



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:34 AM UTC

PDB ID : 4Y8W / pdb_00004y8w
Title : Crystal Structure of Human Cytochrome P450 21A2 Progesterone Complex
Authors : Pallan, P.S.; Lei, L.; Egli, M.
Deposited on : 2015-02-16
Resolution : 2.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

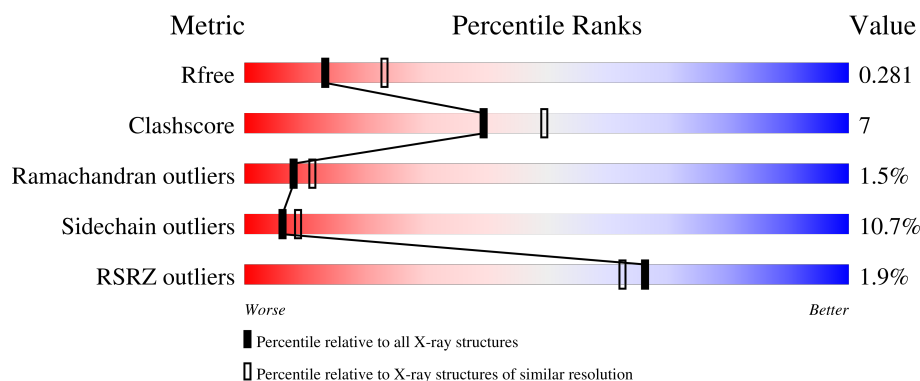
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	482	2% 68% 21% 9%
1	B	482	2% 70% 18% 9%
1	C	482	% 74% 15% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10832 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 21-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3493	2258	606	612	17			
1	B	440	Total	C	N	O	S	0	0	0
			3513	2270	611	615	17			
1	C	442	Total	C	N	O	S	0	0	0
			3531	2279	617	618	17			

There are 48 discrepancies between the modelled and reference sequences:

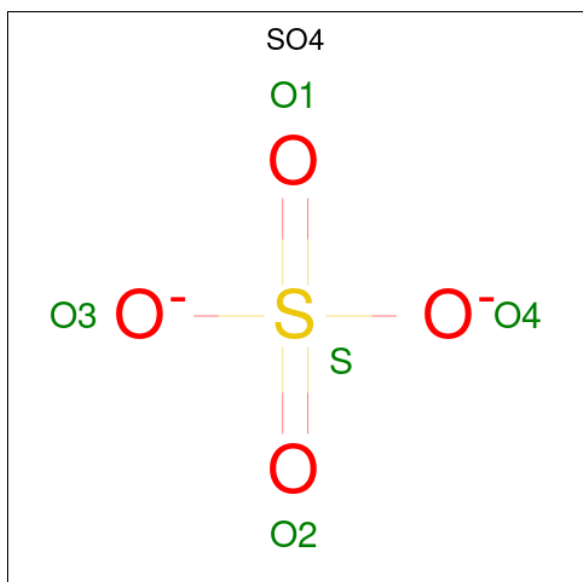
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q16874
A	21	ALA	-	expression tag	UNP Q16874
A	22	LYS	-	expression tag	UNP Q16874
A	23	LYS	-	expression tag	UNP Q16874
A	24	THR	-	expression tag	UNP Q16874
A	25	SER	-	expression tag	UNP Q16874
A	26	SER	-	expression tag	UNP Q16874
A	27	LYS	-	expression tag	UNP Q16874
A	28	GLY	-	expression tag	UNP Q16874
A	29	LYS	-	expression tag	UNP Q16874
A	496	HIS	-	expression tag	UNP Q16874
A	497	HIS	-	expression tag	UNP Q16874
A	498	HIS	-	expression tag	UNP Q16874
A	499	HIS	-	expression tag	UNP Q16874
A	500	HIS	-	expression tag	UNP Q16874
A	501	HIS	-	expression tag	UNP Q16874
B	20	MET	-	initiating methionine	UNP Q16874
B	21	ALA	-	expression tag	UNP Q16874
B	22	LYS	-	expression tag	UNP Q16874
B	23	LYS	-	expression tag	UNP Q16874
B	24	THR	-	expression tag	UNP Q16874
B	25	SER	-	expression tag	UNP Q16874
B	26	SER	-	expression tag	UNP Q16874

