



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 05:02 am BST

PDB ID : 6O5Y
Title : Structure of Human Cytochrome P450 1A1 with 5-amino-N-(5-((4R,5R)-4-amino-5-fluoroazepan-1-yl)-1-methyl-1H-pyrazol-4-yl)-2-(2,6-difluorophenyl)thiazole-4-carboxamide)
Authors : Bart, A.G.; Scott, E.E.
Deposited on : 2019-03-04
Resolution : 3.17 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

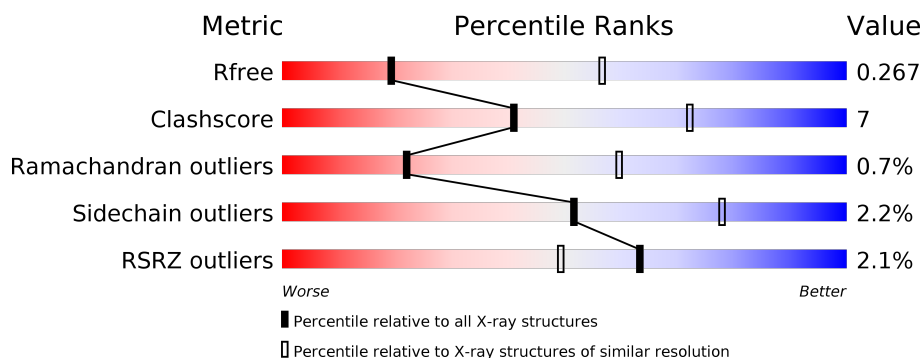
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	491	<div> <div></div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	B	491	<div> <div></div> <div> <div></div> <div>82%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	491	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	D	491	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30187 atoms, of which 15051 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 1A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	464	Total	C	H	N	O	S	0	0	0
			7441	2387	3720	647	666	21			
1	B	470	Total	C	H	N	O	S	0	0	0
			7552	2421	3776	657	678	20			
1	C	468	Total	C	H	N	O	S	0	0	0
			7488	2400	3743	651	673	21			
1	D	458	Total	C	H	N	O	S	0	0	0
			7346	2359	3670	639	658	20			

There are 52 discrepancies between the modelled and reference sequences:

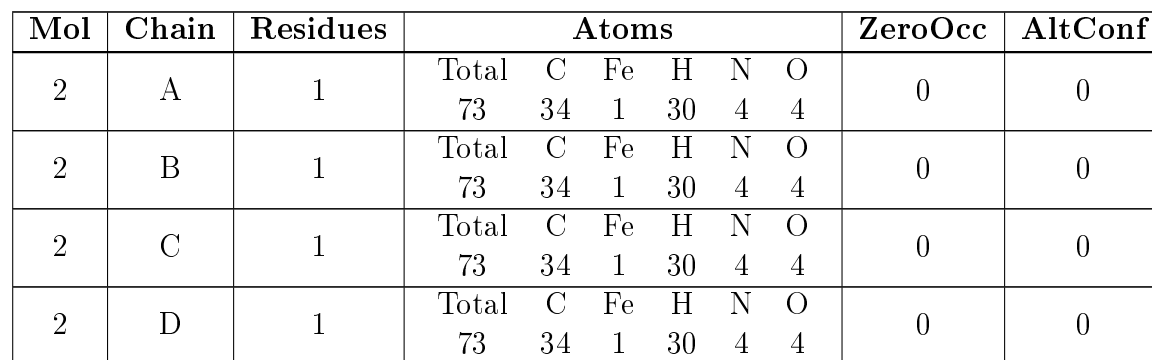
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP P04798
A	29	ALA	-	expression tag	UNP P04798
A	30	LYS	-	expression tag	UNP P04798
A	31	LYS	-	expression tag	UNP P04798
A	32	THR	-	expression tag	UNP P04798
A	33	SER	-	expression tag	UNP P04798
A	34	SER	-	expression tag	UNP P04798
A	513	HIS	-	expression tag	UNP P04798
A	514	HIS	-	expression tag	UNP P04798
A	515	HIS	-	expression tag	UNP P04798
A	516	HIS	-	expression tag	UNP P04798
A	517	HIS	-	expression tag	UNP P04798
A	518	HIS	-	expression tag	UNP P04798
B	28	MET	-	initiating methionine	UNP P04798
B	29	ALA	-	expression tag	UNP P04798
B	30	LYS	-	expression tag	UNP P04798
B	31	LYS	-	expression tag	UNP P04798
B	32	THR	-	expression tag	UNP P04798
B	33	SER	-	expression tag	UNP P04798
B	34	SER	-	expression tag	UNP P04798
B	513	HIS	-	expression tag	UNP P04798

