2.30	0.52
1:B:92:ARG:O	1:B:223:ASN:ND2	2.39	0.52
1:C:4:ARG:NE	1:C:9:ASP:OD1	2.39	0.52
1:B:456:LYS:O	1:B:460:GLU:HG3	2.11	0.51
1:D:368:ASN:ND2	1:D:390:PRO:O	2.37	0.51
1:B:404:TYR:CD1	1:B:405:PRO:HA	2.46	0.51
1:D:222:VAL:HG21	1:D:420:HIS:HB2	1.93	0.51
1:B:237:THR:HA	1:B:276:TRP:CD1	2.45	0.51
1:D:212:ASN:ND2	1:D:241:ILE:HD11	2.26	0.51
1:B:165:HIS:NE2	1:C:66:GLU:OE2	2.35	0.51
1:B:212:ASN:OD1	1:B:237:THR:HG22	2.11	0.50
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.92	0.50
1:D:327:GLU:HA	1:D:374:VAL:HG11	1.94	0.50
1:B:26:LEU:HD21	1:B:37:LYS:HD3	1.93	0.50
2:C:601:HEM:HMC1	2:C:601:HEM:HBC2	1.93	0.50
1:B:15:LYS:HD2	1:D:408:PHE:HA	1.94	0.50
1:C:429:GLN:OE1	1:D:421:ARG:HD2	2.12	0.50
1:D:285:PHE:O	1:D:289:GLU:HG3	2.12	0.50
1:C:179:ASP:OD1	1:C:469:ALA:HA	2.12	0.50
1:D:447:LEU:HD11	1:D:485:HIS:CD2	2.47	0.49
1:B:149:THR:HG21	1:B:194:GLN:HE22	1.77	0.49
1:D:446:TYR:HD2	1:D:447:LEU:HD12	1.77	0.49
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.94	0.49
1:C:217:HIS:HB2	1:C:219:PHE:CZ	2.47	0.49
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.94	0.49
1:D:446:TYR:O	1:D:455:ARG:HD3	2.13	0.49
1:B:261:LEU:HD21	1:C:174:HIS:HB3	1.95	0.48
1:D:404:TYR:CD1	1:D:405:PRO:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:NH1	1:A:299:THR:OG1	2.46	0.48
1:A:217:HIS:CD2	1:A:353:ARG:HH11	2.31	0.48
1:B:235:TYR:CZ	1:B:276:TRP:CB	2.91	0.48
1:C:43:VAL:HG23	1:C:48:PRO:HD2	1.96	0.48
1:D:80:ALA:HB3	1:D:317:LEU:HD13	1.94	0.48
1:D:217:HIS:CD2	1:D:353:ARG:HH11	2.31	0.48
1:B:258:ASP:HB3	1:B:261:LEU:HB3	1.96	0.47
1:C:467:LYS:HD3	1:C:499:TYR:CD1	2.49	0.47
1:D:179:ASP:OD1	1:D:469:ALA:HA	2.14	0.47
1:A:349:MET:O	1:A:353:ARG:HG3	2.14	0.47
1:D:395:ASP:OD1	1:D:395:ASP:N	2.44	0.47
1:B:446:TYR:O	1:B:455:ARG:HD3	2.13	0.47
1:B:55:VAL:HB	1:C:430:ARG:HH22	1.79	0.47
1:B:74:HIS:HA	1:B:114:THR:O	2.14	0.47
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.50	0.47
1:A:390:PRO:HG3	1:C:68:ILE:HG22	1.97	0.47
1:B:428:VAL:HG22	1:C:43:VAL:HG12	1.95	0.47
1:C:447:LEU:HD11	1:C:485:HIS:CE1	2.50	0.47
1:D:129:ARG:HG3	1:D:205:PRO:HG2	1.97	0.47
1:C:82:GLY:HA3	1:C:316:VAL:O	2.14	0.47
1:A:137:THR:OG1	1:A:140:GLY:O	2.16	0.47
1:B:55:VAL:HB	1:C:430:ARG:NH2	2.30	0.47
1:A:437:ASP:OD2	1:A:440:THR:OG1	2.30	0.46
1:B:301:VAL:HG21	3:B:602:NDP:H2D	1.96	0.46
1:A:238:ASP:OD2	1:A:314:LYS:HE2	2.15	0.46
1:A:144:LEU:HG	1:A:235:TYR:OH	2.14	0.46
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.97	0.46
1:A:213:GLY:HA3	1:A:235:TYR:CD2	2.50	0.46
1:A:43:VAL:O	1:A:47:GLY:HA3	2.15	0.46
1:A:43:VAL:HG21	1:B:43:VAL:HG21	1.98	0.46
1:D:26:LEU:HD21	1:D:37:LYS:HD3	1.97	0.46
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.97	0.46
1:A:429:GLN:OE1	1:B:421:ARG:NH1	2.49	0.46
1:B:108:ILE:HD13	1:B:315:LEU:HD22	1.96	0.46
1:B:163:PHE:HE1	1:B:185:TRP:HE1	1.64	0.46
1:A:142:TRP:CH2	1:A:144:LEU:HD22	2.51	0.46
1:B:52:GLN:NE2	1:D:351:GLN:HE22	2.14	0.46
1:B:66:GLU:OE2	1:C:165:HIS:NE2	2.48	0.46
1:C:74:HIS:HA	1:C:114:THR:O	2.16	0.46
1:C:151:ILE:HG13	1:C:194:GLN:OE1	2.16	0.46
1:C:161:PRO:O	1:C:165:HIS:ND1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:THR:HG23	1:D:448:LYS:HD3	1.96	0.46
1:B:84:PHE:HB2	1:B:315:LEU:CD2	2.46	0.45
1:D:77:GLY:HA2	1:D:112:PHE:O	2.15	0.45
1:A:421:ARG:HD2	1:B:429:GLN:OE1	2.16	0.45
1:D:346:PRO:HA	1:D:351:GLN:NE2	2.32	0.45
1:D:137:THR:OG1	1:D:140:GLY:O	2.28	0.45
1:A:213:GLY:HA3	1:A:235:TYR:HD2	1.80	0.45
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.21	0.45
1:A:294:ASN:HB3	1:A:297:ASP:HB2	1.97	0.45
1:B:215:GLY:C	1:B:216:SER:HG	2.19	0.45
1:C:160:PHE:HB3	1:C:161:PRO:HD3	1.98	0.45
1:C:349:MET:O	1:C:353:ARG:HG3	2.16	0.45
1:B:76:LYS:NZ	1:B:258:ASP:OD1	2.42	0.45
1:B:446:TYR:CE2	1:B:488:TYR:HB2	2.51	0.45
1:C:294:ASN:HB3	1:C:297:ASP:HB2	1.99	0.45
1:D:110:VAL:HG22	1:D:133:VAL:HG22	1.99	0.45
1:B:355:PHE:CZ	1:C:57:THR:HG23	2.52	0.45
1:B:179:ASP:OD1	1:B:180:MET:N	2.50	0.45
1:B:456:LYS:HB3	1:B:456:LYS:HE2	1.83	0.44
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.97	0.44
1:B:41:LEU:HB3	1:B:53:ASP:HB2	1.99	0.44
1:A:424:PHE:O	1:A:425:SER:OG	2.29	0.44
1:A:454:GLN:HG2	1:A:457:ARG:HH21	1.81	0.44
1:B:217:HIS:CD2	1:B:350:LEU:HD13	2.52	0.44
1:D:215:GLY:C	1:D:216:SER:HG	2.20	0.44
1:A:56:PHE:CE1	1:A:60:MET:HE3	2.52	0.44
1:B:32:ASN:ND2	1:D:139:ASP:O	2.36	0.44
1:C:456:LYS:O	1:C:460:GLU:HG3	2.17	0.44
1:D:155:ARG:NH2	1:D:438:ASN:OD1	2.38	0.44
1:A:301:VAL:HG21	3:A:602:NDP:H2D	1.98	0.44
1:C:89:ASP:OD1	1:C:102:ILE:HG13	2.17	0.44
1:B:447:LEU:HD11	1:B:485:HIS:CD2	2.53	0.44
1:C:497:ASP:OD1	1:C:498:LYS:N	2.51	0.44
1:D:454:GLN:HG2	1:D:457:ARG:NH2	2.32	0.44
1:A:26:LEU:O	1:A:34:VAL:HG22	2.18	0.44
1:B:294:ASN:HB3	1:B:297:ASP:HB2	2.00	0.44
1:D:143:ASP:HB2	1:D:334:ASP:O	2.18	0.44
3:B:602:NDP:H1B	3:B:602:NDP:C5N	2.48	0.44
1:A:52:GLN:HA	1:C:354:LEU:HD13	2.00	0.43
1:D:349:MET:O	1:D:353:ARG:HG3	2.19	0.43
1:D:192:LEU:HD11	1:D:480:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TYR:CE1	1:B:276:TRP:HB2	2.51	0.43
1:B:248:ASP:HB2	1:B:251:ARG:HH21	1.82	0.43
1:C:74:HIS:CE1	1:C:115:VAL:HG22	2.53	0.43
1:C:414:GLN:HA	1:C:415:PRO:HD3	1.80	0.43
1:A:35:GLY:HA2	1:C:414:GLN:O	2.18	0.43
1:A:215:GLY:O	1:A:217:HIS:N	2.45	0.43
3:C:602:NDP:H71N	3:C:602:NDP:H2N	1.63	0.43
1:A:414:GLN:O	1:C:35:GLY:HA2	2.18	0.43
1:C:395:ASP:OD1	1:C:395:ASP:N	2.51	0.43
1:B:467:LYS:HD3	1:B:499:TYR:CG	2.53	0.43
1:C:37:LYS:HB3	1:C:37:LYS:HE3	1.84	0.43
1:D:74:HIS:HA	1:D:114:THR:O	2.19	0.43
1:D:357:TYR:HB2	1:D:358:PRO:HD3	2.01	0.43
1:A:102:ILE:HD12	1:A:102:ILE:H	1.84	0.42
1:B:168:LYS:HE2	1:C:67:ARG:NH2	2.33	0.42
1:D:448:LYS:NZ	1:D:448:LYS:HB3	2.32	0.42
1:A:212:ASN:OD1	1:A:237:THR:HG22	2.19	0.42
1:A:143:ASP:HB2	1:A:334:ASP:O	2.19	0.42
1:B:108:ILE:HG21	1:B:315:LEU:HD22	2.00	0.42
1:B:177:ASP:HB3	1:B:180:MET:SD	2.59	0.42
1:D:338:MET:SD	1:D:344:PRO:HD3	2.59	0.42
1:C:73:VAL:HG12	1:C:74:HIS:CD2	2.54	0.42
1:B:248:ASP:HB2	1:B:251:ARG:NH2	2.35	0.42
1:B:414:GLN:HA	1:B:415:PRO:HD3	1.89	0.42
1:D:18:ARG:HG2	1:D:18:ARG:O	2.19	0.42
1:D:95:LYS:HG2	1:D:222:VAL:O	2.20	0.42
1:D:135:PHE:HB2	1:D:142:TRP:HB3	2.00	0.42
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	2.01	0.42
1:C:217:HIS:ND1	1:C:350:LEU:HB2	2.34	0.42
1:D:131:PHE:HZ	1:D:276:TRP:CE2	2.38	0.42
1:A:173:THR:HG22	1:D:265:PHE:CZ	2.55	0.42
1:A:410:ALA:HB1	1:A:411:PRO:HD2	2.02	0.42
1:A:421:ARG:NH1	1:B:427:ASP:OD2	2.53	0.42
1:D:451:ASN:OD1	1:D:454:GLN:HG3	2.18	0.42
1:C:84:PHE:O	1:C:105:ARG:HA	2.20	0.42
1:A:37:LYS:HG2	1:D:158:LEU:HD22	2.02	0.41
1:A:262:ARG:NH1	1:D:175:LEU:HD13	2.34	0.41
1:A:446:TYR:CZ	1:A:455:ARG:HD2	2.55	0.41
1:C:186:SER:O	1:C:480:ASN:ND2	2.50	0.41
1:D:41:LEU:O	1:D:49:LEU:HD12	2.20	0.41
1:A:135:PHE:HB2	1:A:142:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LYS:HE3	1:A:309:LEU:CD2	2.50	0.41
1:B:466:LEU:HD23	1:B:496:LEU:HD11	2.02	0.41
1:B:349:MET:CE	2:B:601:HEM:HAB	2.50	0.41
1:C:427:ASP:CG	1:C:429:GLN:HG2	2.41	0.41
1:A:162:SER:HB3	1:B:404:TYR:H	1.86	0.41
1:B:333:PHE:O	1:B:361:HIS:HE1	2.04	0.41
1:C:127:ASP:O	1:C:129:ARG:NH1	2.54	0.41
1:A:367:PRO:HG3	1:C:65:ARG:HD3	2.03	0.41
1:A:429:GLN:HG2	1:A:431:PHE:CZ	2.55	0.41
1:B:14:TRP:O	1:B:17:GLN:HG2	2.19	0.41
1:B:234:HIS:NE2	1:B:281:GLN:OE1	2.54	0.41
1:C:135:PHE:HB2	1:C:142:TRP:HB3	2.03	0.41
1:C:200:SER:OG	1:C:201:ASP:N	2.54	0.41
1:B:235:TYR:CE2	1:B:276:TRP:CG	3.09	0.41
1:B:353:ARG:NH2	1:B:357:TYR:OH	2.47	0.41
1:C:80:ALA:HB3	1:C:317:LEU:HD13	2.02	0.41
1:D:485:HIS:O	1:D:488:TYR:HB3	2.21	0.41
1:A:460:GLU:HG2	1:A:495:LEU:HD11	2.02	0.41
1:B:217:HIS:ND1	1:B:350:LEU:HB2	2.36	0.41
1:C:145:VAL:HB	1:C:353:ARG:HH22	1.86	0.41
1:C:446:TYR:O	1:C:455:ARG:HD3	2.20	0.41
1:A:158:LEU:HD21	1:D:56:PHE:HA	2.03	0.40
1:A:376:CYS:HA	1:A:377:PRO:HD3	1.94	0.40
1:A:80:ALA:HB3	1:A:317:LEU:HD13	2.03	0.40
1:C:220:LYS:NZ	1:C:420:HIS:HB3	2.36	0.40
1:C:427:ASP:OD1	1:C:428:VAL:N	2.53	0.40
1:A:220:LYS:HB3	1:A:343:GLU:HB2	2.03	0.40
1:C:425:SER:HB2	1:D:425:SER:HB2	2.03	0.40
1:A:470:GLN:HE22	1:D:12:LYS:HB2	1.87	0.40
1:B:84:PHE:O	1:B:105:ARG:HA	2.22	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 PDB entries followed by that with respect to all EM entries.