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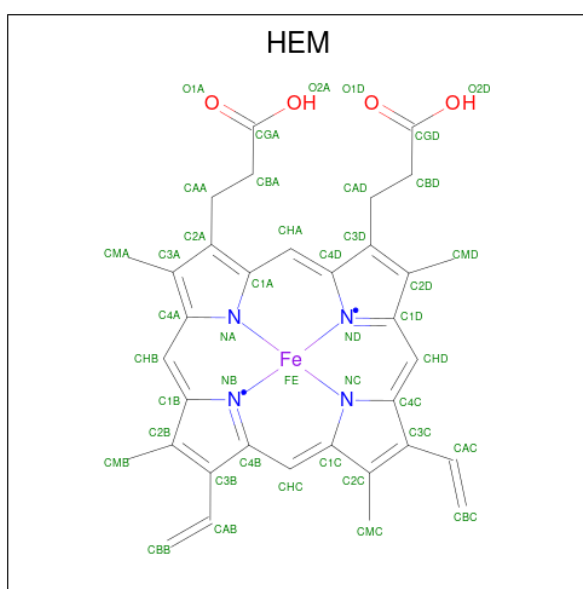
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	LYS	-	expression tag	UNP Q16874
B	28	GLY	-	expression tag	UNP Q16874
B	29	LYS	-	expression tag	UNP Q16874
B	496	HIS	-	expression tag	UNP Q16874
B	497	HIS	-	expression tag	UNP Q16874
B	498	HIS	-	expression tag	UNP Q16874
B	499	HIS	-	expression tag	UNP Q16874
B	500	HIS	-	expression tag	UNP Q16874
B	501	HIS	-	expression tag	UNP Q16874
C	20	MET	-	initiating methionine	UNP Q16874
C	21	ALA	-	expression tag	UNP Q16874
C	22	LYS	-	expression tag	UNP Q16874
C	23	LYS	-	expression tag	UNP Q16874
C	24	THR	-	expression tag	UNP Q16874
C	25	SER	-	expression tag	UNP Q16874
C	26	SER	-	expression tag	UNP Q16874
C	27	LYS	-	expression tag	UNP Q16874
C	28	GLY	-	expression tag	UNP Q16874
C	29	LYS	-	expression tag	UNP Q16874
C	496	HIS	-	expression tag	UNP Q16874
C	497	HIS	-	expression tag	UNP Q16874
C	498	HIS	-	expression tag	UNP Q16874
C	499	HIS	-	expression tag	UNP Q16874
C	500	HIS	-	expression tag	UNP Q16874
C	501	HIS	-	expression tag	UNP Q16874

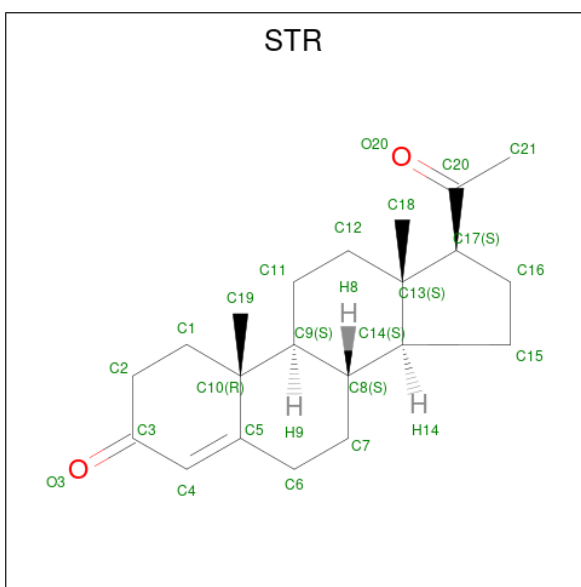
- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	21	2		
4	B	1	Total	C	O	0	0
			23	21	2		
4	C	1	Total	C	O	0	0
			23	21	2		

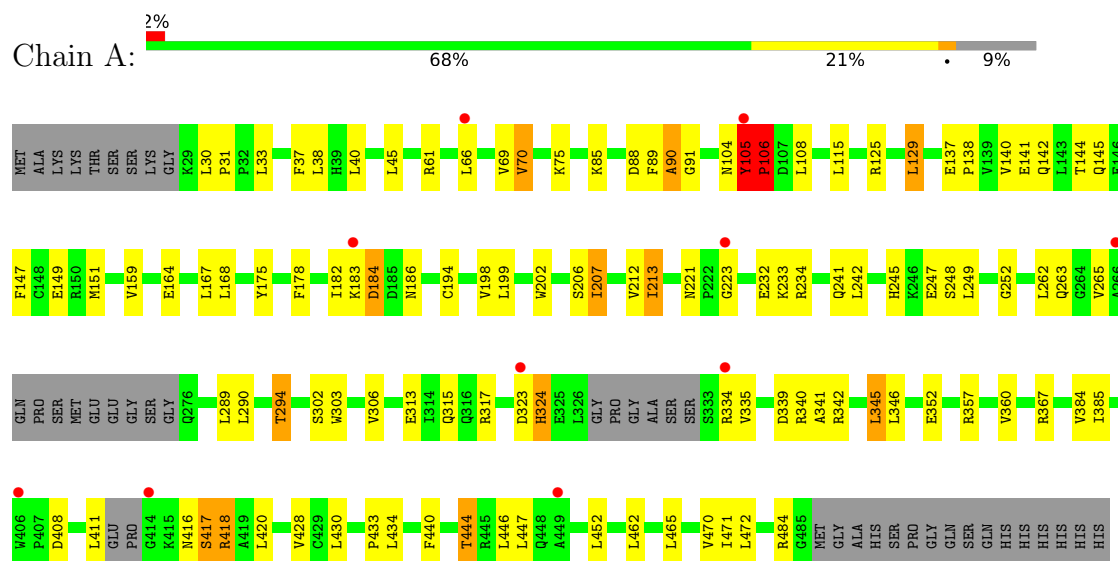
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	25	Total	O	0	0
			25	25		
5	C	30	Total	O	0	0
			30	30		