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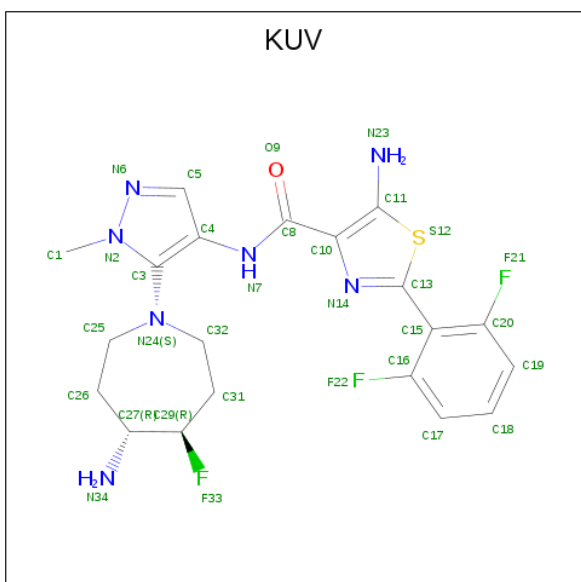
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Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	initiating methionine	UNP P04798
C	29	ALA	-	expression tag	UNP P04798
C	30	LYS	-	expression tag	UNP P04798
C	31	LYS	-	expression tag	UNP P04798
C	32	THR	-	expression tag	UNP P04798
C	33	SER	-	expression tag	UNP P04798
C	34	SER	-	expression tag	UNP P04798
C	513	HIS	-	expression tag	UNP P04798
C	514	HIS	-	expression tag	UNP P04798
C	515	HIS	-	expression tag	UNP P04798
C	516	HIS	-	expression tag	UNP P04798
C	517	HIS	-	expression tag	UNP P04798
C	518	HIS	-	expression tag	UNP P04798
D	28	MET	-	initiating methionine	UNP P04798
D	29	ALA	-	expression tag	UNP P04798
D	30	LYS	-	expression tag	UNP P04798
D	31	LYS	-	expression tag	UNP P04798
D	32	THR	-	expression tag	UNP P04798
D	33	SER	-	expression tag	UNP P04798
D	34	SER	-	expression tag	UNP P04798
D	513	HIS	-	expression tag	UNP P04798
D	514	HIS	-	expression tag	UNP P04798
D	515	HIS	-	expression tag	UNP P04798
D	516	HIS	-	expression tag	UNP P04798
D	517	HIS	-	expression tag	UNP P04798
D	518	HIS	-	expression tag	UNP P04798

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

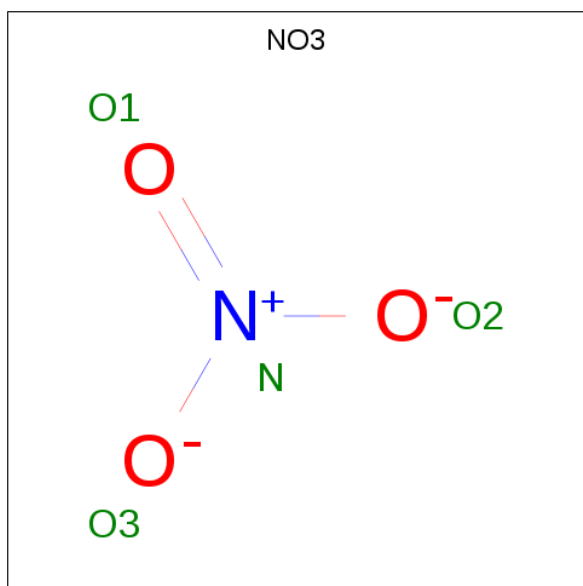


- Molecule 3 is 5-amino-N-{5-[(4R,5R)-4-amino-5-fluoroazepan-1-yl]-1-methyl-1H-pyrazol-4-yl}-2-(2,6-difluorophenyl)-1,3-thiazole-4-carboxamide (three-letter code: KUV) (formula: C₂₀H₂₂F₃N₇OS).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	S	0	0
			54	20	3	22	7	1	1		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		

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 ($\text{RSRZ} > 2$). 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.

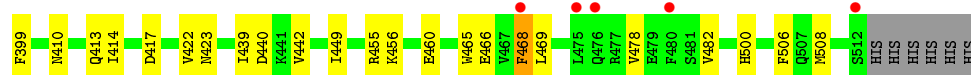
Chain A:

75% 18% 5%

100

191 192 193 194 206 207 214 215 216 220 221 222 223 224 225 226 227 235 236 237 238 239 240 242 251 262 265 266 269 272 278 279 283 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000

[illegible][illegible]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.15Å 195.90Å 236.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.17 49.32 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.32-3.17) 85.9 (49.32-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14 _3260)	Depositor
R, R_{free}	0.239 , 0.267 0.240 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	30187	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: KUV, HEM, NO3

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	0.29	0/3814	0.47	0/5165
1	B	0.29	0/3870	0.48	0/5243
1	C	0.27	0/3839	0.45	0/5201
1	D	0.28	0/3769	0.45	0/5106
All	All	0.28	0/15292	0.46	0/20715

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 [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	3721	3720	3718	54	0
1	B	3776	3776	3773	37	0
1	C	3745	3743	3741	40	0
1	D	3676	3670	3667	61	0
2	A	43	30	30	9	0
2	B	43	30	30	4	0
2	C	43	30	30	6	0
2	D	43	30	30	6	0
3	A	32	22	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
5	A	6	0	0	0	0
5	B	4	0	0	0	0
All	All	15136	15051	15019	213	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 7.

The worst 5 of 213 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:C:119:GLN:O	1:C:309:ASN:ND2	2.06	0.89
1:D:351:ILE:HD11	1:D:365:LEU:HD11	1.65	0.77
1:A:359:LEU:HD21	1:A:465:TRP:CE3	2.19	0.76
1:B:478:VAL:HG13	1:B:508:MET:HG3	1.73	0.71
1:C:207:TYR:HB2	1:C:214:LEU:HD22	1.72	0.71

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	458/491 (93%)	430 (94%)	25 (6%)	3 (1%)	22	60
1	B	466/491 (95%)	435 (93%)	29 (6%)	2 (0%)	34	69
1	C	464/491 (94%)	421 (91%)	40 (9%)	3 (1%)	25	63
1	D	452/491 (92%)	415 (92%)	32 (7%)	5 (1%)	14	50
All	All	1840/1964 (94%)	1701 (92%)	126 (7%)	13 (1%)	22	60