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	497/527 (94%)	481 (97%)	16 (3%)	0	100 100
1	B	497/527 (94%)	480 (97%)	17 (3%)	0	100 100
1	C	497/527 (94%)	481 (97%)	15 (3%)	1 (0%)	47 79
1	D	497/527 (94%)	479 (96%)	17 (3%)	1 (0%)	47 79
All	All	1988/2108 (94%)	1921 (97%)	65 (3%)	2 (0%)	54 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	427	ASP
1	D	216	SER

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 PDB entries followed by that with respect to all EM entries.

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	431/454 (95%)	424 (98%)	7 (2%)	62 84
1	B	431/454 (95%)	431 (100%)	0	100 100
1	C	431/454 (95%)	428 (99%)	3 (1%)	84 94
1	D	431/454 (95%)	427 (99%)	4 (1%)	78 91
All	All	1724/1816 (95%)	1710 (99%)	14 (1%)	82 93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	131	PHE
1	A	235	TYR
1	A	413	HIS
1	A	423	HIS
1	A	433	SER

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Mol	Chain	Res	Type
1	A	490	SER
1	C	89	ASP
1	C	131	PHE
1	C	427	ASP
1	D	131	PHE
1	D	254	HIS
1	D	498	LYS
1	D	499	TYR

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

Mol	Chain	Res	Type
1	B	52	GLN
1	D	39	ASN
1	D	167	GLN
1	D	413	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

8 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	D	601	1	41,50,50	1.90	6 (14%)	45,82,82	1.63	10 (22%)
3	NDP	A	602	-	45,52,52	2.38	6 (13%)	53,80,80	1.70	13 (24%)
2	HEM	A	601	1	41,50,50	1.90	7 (17%)	45,82,82	1.61	5 (11%)
2	HEM	B	601	1	41,50,50	2.07	8 (19%)	45,82,82	1.53	9 (20%)
2	HEM	C	601	1	41,50,50	1.92	6 (14%)	45,82,82	1.95	13 (28%)
3	NDP	D	602	-	45,52,52	2.55	5 (11%)	53,80,80	1.65	11 (20%)
3	NDP	C	602	-	45,52,52	2.58	5 (11%)	53,80,80	1.71	11 (20%)
3	NDP	B	602	-	45,52,52	2.33	6 (13%)	53,80,80	1.71	12 (22%)

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	D	601	1	-	2/12/54/54	-
3	NDP	A	602	-	-	12/30/77/77	0/5/5/5
2	HEM	A	601	1	-	5/12/54/54	-
2	HEM	B	601	1	-	5/12/54/54	-
2	HEM	C	601	1	-	2/12/54/54	-
3	NDP	D	602	-	-	10/30/77/77	0/5/5/5
3	NDP	C	602	-	-	12/30/77/77	0/5/5/5
3	NDP	B	602	-	-	12/30/77/77	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	NDP	P2B-O2B	14.88	1.87	1.59
3	D	602	NDP	P2B-O2B	14.79	1.87	1.59
3	A	602	NDP	P2B-O2B	13.45	1.84	1.59
3	B	602	NDP	P2B-O2B	12.94	1.83	1.59
2	B	601	HEM	C3D-C2D	8.68	1.55	1.36
2	C	601	HEM	C3D-C2D	7.84	1.53	1.36
2	A	601	HEM	C3D-C2D	7.84	1.53	1.36
2	D	601	HEM	C3D-C2D	7.62	1.52	1.36
2	B	601	HEM	C3C-C2C	-4.31	1.34	1.40
3	B	602	NDP	PN-O5D	4.17	1.76	1.59
2	D	601	HEM	C3C-C2C	-4.08	1.34	1.40
3	C	602	NDP	PN-O5D	4.00	1.75	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NDP	PN-O5D	3.90	1.75	1.59
2	A	601	HEM	C3C-CAC	3.88	1.55	1.47
3	D	602	NDP	PN-O5D	3.78	1.74	1.59
2	C	601	HEM	C3C-CAC	3.77	1.55	1.47
2	B	601	HEM	C3C-CAC	3.73	1.55	1.47
2	A	601	HEM	C3C-C2C	-3.69	1.35	1.40
2	C	601	HEM	C3C-C2C	-3.60	1.35	1.40
2	D	601	HEM	C3C-CAC	3.45	1.54	1.47
2	B	601	HEM	CAB-C3B	3.09	1.55	1.47
3	B	602	NDP	O2B-C2B	-2.93	1.33	1.44
2	D	601	HEM	FE-NB	2.91	2.11	1.96
3	A	602	NDP	O2B-C2B	-2.89	1.33	1.44
2	A	601	HEM	CAB-C3B	2.88	1.55	1.47
2	D	601	HEM	CAB-C3B	2.82	1.55	1.47
3	D	602	NDP	O2B-C2B	-2.78	1.34	1.44
2	C	601	HEM	CAB-C3B	2.78	1.55	1.47
3	C	602	NDP	O2B-C2B	-2.66	1.34	1.44
2	C	601	HEM	FE-NB	2.62	2.09	1.96
2	C	601	HEM	FE-ND	2.58	2.09	1.96
2	B	601	HEM	FE-NB	2.44	2.08	1.96
2	B	601	HEM	FE-ND	2.42	2.08	1.96
3	D	602	NDP	C2A-N1A	2.41	1.38	1.33
2	B	601	HEM	CAA-C2A	2.40	1.55	1.52
3	C	602	NDP	C2A-N1A	2.40	1.38	1.33
3	B	602	NDP	C2A-N1A	2.32	1.38	1.33
2	D	601	HEM	FE-ND	2.24	2.08	1.96
3	B	602	NDP	C7N-N7N	2.24	1.39	1.33
2	A	601	HEM	CAA-C2A	2.22	1.55	1.52
2	B	601	HEM	CMD-C2D	2.20	1.55	1.50
2	A	601	HEM	FE-NB	2.19	2.07	1.96
3	A	602	NDP	C2A-N1A	2.19	1.38	1.33
3	D	602	NDP	O5D-C5D	-2.15	1.36	1.44
2	A	601	HEM	FE-ND	2.14	2.07	1.96
3	A	602	NDP	C7N-N7N	2.12	1.39	1.33
3	B	602	NDP	C4A-N3A	2.09	1.38	1.35
3	A	602	NDP	O5D-C5D	-2.07	1.36	1.44
3	C	602	NDP	C2A-N3A	2.07	1.35	1.32