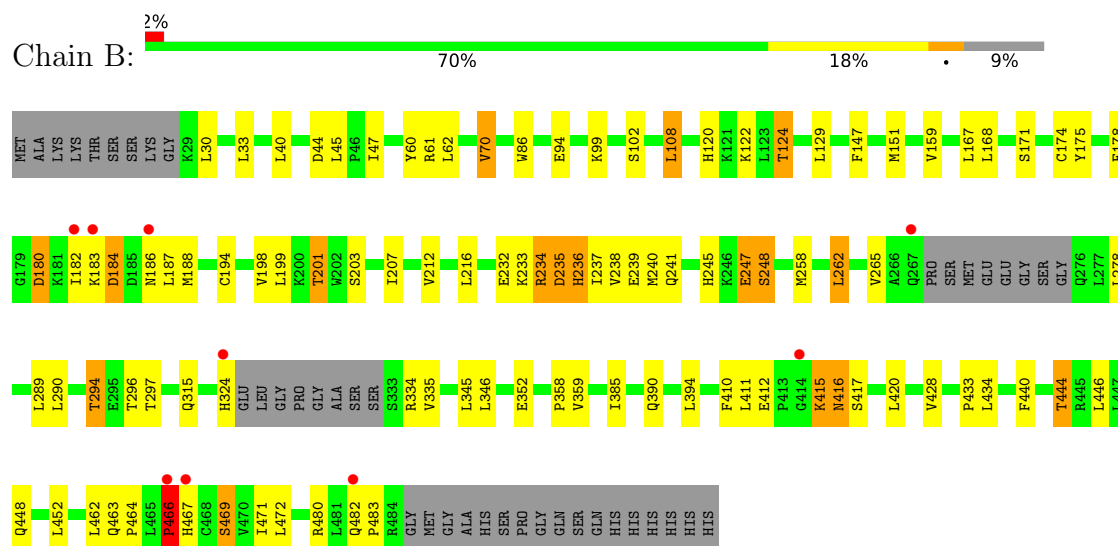
3 Residue-property plots

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

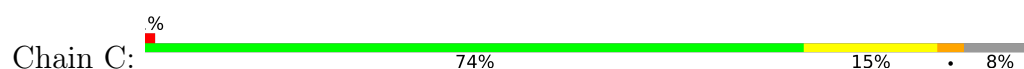
• Molecule 1: Cytochrome P450 21-hydroxylase

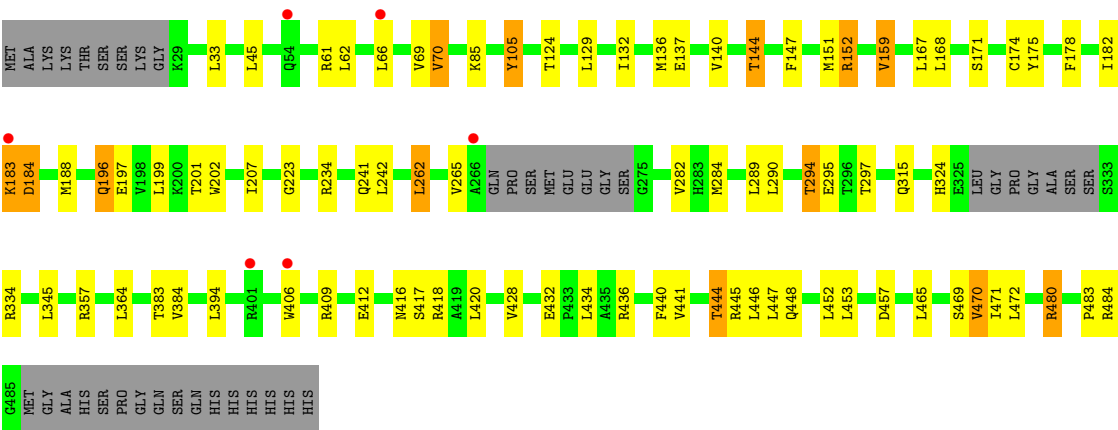


• Molecule 1: Cytochrome P450 21-hydroxylase



• Molecule 1: Cytochrome P450 21-hydroxylase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.38Å 86.86Å 108.92Å 90.00° 102.11° 90.00°	Depositor
Resolution (Å)	30.00 – 2.64 30.00 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.64) 99.6 (30.00-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.231 , 0.281 0.231 , 0.281	Depositor DCC
R_{free} test set	3087 reflections (7.62%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10832	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: SO4, HEM, STR

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	0.61	1/3581 (0.0%)	1.06	8/4875 (0.2%)
1	B	0.58	0/3603	1.04	7/4905 (0.1%)
1	C	0.56	0/3621	0.99	1/4927 (0.0%)
All	All	0.58	1/10805 (0.0%)	1.03	16/14707 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	TYR	CA-C	-5.35	1.46	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	GLU	CA-C-N	7.06	134.41	121.70
1	B	247	GLU	C-N-CA	7.06	134.41	121.70
1	B	247	GLU	N-CA-C	6.51	121.52	111.56
1	A	233	LYS	N-CA-C	-6.20	98.79	108.90
1	A	90	ALA	N-CA-C	6.07	123.72	110.80
1	A	105	TYR	C-N-CD	5.97	133.73	120.60
1	A	106	PRO	CA-N-CD	-5.84	103.32	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	PRO	CA-C-N	5.76	132.06	121.70
1	B	466	PRO	C-N-CA	5.76	132.06	121.70
1	A	233	LYS	CA-C-N	5.48	131.56	121.70
1	A	233	LYS	C-N-CA	5.48	131.56	121.70
1	B	466	PRO	N-CA-C	5.47	123.74	112.47
1	A	416	ASN	N-CA-C	5.20	117.77	110.23
1	A	105	TYR	CA-CB-CG	5.07	123.03	113.90
1	B	180	ASP	N-CA-C	5.02	117.49	111.71
1	C	417	SER	N-CA-C	5.00	116.56	110.41