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	VAL
1	D	150	ASP
1	D	351	ILE
1	A	222	ASN
1	A	449	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/439 (94%)	405 (98%)	10 (2%)	49	76
1	B	421/439 (96%)	416 (99%)	5 (1%)	71	87
1	C	418/439 (95%)	409 (98%)	9 (2%)	52	78
1	D	409/439 (93%)	397 (97%)	12 (3%)	42	72
All	All	1663/1756 (95%)	1627 (98%)	36 (2%)	52	78

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	153	SER
1	C	245	ASN
1	D	336	ASN
1	C	223	ASN
1	C	259	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	C	601	-	27,50,50	1.85	5 (18%)	17,82,82	1.61	3 (17%)
2	HEM	A	601	-	27,50,50	1.84	4 (14%)	17,82,82	1.77	5 (29%)
2	HEM	D	601	-	27,50,50	1.85	4 (14%)	17,82,82	1.74	5 (29%)
3	KUV	A	602	-	27,35,35	2.97	12 (44%)	19,51,51	2.85	8 (42%)
4	NO3	B	602	-	1,3,3	0.61	0	0,3,3	0.00	-
2	HEM	B	601	1	27,50,50	1.83	4 (14%)	17,82,82	1.89	5 (29%)

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	601	-	-	4/6/54/54	-
3	KUV	A	602	-	-	0/2/30/30	0/4/4/4
2	HEM	D	601	-	-	4/6/54/54	-
2	HEM	C	601	-	-	3/6/54/54	-
2	HEM	B	601	1	-	4/6/54/54	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	KUV	C13-S12	6.63	1.82	1.73
3	A	602	KUV	C5-C4	5.58	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	KUV	C11-S12	5.52	1.81	1.72
3	A	602	KUV	C31-C32	5.33	1.61	1.52
3	A	602	KUV	C1-N2	-5.20	1.37	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	KUV	C20-C15-C16	-6.23	108.44	114.56
3	A	602	KUV	C31-C32-N24	5.79	123.46	113.48
3	A	602	KUV	C26-C25-N24	4.56	121.34	113.48
3	A	602	KUV	C16-C15-C13	3.87	127.69	121.78
2	B	601	HEM	CAA-CBA-CGA	-3.67	106.51	112.67

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	HEM	C2D-C3D-CAD-CBD
2	C	601	HEM	C4D-C3D-CAD-CBD
2	A	601	HEM	C1A-C2A-CAA-CBA
2	A	601	HEM	C3A-C2A-CAA-CBA
2	A	601	HEM	C2D-C3D-CAD-CBD

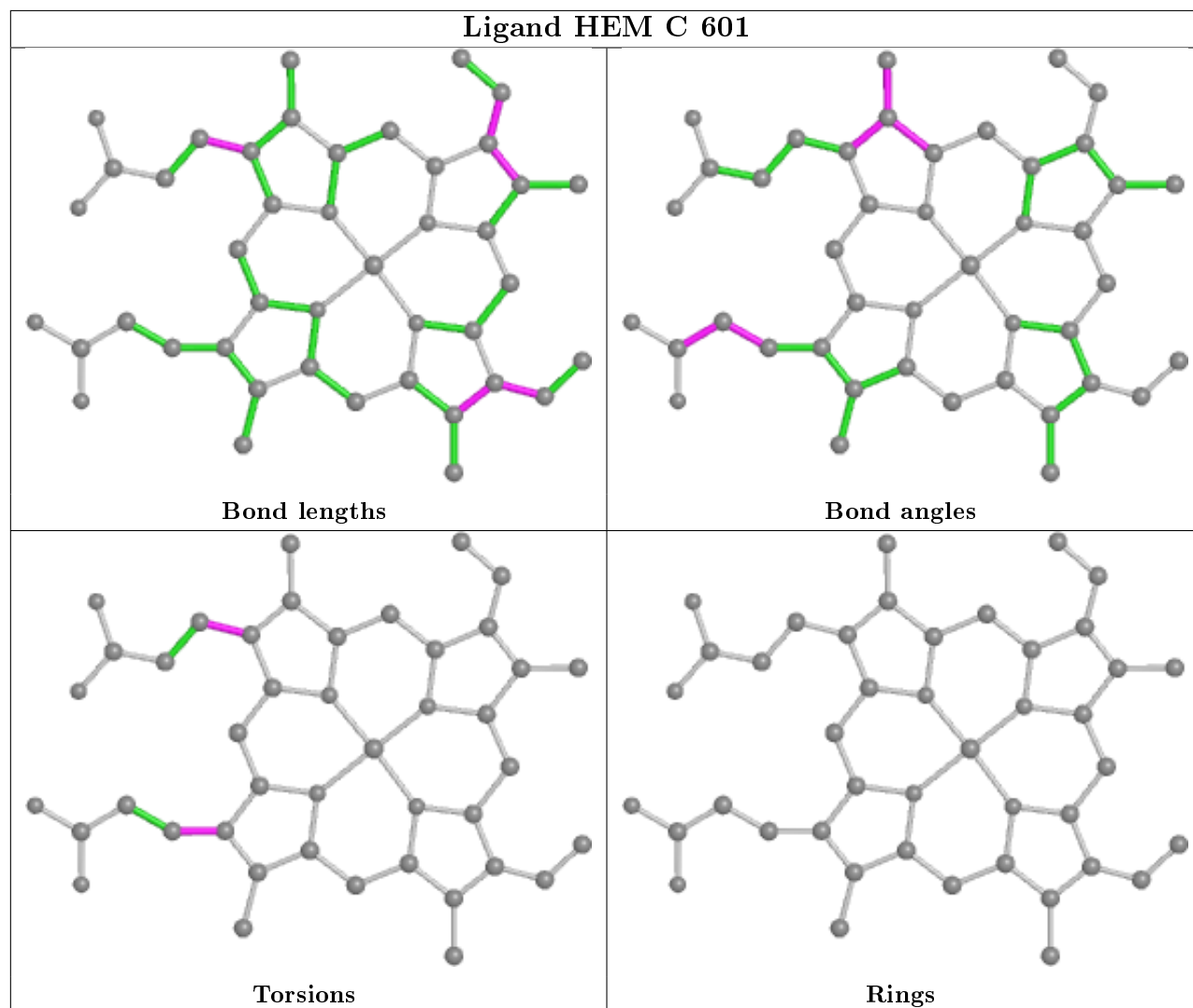
There are no ring outliers.