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	NDP	PN-O3-PA	-7.14	108.32	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	HEM	C4D-ND-C1D	6.73	112.03	105.07
3	A	602	NDP	PN-O3-PA	-6.69	109.86	132.83
3	C	602	NDP	PN-O3-PA	-6.60	110.19	132.83
3	D	602	NDP	PN-O3-PA	-6.55	110.34	132.83
2	A	601	HEM	C4D-ND-C1D	6.29	111.57	105.07
2	D	601	HEM	C4D-ND-C1D	6.07	111.34	105.07
2	B	601	HEM	C4D-ND-C1D	5.75	111.01	105.07
2	C	601	HEM	C3B-C2B-C1B	3.35	108.97	106.49
3	A	602	NDP	PA-O5B-C5B	-3.28	102.43	121.68
2	C	601	HEM	C1B-NB-C4B	3.28	108.46	105.07
3	A	602	NDP	O2B-P2B-O1X	-3.09	97.48	109.39
3	B	602	NDP	O2B-P2B-O1X	-3.07	97.52	109.39
3	C	602	NDP	O2B-P2B-O1X	-3.05	97.61	109.39
3	B	602	NDP	PA-O5B-C5B	-3.02	103.95	121.68
2	C	601	HEM	CHC-C4B-C3B	3.02	129.19	124.57
2	C	601	HEM	CAD-CBD-CGD	-3.01	107.14	113.60
3	C	602	NDP	PA-O5B-C5B	-3.00	104.08	121.68
2	A	601	HEM	C4C-CHD-C1D	3.00	126.52	122.56
2	D	601	HEM	CAD-CBD-CGD	-2.98	107.20	113.60
3	D	602	NDP	PA-O5B-C5B	-2.93	104.52	121.68
3	D	602	NDP	O2B-P2B-O1X	-2.85	98.38	109.39
2	C	601	HEM	CBA-CAA-C2A	-2.84	107.77	112.62
3	C	602	NDP	PN-O5D-C5D	-2.79	105.30	121.68
3	D	602	NDP	PN-O5D-C5D	-2.76	105.50	121.68
2	B	601	HEM	C4C-CHD-C1D	2.75	126.19	122.56
2	A	601	HEM	C1B-NB-C4B	2.72	107.88	105.07
2	C	601	HEM	C4C-CHD-C1D	2.70	126.11	122.56
3	A	602	NDP	O3X-P2B-O2X	2.59	117.55	107.64
3	B	602	NDP	PN-O5D-C5D	-2.59	106.52	121.68
3	B	602	NDP	O3X-P2B-O2X	2.58	117.51	107.64
3	A	602	NDP	PN-O5D-C5D	-2.56	106.66	121.68
2	D	601	HEM	C1B-NB-C4B	2.53	107.68	105.07
3	D	602	NDP	O3X-P2B-O2X	2.52	117.27	107.64
3	C	602	NDP	O5D-PN-O1N	-2.51	99.26	109.07
3	D	602	NDP	C2A-N1A-C6A	-2.51	114.47	118.75
3	C	602	NDP	O3X-P2B-O2X	2.51	117.21	107.64
3	C	602	NDP	C2A-N1A-C6A	-2.45	114.56	118.75
2	B	601	HEM	C1B-NB-C4B	2.45	107.60	105.07
3	D	602	NDP	O5D-PN-O1N	-2.41	99.67	109.07
2	C	601	HEM	CMA-C3A-C4A	-2.41	124.77	128.46
3	A	602	NDP	C2A-N1A-C6A	-2.36	114.72	118.75
2	D	601	HEM	CAD-C3D-C4D	2.35	128.77	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	CAD-CBD-CGD	-2.35	108.54	113.60
3	A	602	NDP	C5D-C4D-C3D	-2.33	106.44	115.18
2	B	601	HEM	C4A-C3A-C2A	2.33	108.62	107.00
3	B	602	NDP	C2A-N1A-C6A	-2.32	114.78	118.75
2	C	601	HEM	CAD-C3D-C4D	2.32	128.71	124.66
3	B	602	NDP	C3B-C2B-C1B	-2.26	98.64	102.89
3	B	602	NDP	O2N-PN-O1N	2.26	123.42	112.24
2	D	601	HEM	CMC-C2C-C3C	2.25	128.88	124.68
3	C	602	NDP	O2N-PN-O1N	2.22	123.19	112.24
3	C	602	NDP	O7N-C7N-C3N	2.21	125.06	120.90
3	C	602	NDP	O4B-C4B-C3B	2.18	109.44	105.11
2	D	601	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
3	D	602	NDP	O2N-PN-O1N	2.18	123.01	112.24
3	B	602	NDP	C5D-C4D-C3D	-2.17	107.06	115.18
2	A	601	HEM	CMC-C2C-C3C	2.16	128.72	124.68
3	B	602	NDP	O5D-PN-O1N	-2.16	100.64	109.07
2	C	601	HEM	CMC-C2C-C3C	2.16	128.71	124.68
3	D	602	NDP	O4B-C4B-C3B	2.15	109.36	105.11
3	B	602	NDP	O7N-C7N-C3N	2.14	124.93	120.90
3	D	602	NDP	O7N-C7N-C3N	2.14	124.93	120.90
2	B	601	HEM	CMA-C3A-C4A	-2.14	125.18	128.46
3	A	602	NDP	O2N-PN-O1N	2.13	122.77	112.24
2	C	601	HEM	CAA-CBA-CGA	-2.12	107.82	113.76
2	D	601	HEM	C4C-CHD-C1D	2.11	125.34	122.56
3	A	602	NDP	C5B-C4B-C3B	-2.10	107.30	115.18
2	C	601	HEM	C3D-C4D-ND	-2.10	107.83	110.17
3	B	602	NDP	O2X-P2B-O2B	-2.09	96.64	105.99
2	A	601	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
2	D	601	HEM	C3B-C2B-C1B	2.08	108.03	106.49
3	A	602	NDP	O5D-PN-O1N	-2.08	100.95	109.07
2	C	601	HEM	CHD-C1D-ND	2.08	126.69	124.43
3	A	602	NDP	O4B-C4B-C3B	2.07	109.20	105.11
3	D	602	NDP	O2X-P2B-O2B	-2.07	96.74	105.99
2	B	601	HEM	C1D-C2D-C3D	-2.06	104.79	106.96
3	A	602	NDP	O2X-P2B-O2B	-2.05	96.80	105.99
2	B	601	HEM	C3B-C2B-C1B	2.05	108.01	106.49
3	C	602	NDP	O2X-P2B-O2B	-2.03	96.90	105.99
3	A	602	NDP	C3N-C2N-N1N	-2.02	120.21	123.10
2	D	601	HEM	CBA-CAA-C2A	-2.02	109.17	112.62
2	B	601	HEM	CAD-C3D-C2D	2.01	131.62	127.88
2	D	601	HEM	C4A-C3A-C2A	2.01	108.39	107.00

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	C3A-C2A-CAA-CBA
2	B	601	HEM	C4D-C3D-CAD-CBD
3	A	602	NDP	C3B-C4B-C5B-O5B
3	B	602	NDP	C3B-C4B-C5B-O5B
3	B	602	NDP	C2N-C3N-C7N-N7N
3	C	602	NDP	C5B-O5B-PA-O1A
3	C	602	NDP	C5B-O5B-PA-O2A
3	D	602	NDP	C5B-O5B-PA-O2A
3	D	602	NDP	C5B-O5B-PA-O3
3	D	602	NDP	PN-O3-PA-O5B
3	D	602	NDP	C3B-C4B-C5B-O5B
2	B	601	HEM	C2D-C3D-CAD-CBD
3	C	602	NDP	O4B-C4B-C5B-O5B
3	C	602	NDP	C3B-C4B-C5B-O5B
3	D	602	NDP	O4B-C4B-C5B-O5B
3	A	602	NDP	C3B-C2B-O2B-P2B
3	A	602	NDP	C1B-C2B-O2B-P2B
3	A	602	NDP	O4B-C4B-C5B-O5B
3	B	602	NDP	O4B-C4B-C5B-O5B
3	B	602	NDP	C2D-C1D-N1N-C6N
3	B	602	NDP	C2D-C1D-N1N-C2N
3	B	602	NDP	O4D-C1D-N1N-C6N
2	B	601	HEM	C3D-CAD-CBD-CGD
3	A	602	NDP	PN-O3-PA-O5B
3	B	602	NDP	PN-O3-PA-O5B
3	A	602	NDP	C5B-O5B-PA-O3
3	B	602	NDP	C2B-O2B-P2B-O3X
3	C	602	NDP	C5D-O5D-PN-O3
2	A	601	HEM	C2A-CAA-CBA-CGA
3	B	602	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	O4D-C1D-N1N-C6N
2	A	601	HEM	C1A-C2A-CAA-CBA
2	A	601	HEM	C3A-C2A-CAA-CBA
3	A	602	NDP	O4D-C1D-N1N-C6N
3	D	602	NDP	O4D-C1D-N1N-C6N
3	C	602	NDP	PA-O3-PN-O2N
3	A	602	NDP	C2D-C1D-N1N-C6N
3	C	602	NDP	C1B-C2B-O2B-P2B
3	D	602	NDP	C2D-C1D-N1N-C6N
3	C	602	NDP	C3B-C2B-O2B-P2B
2	D	601	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	A	602	NDP	O4D-C1D-N1N-C2N
3	A	602	NDP	C2B-O2B-P2B-O3X
3	B	602	NDP	C5B-O5B-PA-O3
3	C	602	NDP	C5B-O5B-PA-O3
3	C	602	NDP	C2B-O2B-P2B-O3X
3	D	602	NDP	C5D-O5D-PN-O3
3	A	602	NDP	C2D-C1D-N1N-C2N
2	A	601	HEM	CAA-CBA-CGA-O2A
2	D	601	HEM	CAD-CBD-CGD-O2D
3	B	602	NDP	C1B-C2B-O2B-P2B
3	A	602	NDP	C5B-O5B-PA-O2A
3	B	602	NDP	C5D-O5D-PN-O1N
3	C	602	NDP	C5D-O5D-PN-O1N
3	D	602	NDP	C5D-O5D-PN-O1N
2	C	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAD-CBD-CGD-O1D
3	D	602	NDP	C3B-C2B-O2B-P2B
2	A	601	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