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLU	Peptide
1	B	235	ASP	Peptide
1	B	466	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3493	0	3528	58	0
1	B	3513	0	3563	48	0
1	C	3531	0	3586	36	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	43	0	30	1	0
3	B	43	0	30	0	0
3	C	43	0	30	2	0
4	A	23	0	30	1	0
4	B	23	0	30	1	0
4	C	23	0	30	0	0
5	A	22	0	0	0	0
5	B	25	0	0	0	0
5	C	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10832	0	10857	144	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.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PHE:HB2	1:A:182:ILE:HD11	1.42	0.96
1:B:315:GLN:HE22	1:B:452:LEU:H	1.14	0.92
1:B:174:CYS:HB2	1:B:188:MET:HE1	1.54	0.88
1:A:151:MET:HE1	1:A:159:VAL:HG11	1.53	0.88
1:A:315:GLN:HE22	1:A:452:LEU:H	1.16	0.87
1:A:418:ARG:HD2	1:A:418:ARG:H	1.43	0.84
1:C:188:MET:HA	1:C:188:MET:HE2	1.63	0.80
1:C:315:GLN:HE22	1:C:452:LEU:H	1.31	0.79
1:A:105:TYR:HB3	1:A:106:PRO:CA	2.14	0.78
1:C:178:PHE:CD1	1:C:241:GLN:HG2	2.18	0.77
1:B:70:VAL:HG22	1:B:385:ILE:HG12	1.70	0.74
1:C:61:ARG:HG2	1:C:70:VAL:HG12	1.70	0.73
1:B:315:GLN:HE22	1:B:452:LEU:N	1.90	0.69
1:B:315:GLN:NE2	1:B:452:LEU:H	1.90	0.68
1:A:252:GLY:H	1:A:263:GLN:HE22	1.40	0.67
1:A:105:TYR:HB3	1:A:106:PRO:HA	1.76	0.66
1:B:236:HIS:O	1:B:238:VAL:N	2.29	0.66
1:B:415:LYS:HB2	1:B:416:ASN:HB3	1.78	0.66
1:B:440:PHE:O	1:B:444:THR:HB	1.96	0.65
1:B:290:LEU:O	1:B:294:THR:HG23	1.97	0.65
1:C:440:PHE:O	1:C:444:THR:HB	2.00	0.62
1:C:140:VAL:O	1:C:144:THR:HG22	1.98	0.62
1:B:194:CYS:O	1:B:198:VAL:HG23	1.99	0.62
1:C:196:GLN:HE21	1:C:196:GLN:HA	1.65	0.61
1:A:178:PHE:CD1	1:A:241:GLN:HG2	2.35	0.61
1:B:151:MET:HE1	1:B:159:VAL:HG11	1.81	0.61
1:B:174:CYS:CB	1:B:188:MET:HE1	2.29	0.61
1:A:75:LYS:HZ3	1:A:418:ARG:HH11	1.49	0.60
1:A:184:ASP:H	1:A:186:ASN:H	1.50	0.60
1:B:247:GLU:H	1:B:248:SER:HB3	1.66	0.60
1:A:151:MET:CE	1:A:159:VAL:HG11	2.28	0.60
1:B:296:THR:HA	1:B:359:VAL:HG11	1.84	0.59
1:C:406:TRP:O	1:C:409:ARG:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:SER:HB2	1:B:469:SER:HB2	1.86	0.58
1:A:138:PRO:HA	1:A:141:GLU:HG2	1.86	0.57
1:A:202:TRP:HZ3	1:A:470:VAL:HG21	1.69	0.57
1:A:290:LEU:O	1:A:294:THR:HG23	2.03	0.57
1:B:175:TYR:OH	1:B:183:LYS:HB2	2.04	0.56
1:A:105:TYR:HB3	1:A:106:PRO:CB	2.36	0.55
3:A:603:HEM:HBC2	3:A:603:HEM:HMC2	1.89	0.55
1:C:290:LEU:O	1:C:294:THR:HG23	2.07	0.54
1:B:178:PHE:CD1	1:B:241:GLN:HG2	2.42	0.54
1:C:201:THR:O	1:C:207:ILE:HD12	2.07	0.54
1:B:40:LEU:HD11	1:B:212:VAL:HG11	1.90	0.53
1:A:61:ARG:HG2	1:A:70:VAL:HG12	1.91	0.53
1:B:178:PHE:CG	1:B:241:GLN:HG2	2.43	0.53
1:C:151:MET:HE1	1:C:159:VAL:HG11	1.90	0.53
1:A:418:ARG:H	1:A:418:ARG:CD	2.17	0.52
1:B:182:ILE:HA	1:B:187:LEU:HD12	1.90	0.52
1:C:69:VAL:HG22	1:C:384:VAL:HB	1.91	0.51
1:A:339:ASP:O	1:A:341:ALA:N	2.43	0.51
1:C:406:TRP:CE3	1:C:409:ARG:HB2	2.45	0.51
1:C:171:SER:O	1:C:175:TYR:HD1	1.93	0.51
1:C:188:MET:HA	1:C:188:MET:CE	2.39	0.50
1:B:415:LYS:HD3	1:B:416:ASN:HB3	1.93	0.50
1:C:178:PHE:CG	1:C:241:GLN:HG2	2.47	0.50
1:C:418:ARG:HD3	1:C:418:ARG:H	1.77	0.50
1:A:252:GLY:H	1:A:263:GLN:NE2	2.07	0.50
1:B:171:SER:HA	1:B:188:MET:CE	2.41	0.50
1:A:105:TYR:HB3	1:A:106:PRO:HB3	1.94	0.50
1:B:184:ASP:H	1:B:186:ASN:H	1.60	0.50
1:A:212:VAL:HG23	1:A:213:ILE:HG13	1.94	0.49
1:C:412:GLU:H	1:C:412:GLU:CD	2.20	0.49
1:A:140:VAL:O	1:A:144:THR:HG23	2.12	0.49
1:C:202:TRP:HZ3	1:C:470:VAL:HG21	1.78	0.49
1:A:89:PHE:O	1:A:91:GLY:N	2.46	0.48
1:A:69:VAL:HG22	1:A:384:VAL:HB	1.96	0.48
1:C:175:TYR:OH	1:C:183:LYS:HB2	2.13	0.48
1:C:105:TYR:HB2	1:C:284:MET:HG2	1.96	0.48