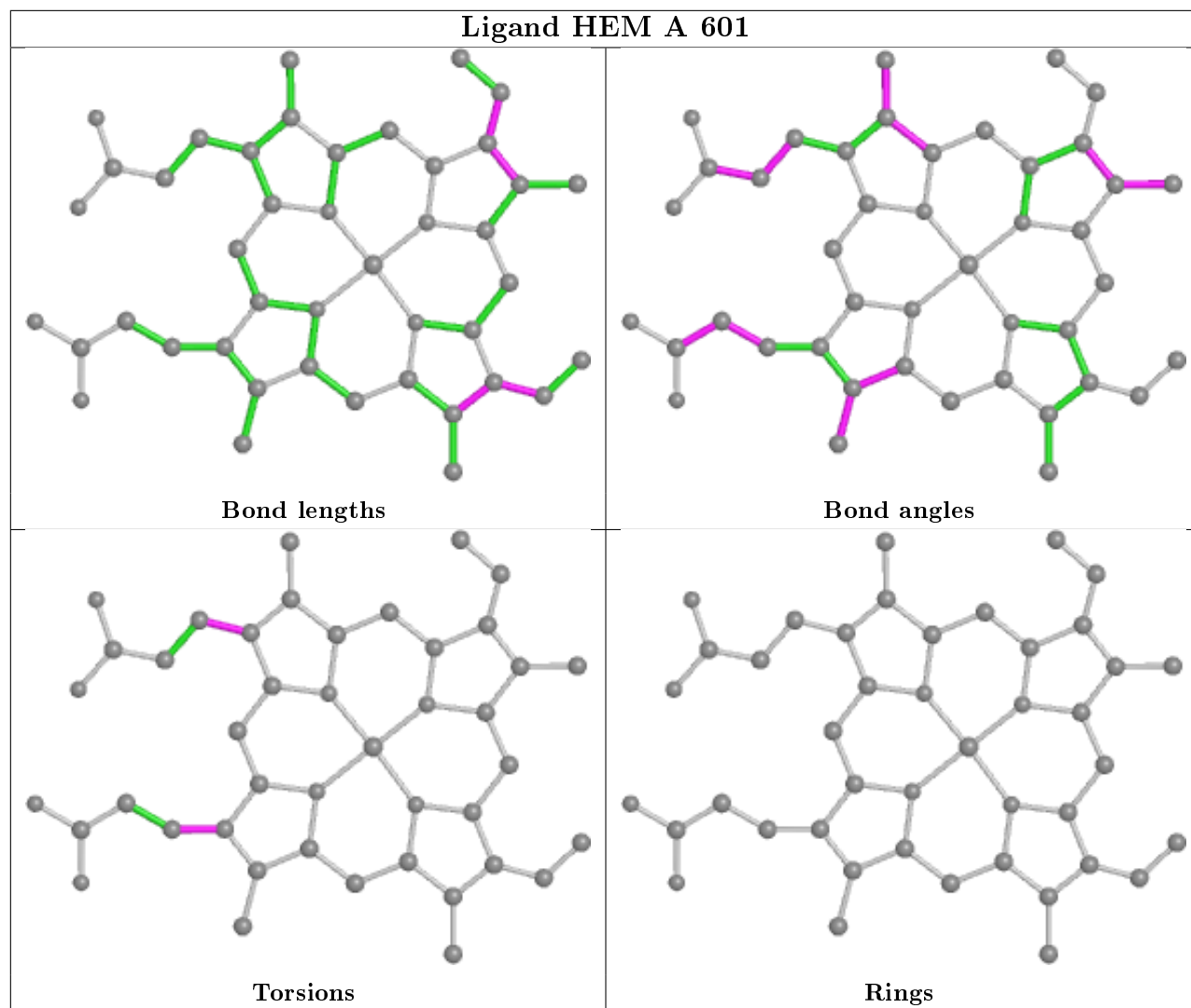
5 monomers are involved in 28 short contacts:

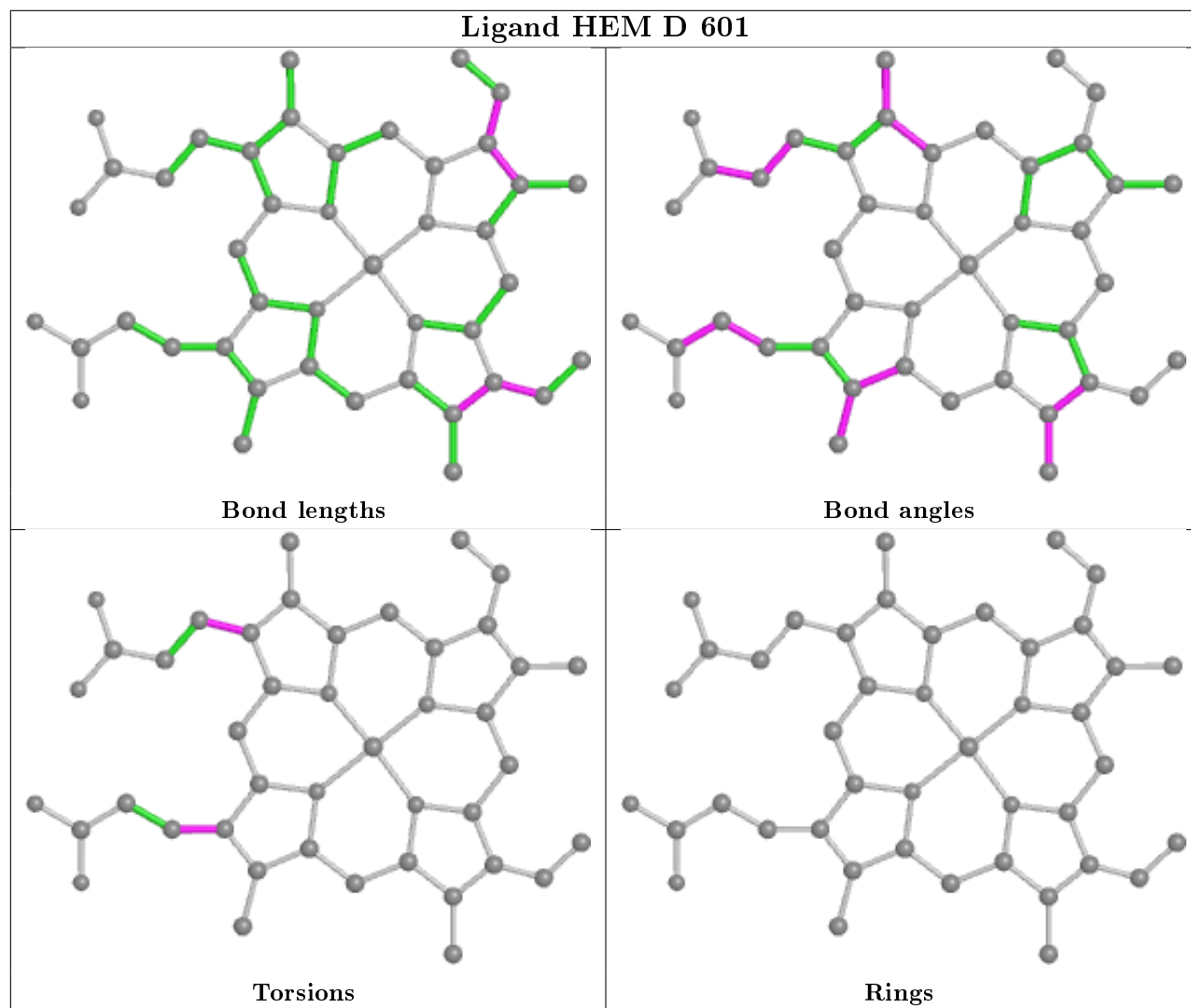
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	6	0
2	A	601	HEM	9	0
2	D	601	HEM	6	0
3	A	602	KUV	3	0
2	B	601	HEM	4	0

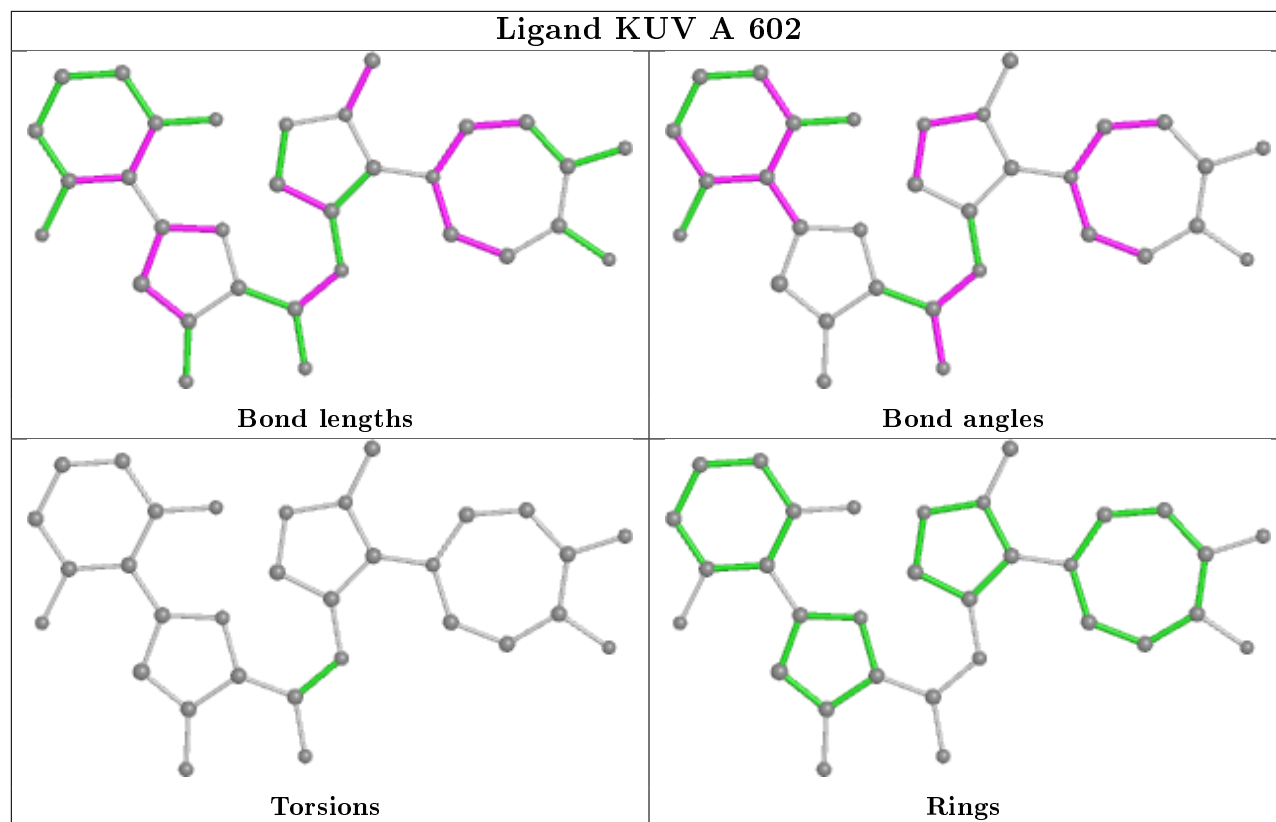
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