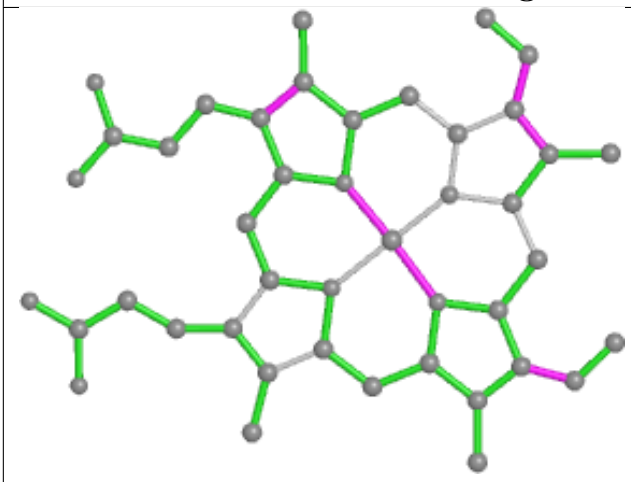
8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	2	0
3	A	602	NDP	2	0
2	A	601	HEM	2	0
2	B	601	HEM	3	0
2	C	601	HEM	1	0
3	D	602	NDP	1	0
3	C	602	NDP	3	0
3	B	602	NDP	3	0

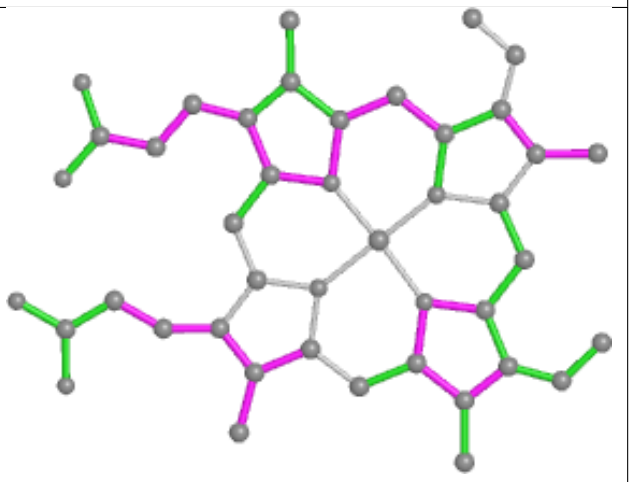
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