1:A:38:LEU:HD23	1:A:40:LEU:HD12	1.95	0.48
1:C:262:LEU:HD13	1:C:282:VAL:HG11	1.95	0.48
1:C:453:LEU:HB2	1:C:480:ARG:HB3	1.96	0.48
1:B:61:ARG:HG2	1:B:70:VAL:HG12	1.96	0.48
1:A:106:PRO:HD2	1:A:106:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ARG:HD2	1:C:445:ARG:HH22	1.78	0.47
1:A:125:ARG:NH1	1:A:430:LEU:O	2.47	0.47
1:A:206:SER:O	1:A:207:ILE:HB	2.15	0.47
1:A:340:ARG:NH1	1:B:412:GLU:O	2.47	0.47
1:A:221:ASN:HD22	1:A:221:ASN:C	2.22	0.47
1:A:247:GLU:O	1:A:248:SER:HB3	2.15	0.47
1:A:315:GLN:NE2	1:A:452:LEU:H	1.98	0.47
1:C:409:ARG:HG3	1:C:416:ASN:HD21	1.80	0.47
1:A:194:CYS:O	1:A:198:VAL:HG23	2.15	0.47
1:A:175:TYR:OH	1:A:183:LYS:HB2	2.16	0.46
1:A:66:LEU:HD13	1:A:213:ILE:HG12	1.98	0.46
3:C:602:HEM:HMB2	3:C:602:HEM:HBB2	1.97	0.46
1:B:147:PHE:O	1:B:151:MET:HG2	2.17	0.45
1:B:463:GLN:HA	1:B:464:PRO:HD3	1.87	0.45
1:A:178:PHE:CG	1:A:241:GLN:HG2	2.51	0.44
1:A:199:LEU:HD21	1:A:471:ILE:HD12	1.98	0.44
1:A:360:VAL:HG21	4:A:604:STR:H211	1.99	0.44
1:B:198:VAL:HG12	4:B:603:STR:H21	2.00	0.44
1:B:171:SER:HA	1:B:188:MET:HE3	1.98	0.44
1:B:201:THR:HG22	1:B:207:ILE:CD1	2.47	0.44
1:B:258:MET:O	1:B:262:LEU:HB2	2.17	0.44
1:A:245:HIS:O	1:A:249:LEU:HB2	2.17	0.44
3:C:602:HEM:HMC1	3:C:602:HEM:HBC2	1.99	0.44
1:C:202:TRP:CZ3	1:C:470:VAL:HG21	2.52	0.44
1:A:147:PHE:O	1:A:151:MET:HG2	2.18	0.44
1:A:147:PHE:HE1	1:A:164:GLU:HB3	1.83	0.44
1:A:440:PHE:O	1:A:444:THR:HB	2.17	0.44
1:B:108:LEU:HD22	1:B:124:THR:HG21	1.99	0.44
1:B:482:GLN:HA	1:B:483:PRO:HD3	1.86	0.44
1:A:129:LEU:HD11	1:A:433:PRO:HG2	1.99	0.44
1:B:60:TYR:HE1	1:B:62:LEU:HD22	1.81	0.44
1:A:31:PRO:HG2	1:A:61:ARG:HG3	2.00	0.43
1:A:145:GLN:O	1:A:149:GLU:HG2	2.18	0.43
1:B:44:ASP:HB3	1:B:47:ILE:HB	2.00	0.43
1:B:129:LEU:HD11	1:B:433:PRO:HG2	2.00	0.43
1:B:247:GLU:N	1:B:248:SER:HB3	2.32	0.43
1:C:199:LEU:HD23	1:C:295:GLU:HG3	2.00	0.43
1:A:207:ILE:HD11	1:A:223:GLY:O	2.19	0.43
1:C:144:THR:HG21	1:C:441:VAL:HG12	2.01	0.43
1:A:85:LYS:HB3	1:A:88:ASP:HB2	2.01	0.43
1:A:302:SER:O	1:A:306:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:TRP:CD2	1:A:357:ARG:HG2	2.54	0.42
1:B:233:LYS:HA	1:B:234:ARG:C	2.45	0.42
1:C:144:THR:HA	1:C:147:PHE:HB3	2.01	0.42
1:B:94:GLU:HG2	1:B:99:LYS:HD2	2.02	0.42
1:B:358:PRO:HD2	1:B:390:GLN:HG3	2.02	0.42
1:C:207:ILE:HD11	1:C:223:GLY:O	2.20	0.42
1:A:206:SER:HB2	1:A:221:ASN:HD21	1.85	0.42
1:B:199:LEU:HD21	1:B:471:ILE:HD12	2.01	0.42
1:C:483:PRO:HA	1:C:484:ARG:HA	1.79	0.42
1:A:317:ARG:HH22	1:A:408:ASP:CG	2.28	0.42
1:A:104:ASN:HD22	1:A:104:ASN:H	1.68	0.42
1:C:152:ARG:O	1:C:152:ARG:HD2	2.19	0.41
1:C:432:GLU:O	1:C:436:ARG:HG3	2.20	0.41
1:A:151:MET:HE1	1:A:159:VAL:CG1	2.38	0.41
1:B:410:PHE:HD1	1:B:416:ASN:HB2	1.85	0.41
1:C:324:HIS:O	1:C:324:HIS:ND1	2.53	0.41
1:B:466:PRO:HB2	1:B:467:HIS:CG	2.56	0.41
1:A:178:PHE:HB2	1:A:182:ILE:CD1	2.32	0.41
1:A:317:ARG:NH2	1:A:408:ASP:OD2	2.54	0.41
1:A:323:ASP:O	1:A:324:HIS:HB2	2.20	0.41
1:B:183:LYS:HD3	1:B:188:MET:HB2	2.03	0.41
1:B:233:LYS:HA	1:B:235:ASP:N	2.36	0.41
1:C:132:ILE:HD12	1:C:136:MET:HB2	2.02	0.41
1:B:182:ILE:HD12	1:B:188:MET:HE2	2.02	0.40
1:A:37:PHE:HD2	1:A:38:LEU:HD12	1.87	0.40
1:B:241:GLN:HG3	1:B:245:HIS:CE1	2.57	0.40
1:A:345:LEU:HD23	1:A:411:LEU:HD11	2.03	0.40
1:C:174:CYS:SG	1:C:188:MET:HE1	2.62	0.40
1:B:120:HIS:O	1:B:124:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/482 (90%)	399 (92%)	24 (6%)	9 (2%)	5	7
1	B	434/482 (90%)	406 (94%)	20 (5%)	8 (2%)	6	9
1	C	436/482 (90%)	422 (97%)	12 (3%)	2 (0%)	24	36
All	All	1302/1446 (90%)	1227 (94%)	56 (4%)	19 (2%)	8	11