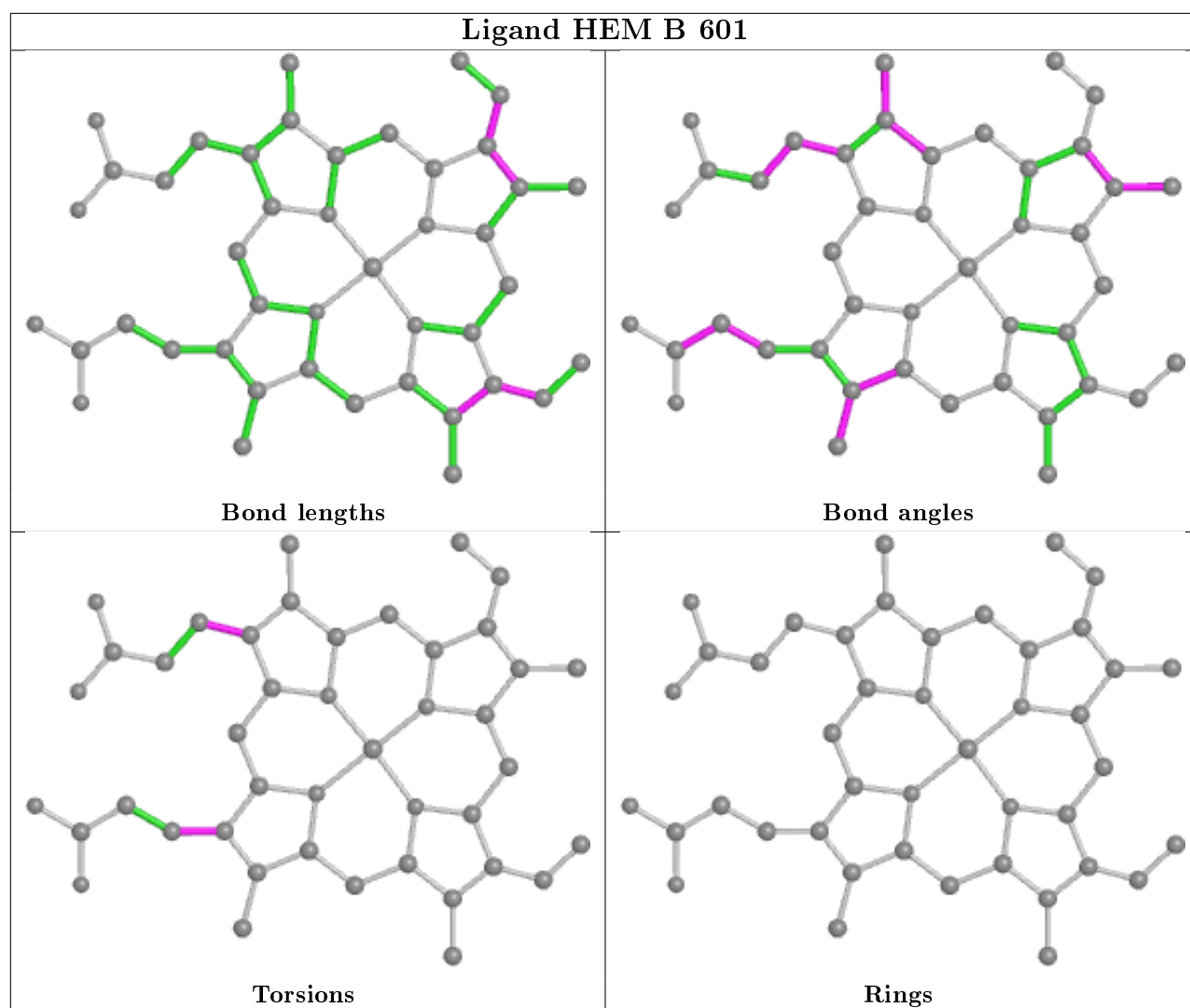
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	464/491 (94%)	0.27	3 (0%) 89 83	49, 71, 96, 120	0
1	B	470/491 (95%)	0.29	5 (1%) 80 69	48, 63, 82, 97	0
1	C	468/491 (95%)	0.34	15 (3%) 47 31	66, 91, 113, 121	0
1	D	458/491 (93%)	0.43	16 (3%) 44 28	72, 97, 112, 121	0
All	All	1860/1964 (94%)	0.33	39 (2%) 63 49	48, 81, 109, 121	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	GLU	4.4
1	C	289	CYS	3.4
1	B	221	ASN	3.2
1	C	153	SER	3.0
1	D	351	ILE	2.9

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](#)