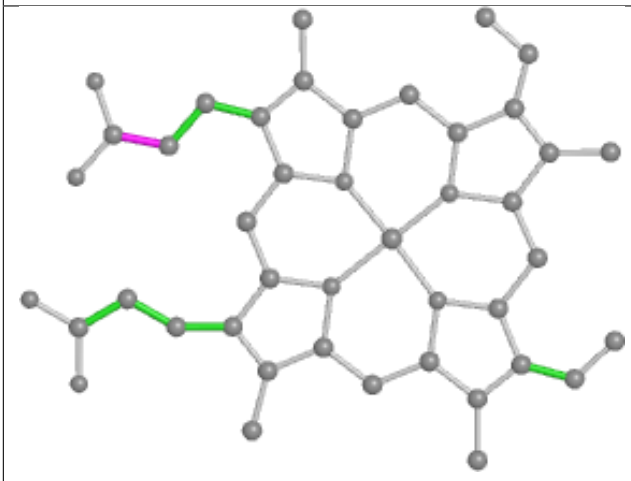
Ligand HEM D 601



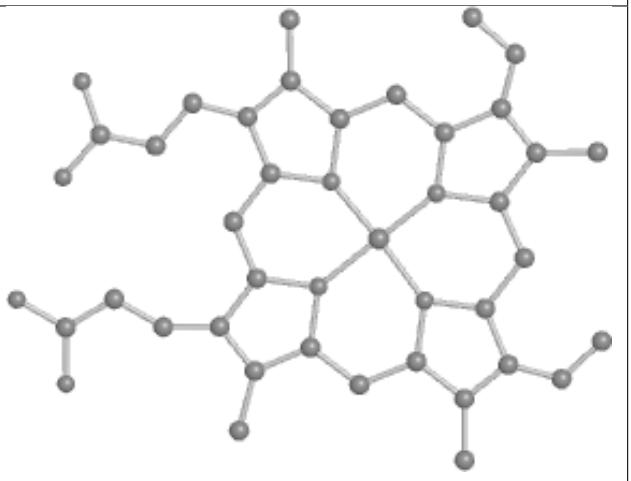
Bond lengths



Bond angles

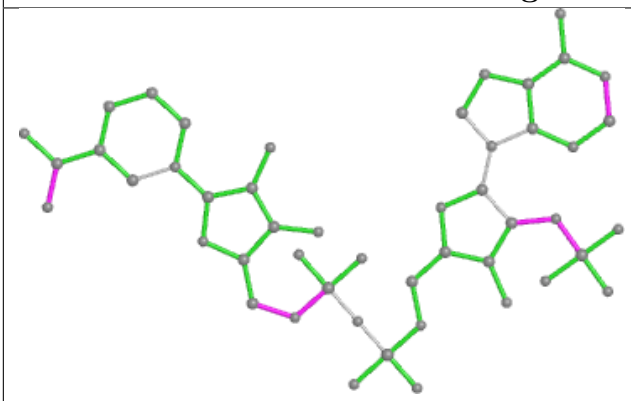


Torsions

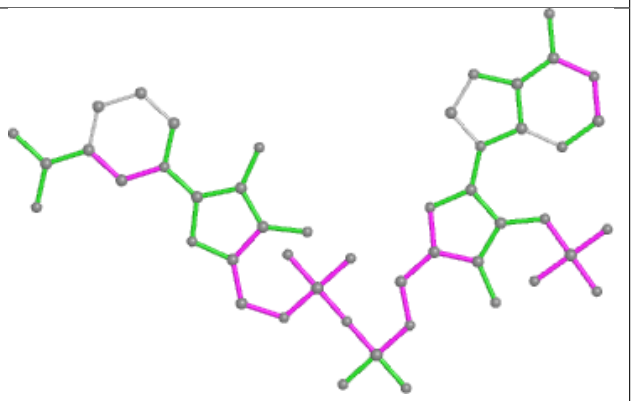


Rings

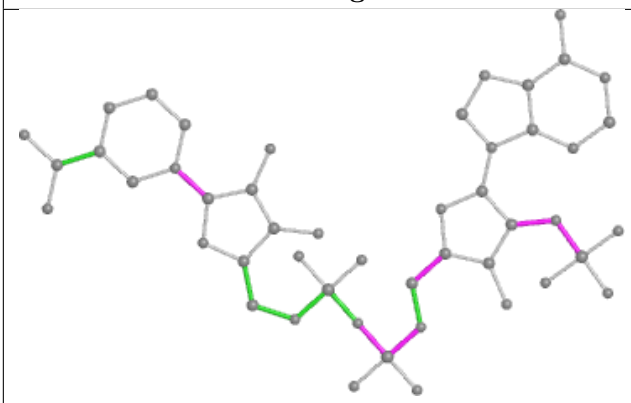
Ligand NDP A 602



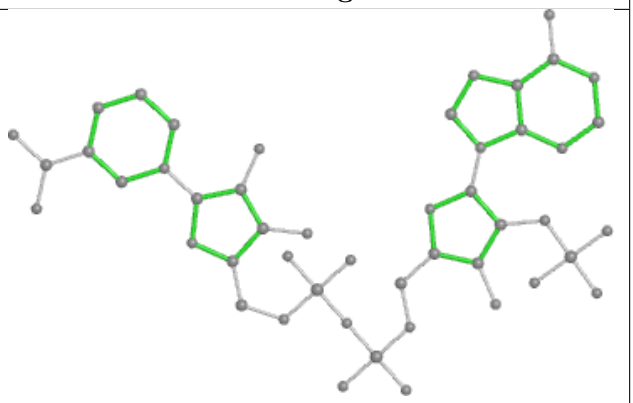
Bond lengths



Bond angles

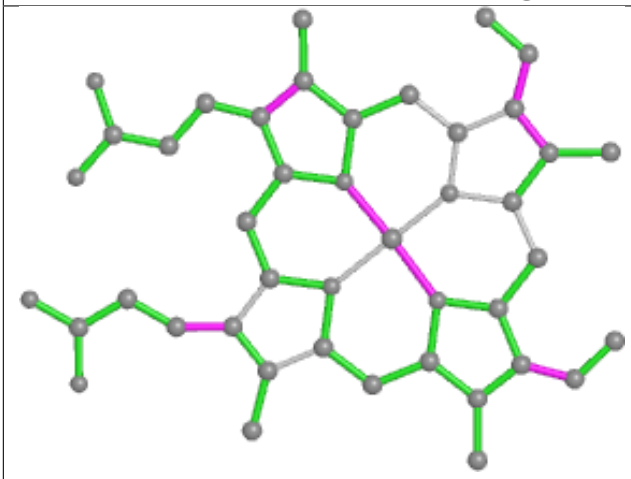


Torsions

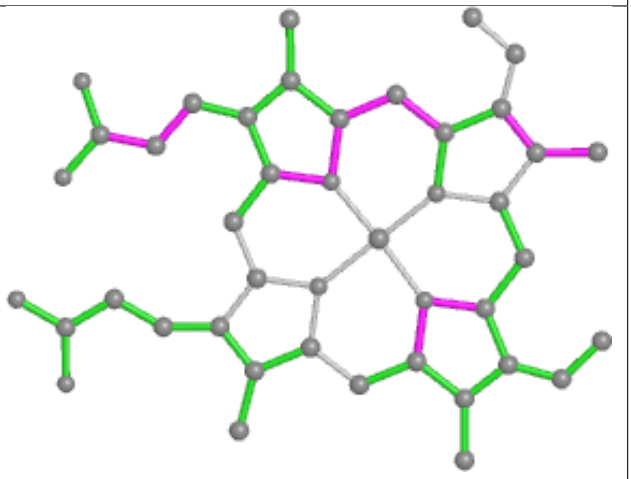


Rings

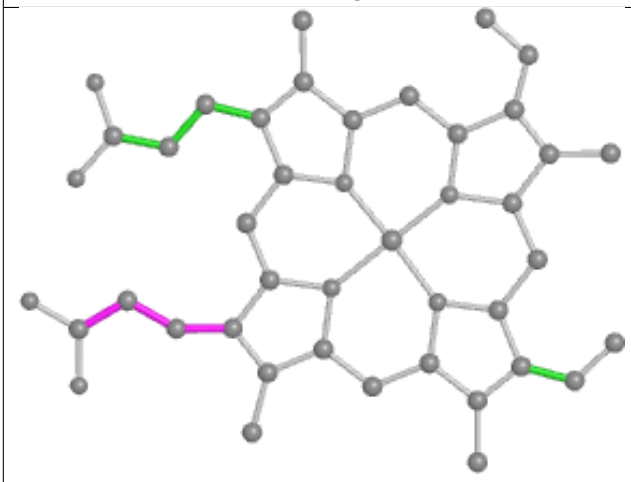
Ligand HEM A 601



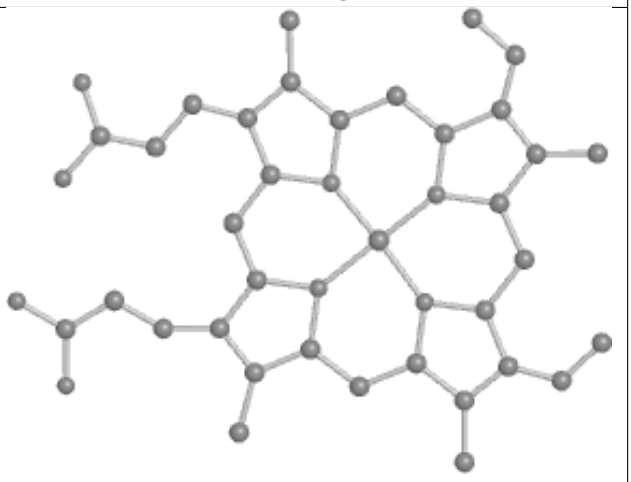
Bond lengths



Bond angles

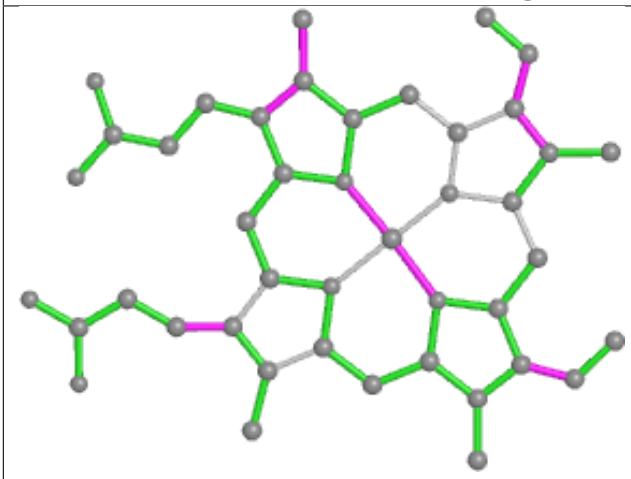


Torsions

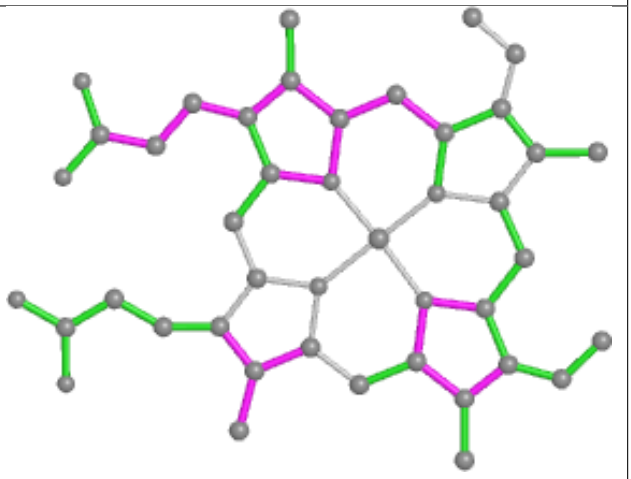


Rings

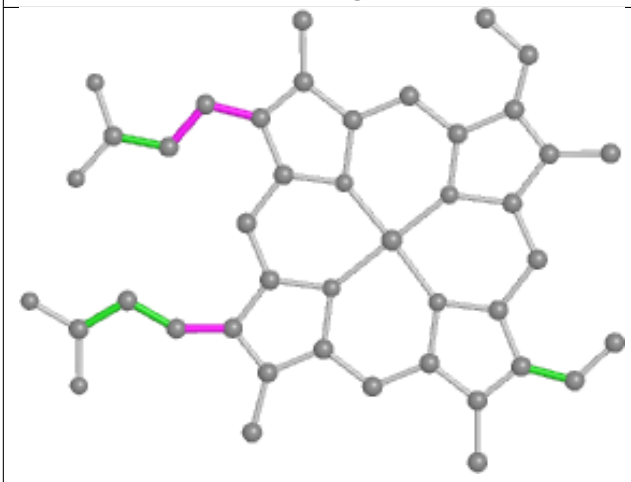
Ligand HEM B 601



Bond lengths



Bond angles



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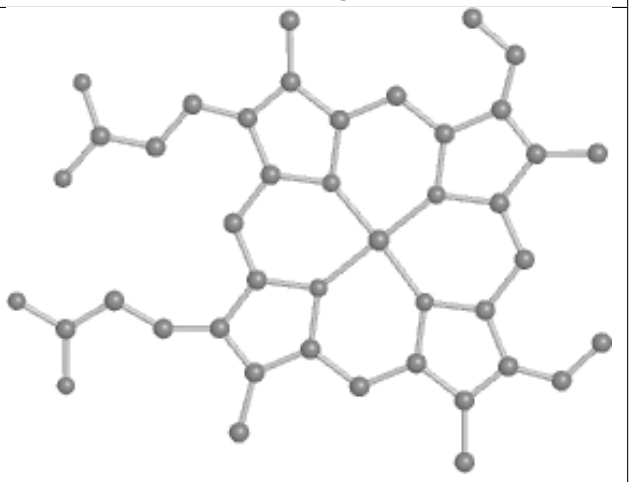
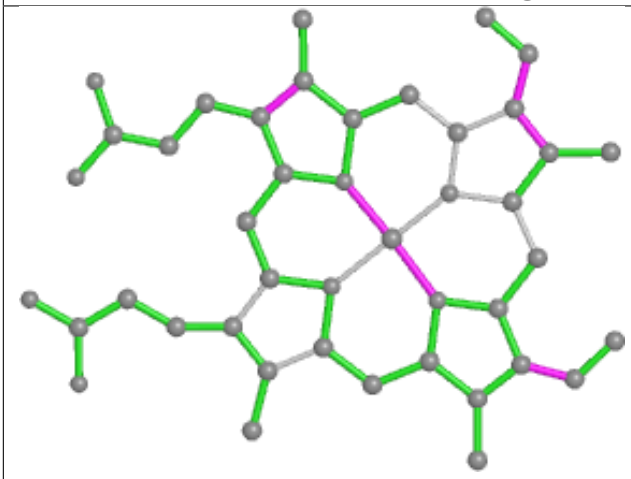
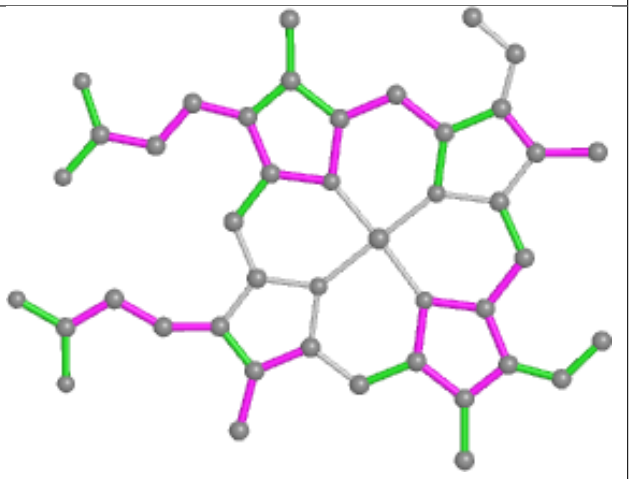