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ALA
1	A	324	HIS
1	B	184	ASP
1	B	236	HIS
1	B	237	ILE
1	A	184	ASP
1	A	207	ILE
1	B	248	SER
1	B	417	SER
1	B	469	SER
1	C	184	ASP
1	A	484	ARG
1	A	105	TYR
1	B	335	VAL
1	A	417	SER
1	B	86	TRP
1	C	469	SER
1	A	335	VAL
1	A	106	PRO

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	379/421 (90%)	342 (90%)	37 (10%)	7	11
1	B	384/421 (91%)	343 (89%)	41 (11%)	6	9
1	C	386/421 (92%)	341 (88%)	45 (12%)	5	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1149/1263 (91%)	1026 (89%)	123 (11%)	6 9

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	LEU
1	A	45	LEU
1	A	70	VAL
1	A	108	LEU
1	A	115	LEU
1	A	129	LEU
1	A	137	GLU
1	A	142	GLN
1	A	167	LEU
1	A	168	LEU
1	A	213	ILE
1	A	234	ARG
1	A	242	LEU
1	A	262	LEU
1	A	265	VAL
1	A	289	LEU
1	A	294	THR
1	A	313	GLU
1	A	334	ARG
1	A	342	ARG
1	A	345	LEU
1	A	346	LEU
1	A	352	GLU
1	A	367	ARG
1	A	385	ILE
1	A	417	SER
1	A	418	ARG
1	A	420	LEU
1	A	428	VAL
1	A	434	LEU
1	A	444	THR
1	A	446	LEU
1	A	447	LEU
1	A	462	LEU
1	A	465	LEU
1	A	472	LEU

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	33	LEU
1	B	45	LEU
1	B	70	VAL
1	B	102	SER
1	B	108	LEU
1	B	122	LYS
1	B	124	THR
1	B	167	LEU
1	B	168	LEU
1	B	180	ASP
1	B	201	THR
1	B	216	LEU
1	B	232	GLU
1	B	234	ARG
1	B	239	GLU
1	B	240	MET
1	B	262	LEU
1	B	265	VAL
1	B	278	LEU
1	B	289	LEU
1	B	294	THR
1	B	297	THR
1	B	324	HIS
1	B	334	ARG
1	B	345	LEU
1	B	346	LEU
1	B	352	GLU
1	B	394	LEU
1	B	411	LEU
1	B	415	LYS
1	B	416	ASN
1	B	420	LEU
1	B	428	VAL
1	B	434	LEU
1	B	444	THR
1	B	446	LEU
1	B	448	GLN
1	B	462	LEU
1	B	472	LEU
1	B	480	ARG
1	C	33	LEU