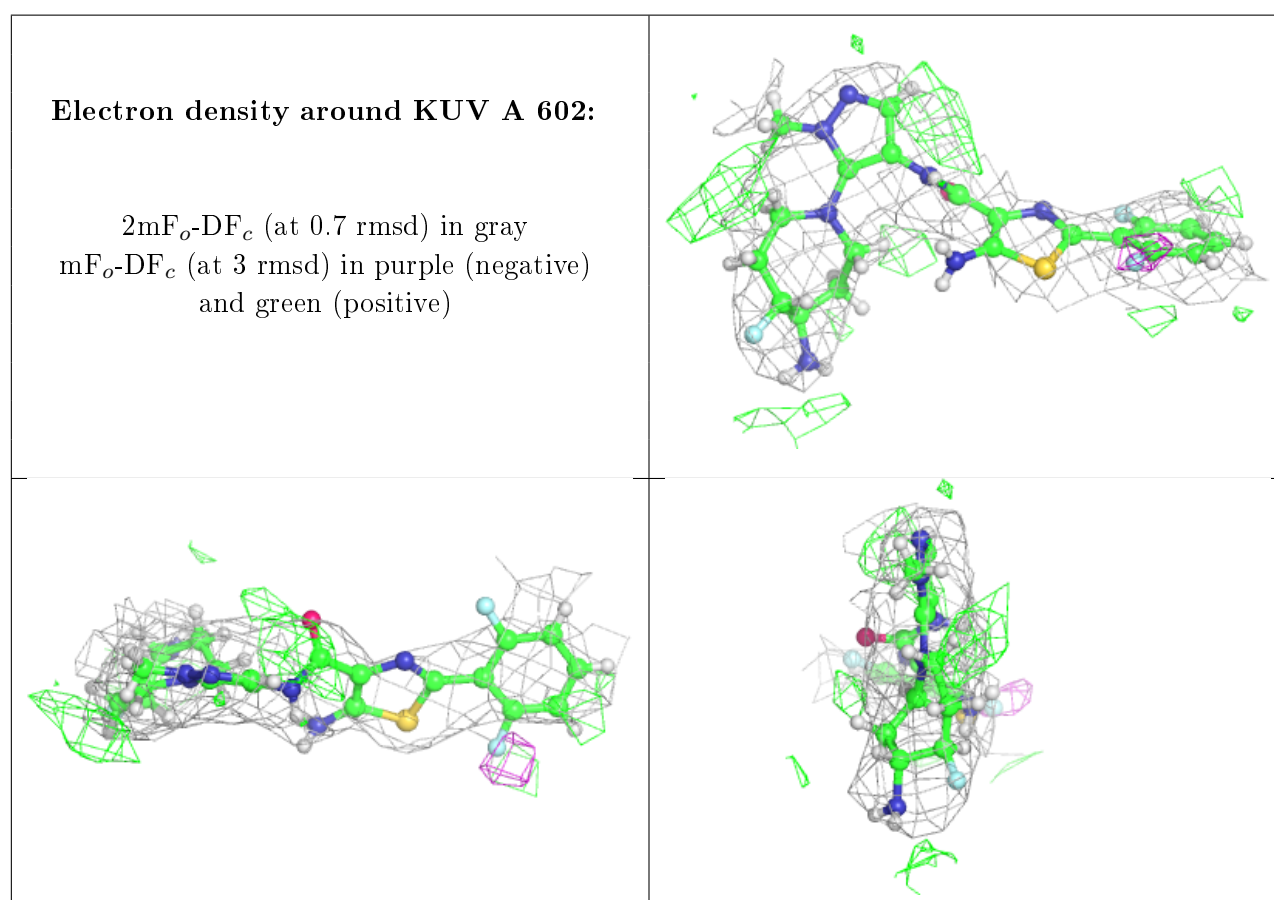
There are no carbohydrates in this entry.

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.

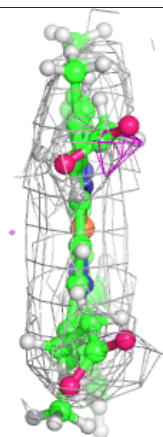
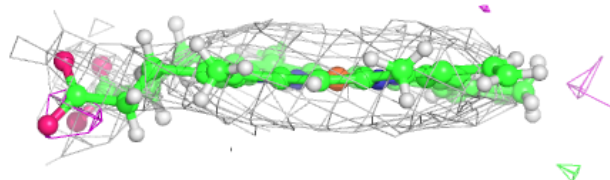
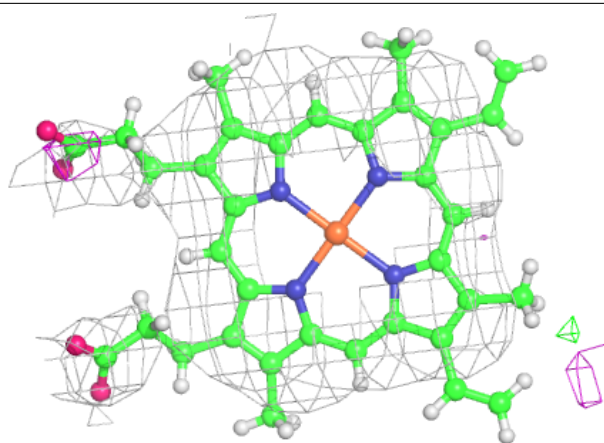
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	KUV	A	602	32/32	0.75	0.35	66,88,114,134	0
4	NO3	B	602	4/4	0.86	0.22	62,63,64,66	0
2	HEM	D	601	43/43	0.94	0.35	79,87,105,107	0
2	HEM	A	601	43/43	0.95	0.32	54,65,80,82	0
2	HEM	C	601	43/43	0.95	0.36	68,81,97,101	0
2	HEM	B	601	43/43	0.95	0.33	49,52,65,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