Rings

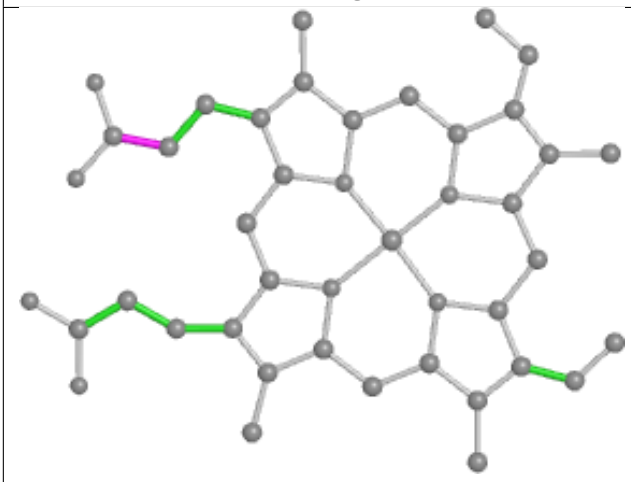
Ligand HEM C 601



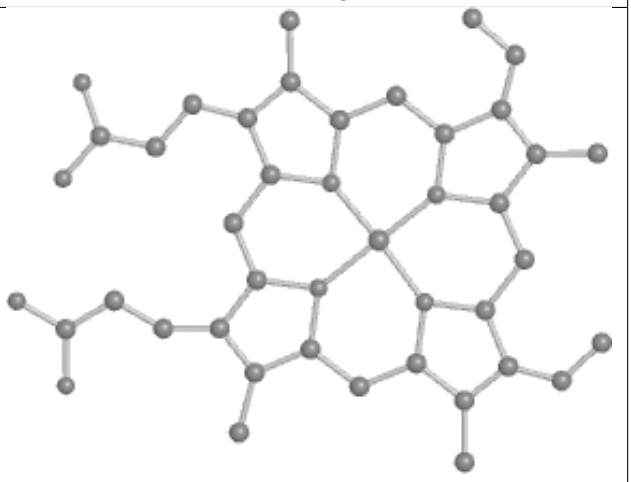
Bond lengths



Bond angles

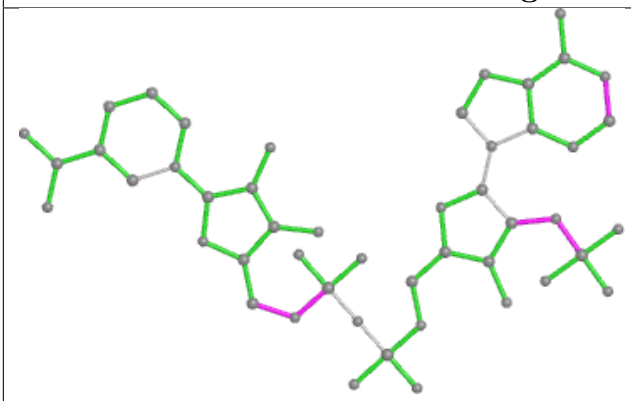


Torsions

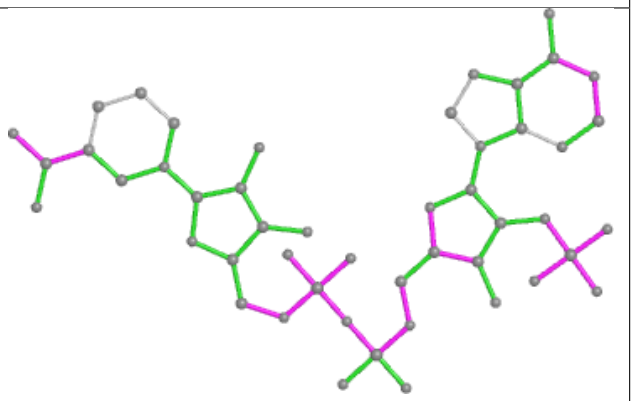


Rings

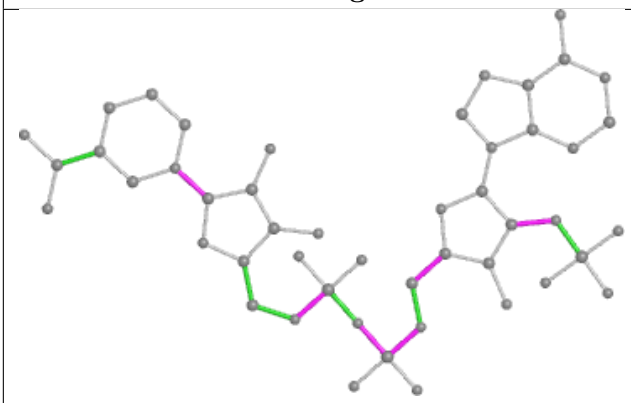
Ligand NDP D 602



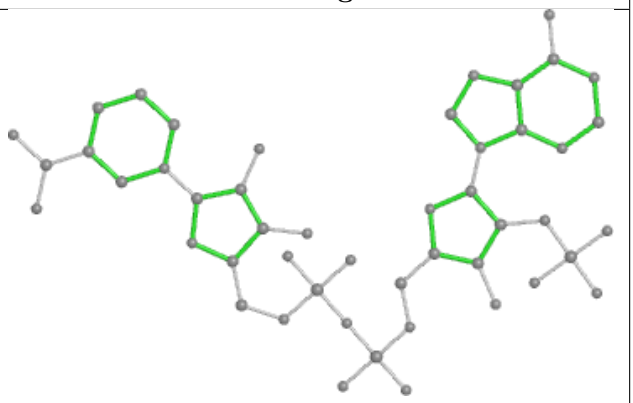
Bond lengths



Bond angles

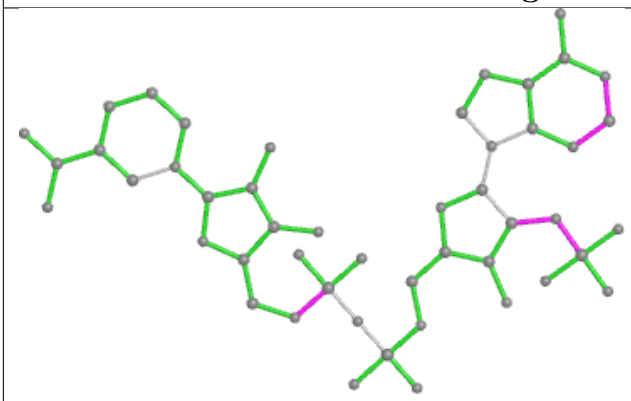


Torsions

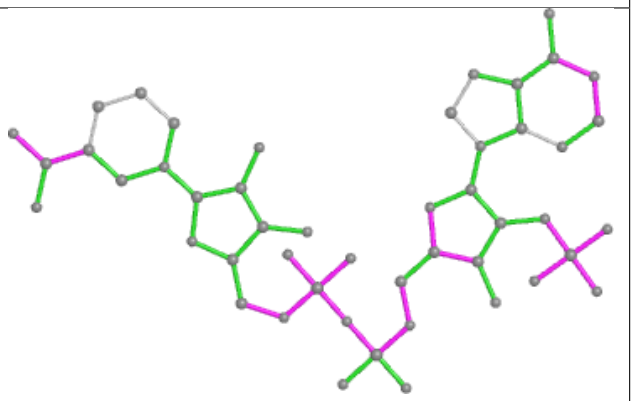


Rings

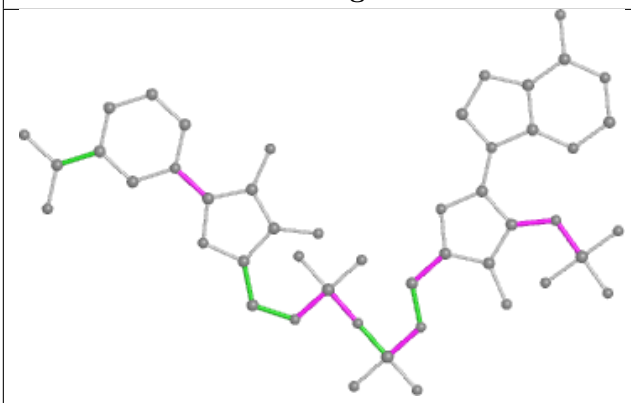
Ligand NDP C 602



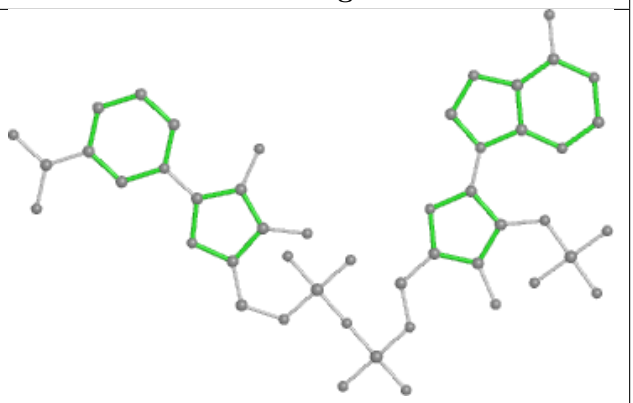
Bond lengths



Bond angles

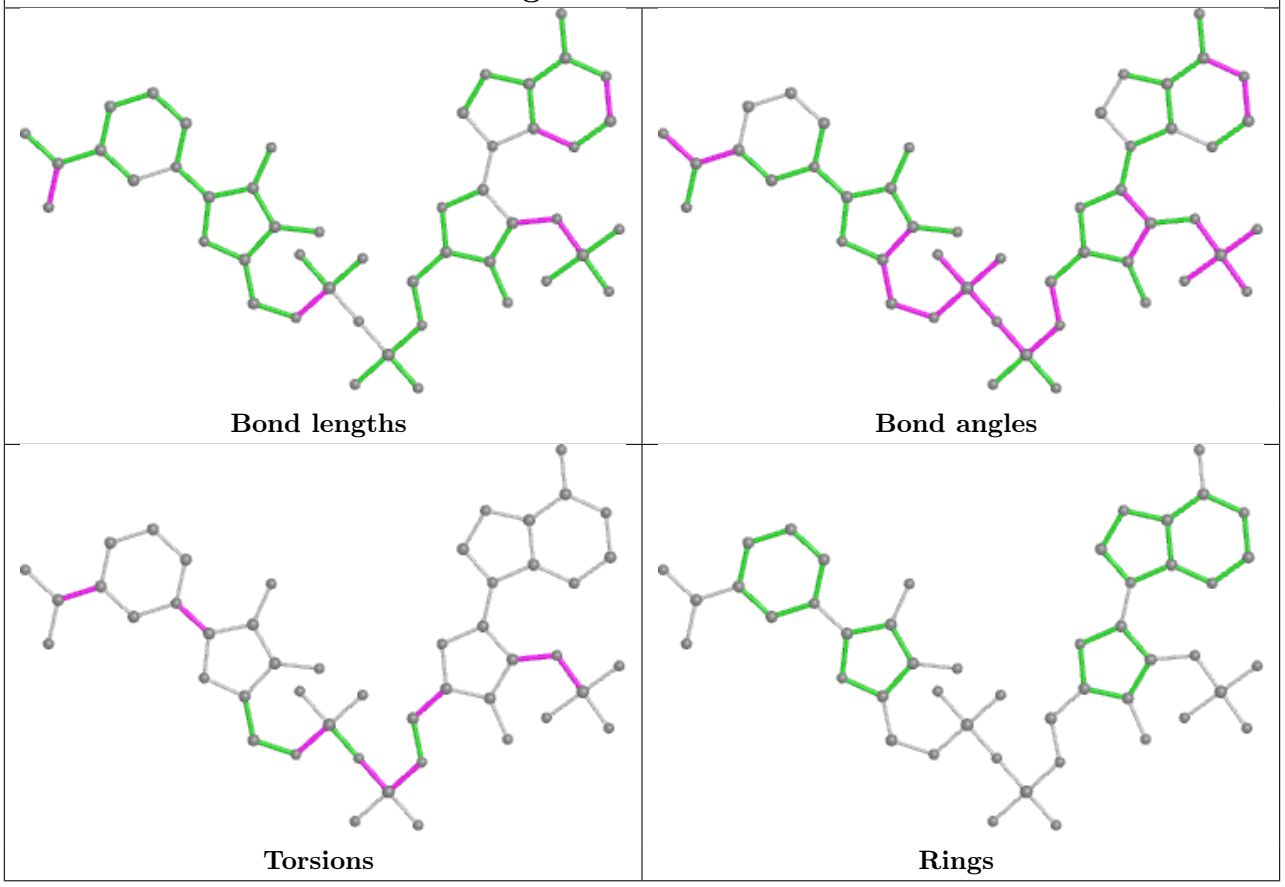


Torsions



Rings

Ligand NDP B 602



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.