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Mol	Chain	Res	Type
1	C	45	LEU
1	C	62	LEU
1	C	66	LEU
1	C	70	VAL
1	C	85	LYS
1	C	105	TYR
1	C	124	THR
1	C	129	LEU
1	C	137	GLU
1	C	144	THR
1	C	152	ARG
1	C	159	VAL
1	C	167	LEU
1	C	168	LEU
1	C	182	ILE
1	C	183	LYS
1	C	184	ASP
1	C	196	GLN
1	C	197	GLU
1	C	234	ARG
1	C	242	LEU
1	C	262	LEU
1	C	265	VAL
1	C	289	LEU
1	C	294	THR
1	C	297	THR
1	C	345	LEU
1	C	357	ARG
1	C	364	LEU
1	C	383	THR
1	C	394	LEU
1	C	420	LEU
1	C	428	VAL
1	C	434	LEU
1	C	444	THR
1	C	446	LEU
1	C	447	LEU
1	C	448	GLN
1	C	457	ASP
1	C	465	LEU
1	C	470	VAL
1	C	471	ILE

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Mol	Chain	Res	Type
1	C	472	LEU
1	C	480	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	73	ASN
1	A	104	ASN
1	A	221	ASN
1	A	263	GLN
1	A	315	GLN
1	A	448	GLN
1	B	67	GLN
1	B	145	GLN
1	B	154	GLN
1	B	196	GLN
1	B	221	ASN
1	B	241	GLN
1	B	244	GLN
1	B	263	GLN
1	B	276	GLN
1	B	283	HIS
1	B	315	GLN
1	B	319	GLN
1	B	347	ASN
1	B	388	ASN
1	B	448	GLN
1	B	482	GLN
1	C	196	GLN
1	C	241	GLN
1	C	253	GLN
1	C	263	GLN
1	C	299	ASN
1	C	311	HIS
1	C	315	GLN
1	C	319	GLN
1	C	347	ASN
1	C	388	ASN
1	C	390	GLN
1	C	448	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	SO4	C	601	-	4,4,4	0.41	0	6,6,6	0.14	0
2	SO4	A	602	2	4,4,4	0.42	0	6,6,6	0.13	0
4	STR	C	603	-	26,26,26	0.69	0	42,42,42	1.32	6 (14%)
3	HEM	B	602	1	50,50,50	1.61	5 (10%)	67,82,82	1.34	9 (13%)
3	HEM	A	603	1	50,50,50	1.59	5 (10%)	67,82,82	1.36	9 (13%)
3	HEM	C	602	1	50,50,50	1.58	5 (10%)	67,82,82	1.39	7 (10%)
2	SO4	B	601	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SO4	A	601	2	4,4,4	0.43	0	6,6,6	0.13	0
4	STR	B	603	-	26,26,26	0.66	0	42,42,42	1.26	5 (11%)
4	STR	A	604	-	26,26,26	0.70	0	42,42,42	1.29	5 (11%)

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
4	STR	C	603	-	-	4/4/62/62	0/4/4/4
3	HEM	B	602	1	-	0/14/54/54	-
3	HEM	A	603	1	-	1/14/54/54	-
3	HEM	C	602	1	-	0/14/54/54	-
4	STR	B	603	-	-	4/4/62/62	0/4/4/4
4	STR	A	604	-	-	4/4/62/62	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	FE-NB	5.66	2.12	1.94
3	A	603	HEM	FE-NB	5.52	2.11	1.94
3	C	602	HEM	FE-NB	5.33	2.11	1.94
3	C	602	HEM	FE-NC	4.66	2.10	1.95
3	A	603	HEM	FE-NC	4.64	2.10	1.95
3	B	602	HEM	FE-NC	4.47	2.09	1.95
3	C	602	HEM	C1B-NB	-3.22	1.34	1.40
3	B	602	HEM	C1B-NB	-3.21	1.34	1.40
3	A	603	HEM	C1B-NB	-3.12	1.34	1.40
3	C	602	HEM	C4D-ND	-2.90	1.35	1.40
3	A	603	HEM	C4D-ND	-2.84	1.35	1.40
3	B	602	HEM	C4D-ND	-2.82	1.35	1.40
3	A	603	HEM	C3B-C4B	2.36	1.49	1.44
3	B	602	HEM	C3B-C4B	2.29	1.49	1.44
3	C	602	HEM	C3B-C4B	2.23	1.49	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	HEM	CHC-C4B-NB	4.28	129.03	124.42
3	C	602	HEM	CHD-C1D-ND	3.98	128.70	124.42
3	A	603	HEM	CHC-C4B-NB	3.86	128.58	124.42
3	B	602	HEM	CHC-C4B-NB	3.86	128.58	124.42
3	A	603	HEM	C1B-NB-C4B	3.79	109.70	105.21
3	B	602	HEM	CHD-C1D-ND	3.57	128.27	124.42
3	B	602	HEM	C1B-NB-C4B	3.41	109.24	105.21
3	C	602	HEM	C1B-NB-C4B	3.39	109.22	105.21
3	A	603	HEM	CHA-C4D-ND	3.30	128.44	124.37
3	B	602	HEM	CHA-C4D-ND	3.27	128.41	124.37
3	C	602	HEM	CHA-C4D-ND	3.22	128.34	124.37
3	A	603	HEM	CHD-C1D-ND	3.07	127.72	124.42
3	C	602	HEM	CHD-C1D-C2D	-2.98	120.32	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	STR	C15-C14-C13	2.97	107.33	103.84
4	A	604	STR	C6-C5-C4	-2.89	116.24	120.86
4	C	603	STR	C15-C14-C13	2.87	107.22	103.84
3	A	603	HEM	CHA-C4D-C3D	-2.84	119.99	125.23
4	B	603	STR	C6-C5-C4	-2.63	116.66	120.86
4	A	604	STR	C15-C14-C13	2.61	106.91	103.84
3	B	602	HEM	CHA-C4D-C3D	-2.56	120.50	125.23
4	C	603	STR	C6-C5-C4	-2.55	116.78	120.86
3	B	602	HEM	CHB-C1B-NB	2.54	127.51	124.37
4	C	603	STR	C2-C3-C4	2.53	120.57	116.73
3	A	603	HEM	C3B-C4B-NB	-2.52	107.66	109.47
3	C	602	HEM	CHA-C4D-C3D	-2.51	120.59	125.23
3	B	602	HEM	CHD-C1D-C2D	-2.50	121.08	125.03
4	A	604	STR	C6-C5-C10	2.47	121.11	116.76
3	A	603	HEM	CHD-C1D-C2D	-2.43	121.20	125.03
4	B	603	STR	C21-C20-C17	2.39	121.78	117.65
4	B	603	STR	C6-C5-C10	2.33	120.88	116.76
4	B	603	STR	C2-C3-C4	2.29	120.21	116.73
3	A	603	HEM	CHB-C1B-NB	2.23	127.12	124.37
3	B	602	HEM	O2D-CGD-O1D	-2.17	117.76	123.33
3	B	602	HEM	C3B-C4B-NB	-2.16	107.92	109.47
4	C	603	STR	C21-C20-C17	2.13	121.33	117.65
4	C	603	STR	C6-C5-C10	2.11	120.48	116.76
4	A	604	STR	C21-C20-C17	2.07	121.22	117.65
4	A	604	STR	C2-C3-C4	2.03	119.82	116.73
3	A	603	HEM	O2D-CGD-O1D	-2.03	118.12	123.33
3	C	602	HEM	C4B-C3B-C2B	-2.02	105.42	107.28
4	C	603	STR	C1-C10-C5	2.00	112.19	108.74