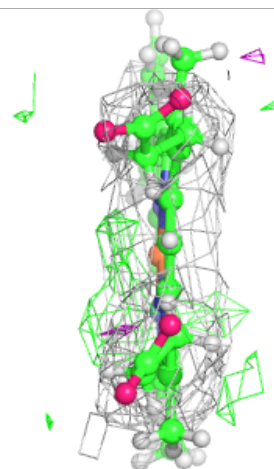
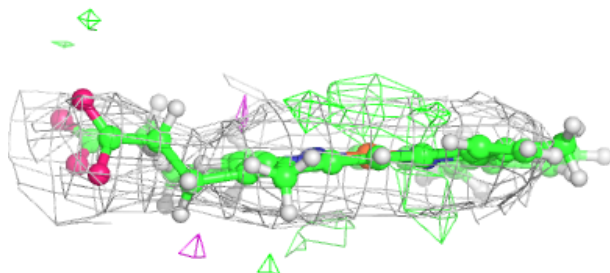
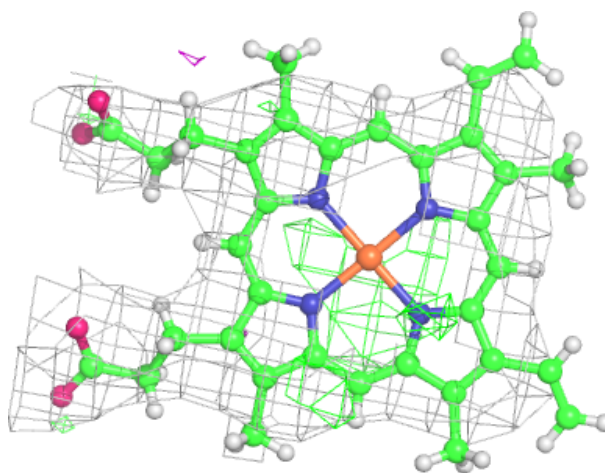
Electron density around HEM D 601:

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



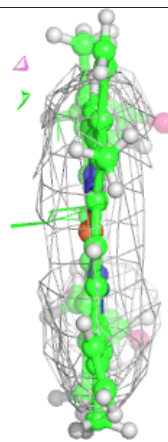
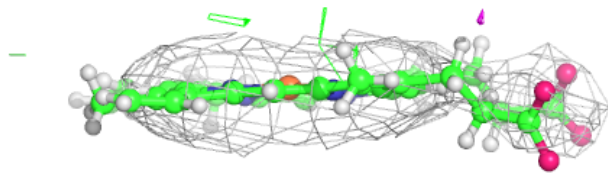
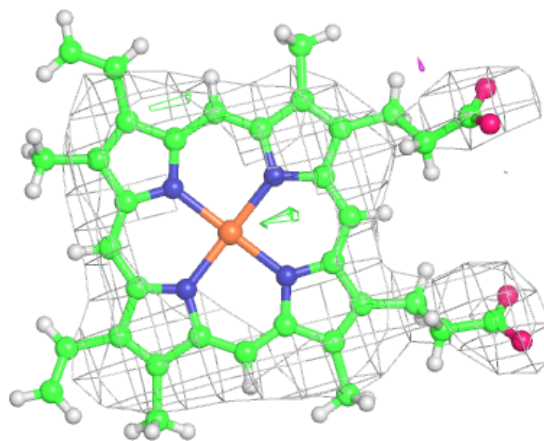
Electron density around HEM A 601:

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



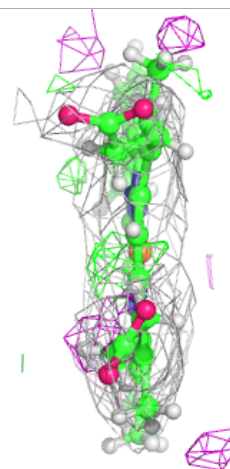
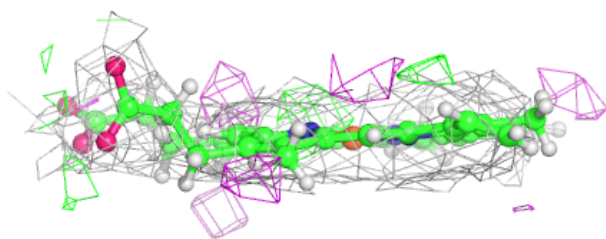
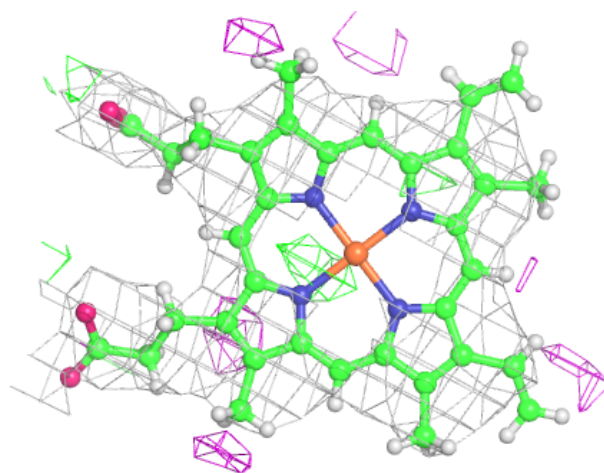
Electron density around HEM C 601:

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



Electron density around HEM B 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 [i](#)

There are no such residues in this entry.