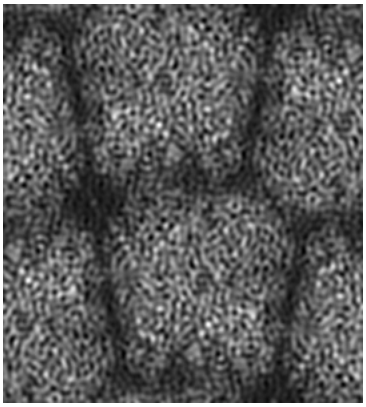
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6314. These allow visual inspection of the internal detail of the map and identification of artifacts.

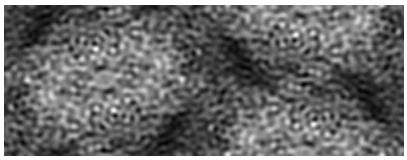
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

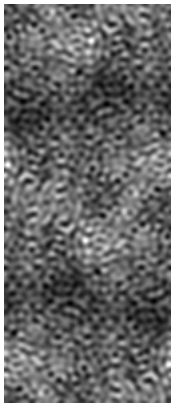
6.1.1 Primary map



X



Y



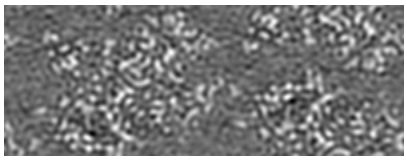
Z

The images above show the map projected in three orthogonal directions.

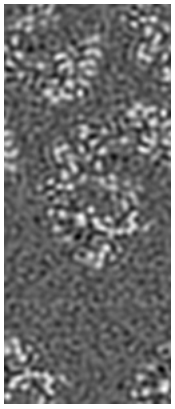
6.2 Central slices

6.2.1 Primary map

X Index: 45



Y Index: 108

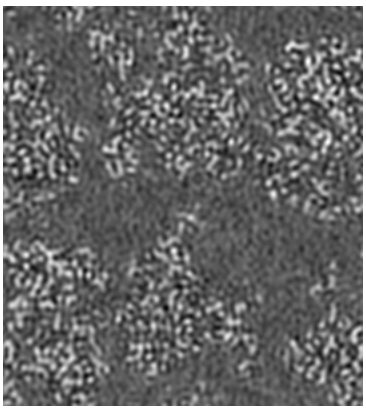


Z Index: 120

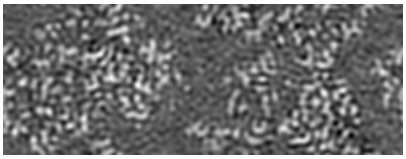
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

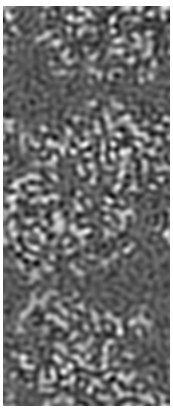
6.3.1 Primary map



X Index: 19



Y Index: 202

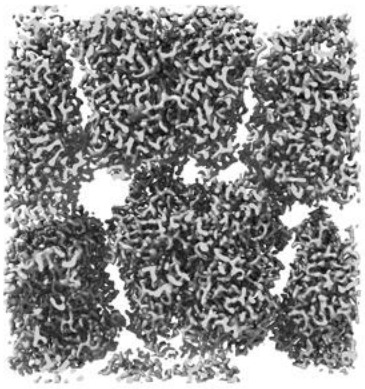


Z Index: 56

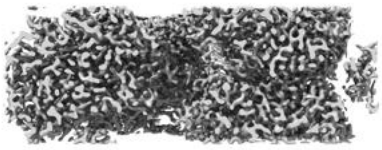
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

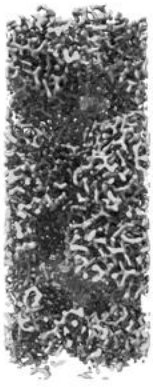
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

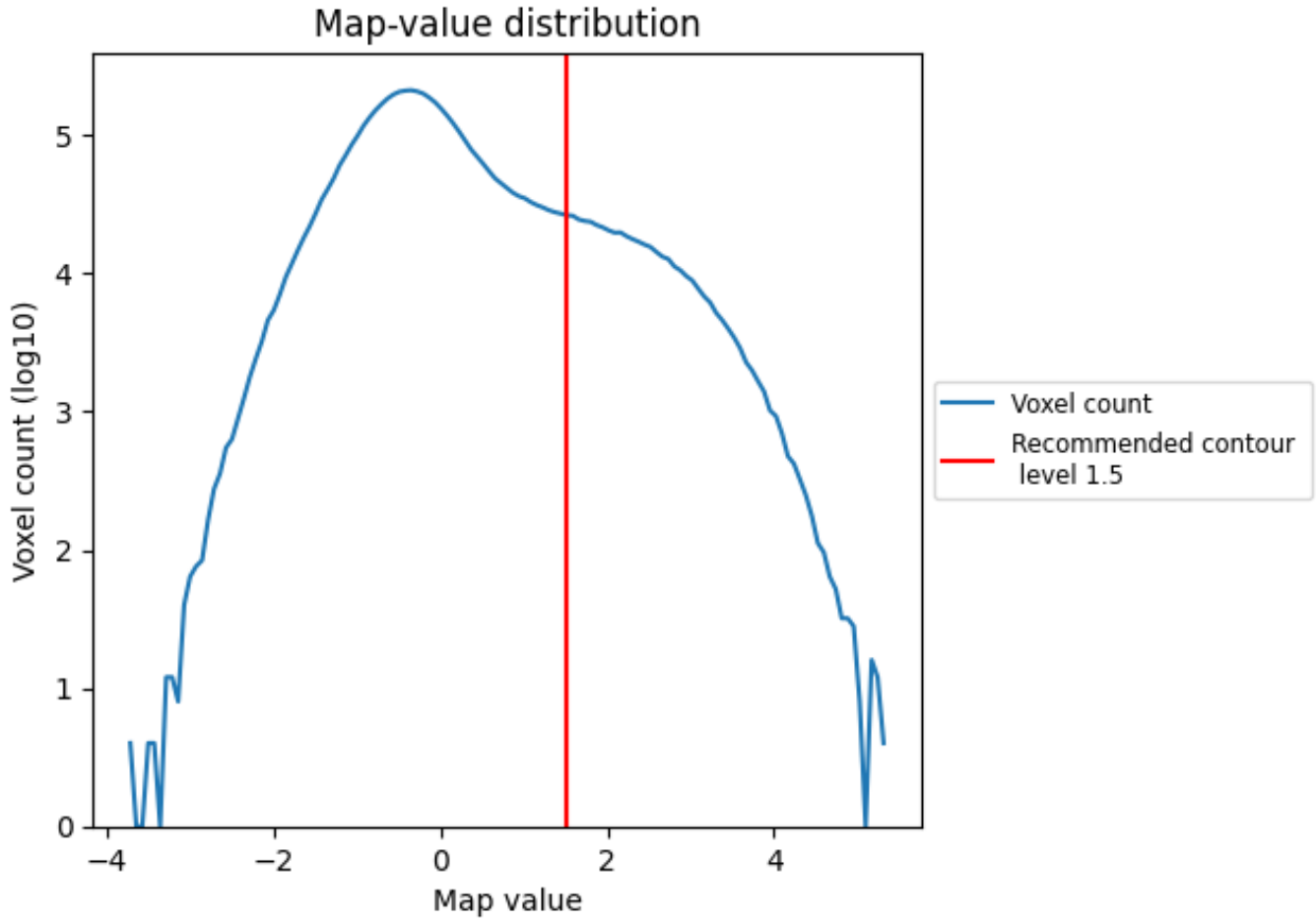
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

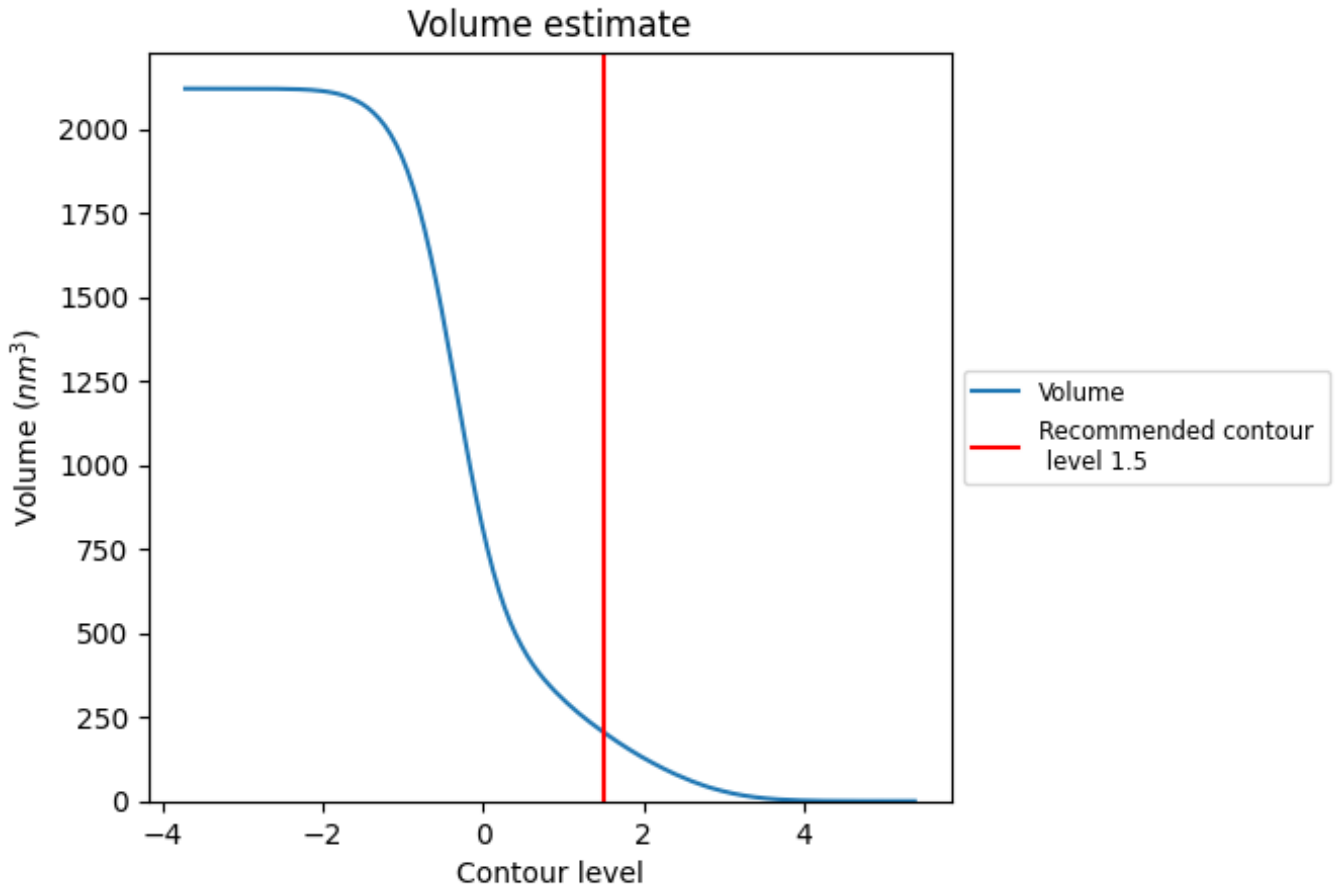
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 206 nm^3; this corresponds to an approximate mass of 186 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

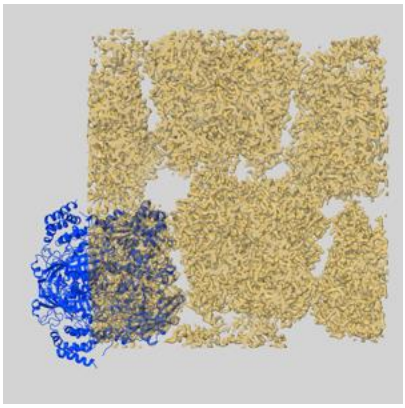
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

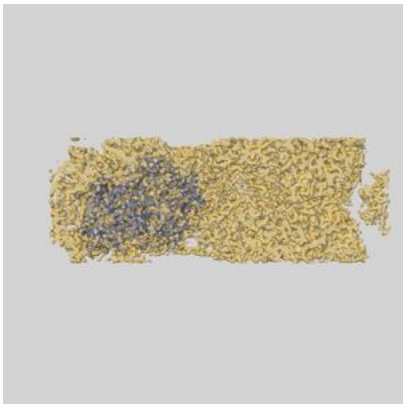
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6314 and PDB model 3J7B. Per-residue inclusion information can be found in section 3 on page 5.

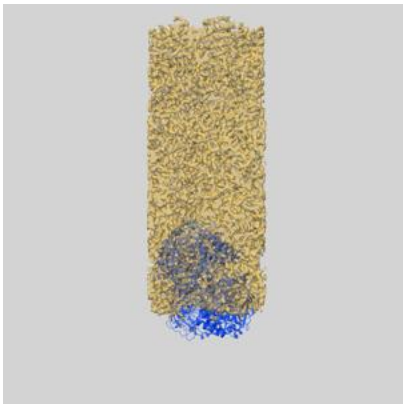
9.1 Map-model overlay



X



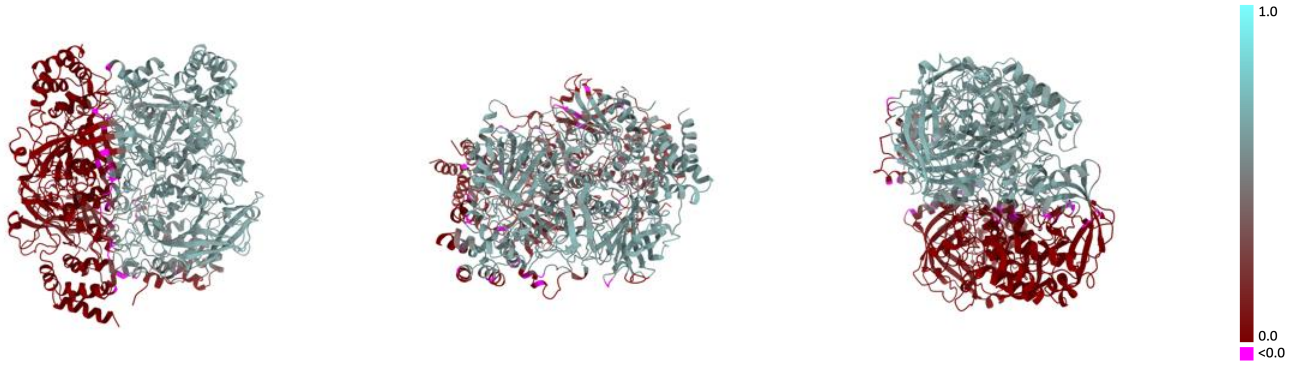
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

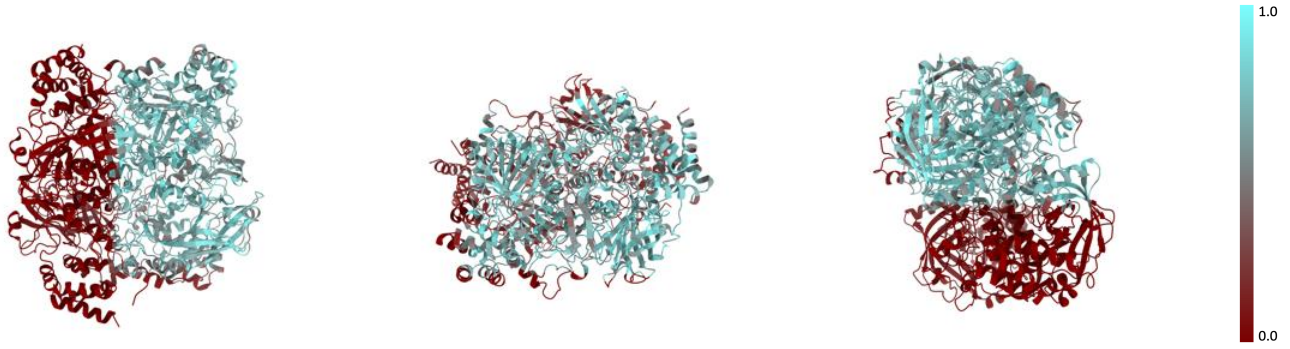
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

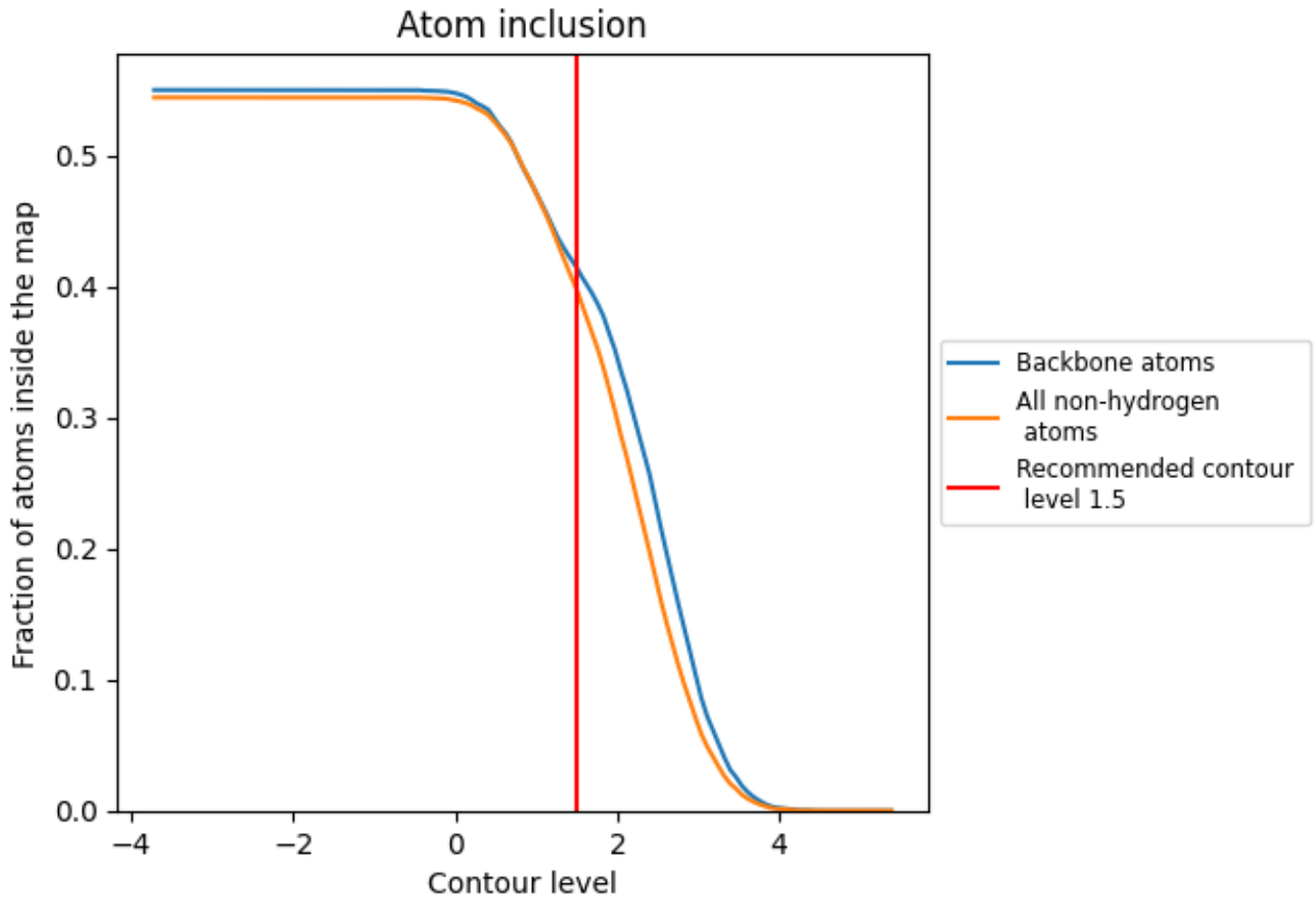
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 41% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3975	0.3340
A	0.6260	0.5130
B	0.5802	0.4900
C	0.1297	0.1150
D	0.2540	0.2190