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	603	STR	C16-C17-C20-C21
4	C	603	STR	C13-C17-C20-C21
4	A	604	STR	C16-C17-C20-C21
4	B	603	STR	C16-C17-C20-C21
4	C	603	STR	C16-C17-C20-O20
4	A	604	STR	C13-C17-C20-O20
4	A	604	STR	C13-C17-C20-C21
4	B	603	STR	C13-C17-C20-O20
4	B	603	STR	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
4	A	604	STR	C16-C17-C20-O20
4	B	603	STR	C16-C17-C20-O20
4	C	603	STR	C13-C17-C20-O20
3	A	603	HEM	C2B-C3B-CAB-CBB

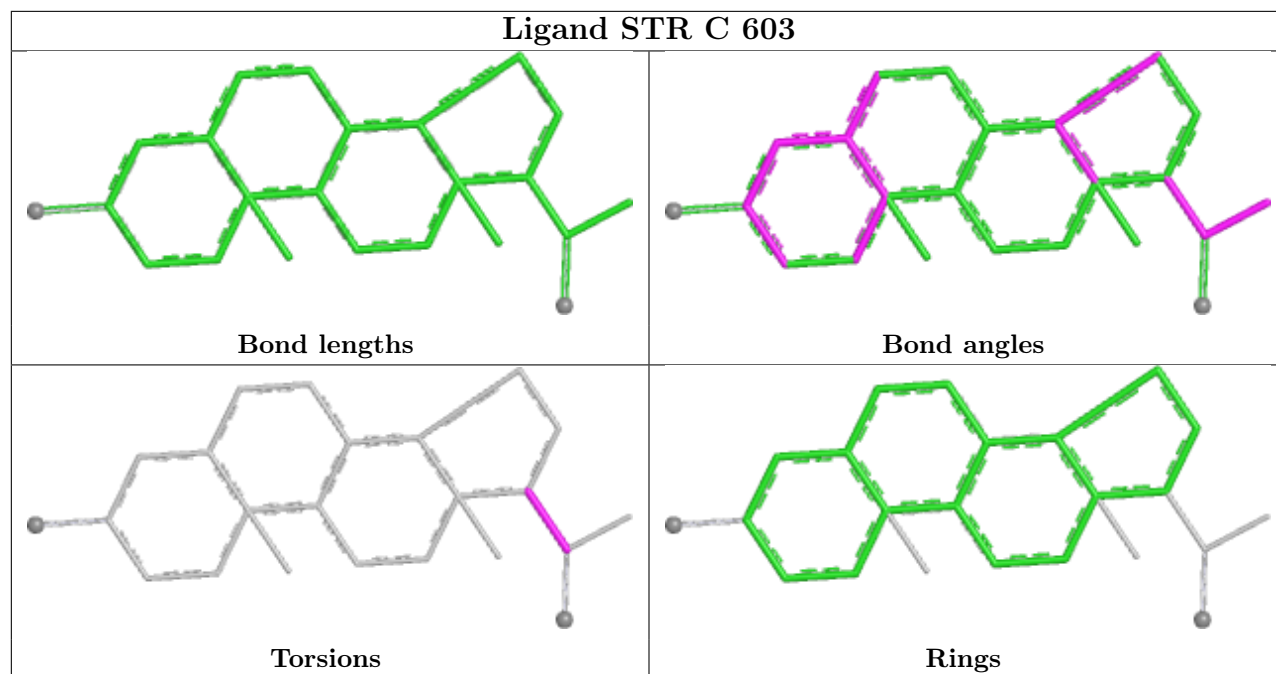
There are no ring outliers.

4 monomers are involved in 5 short contacts:

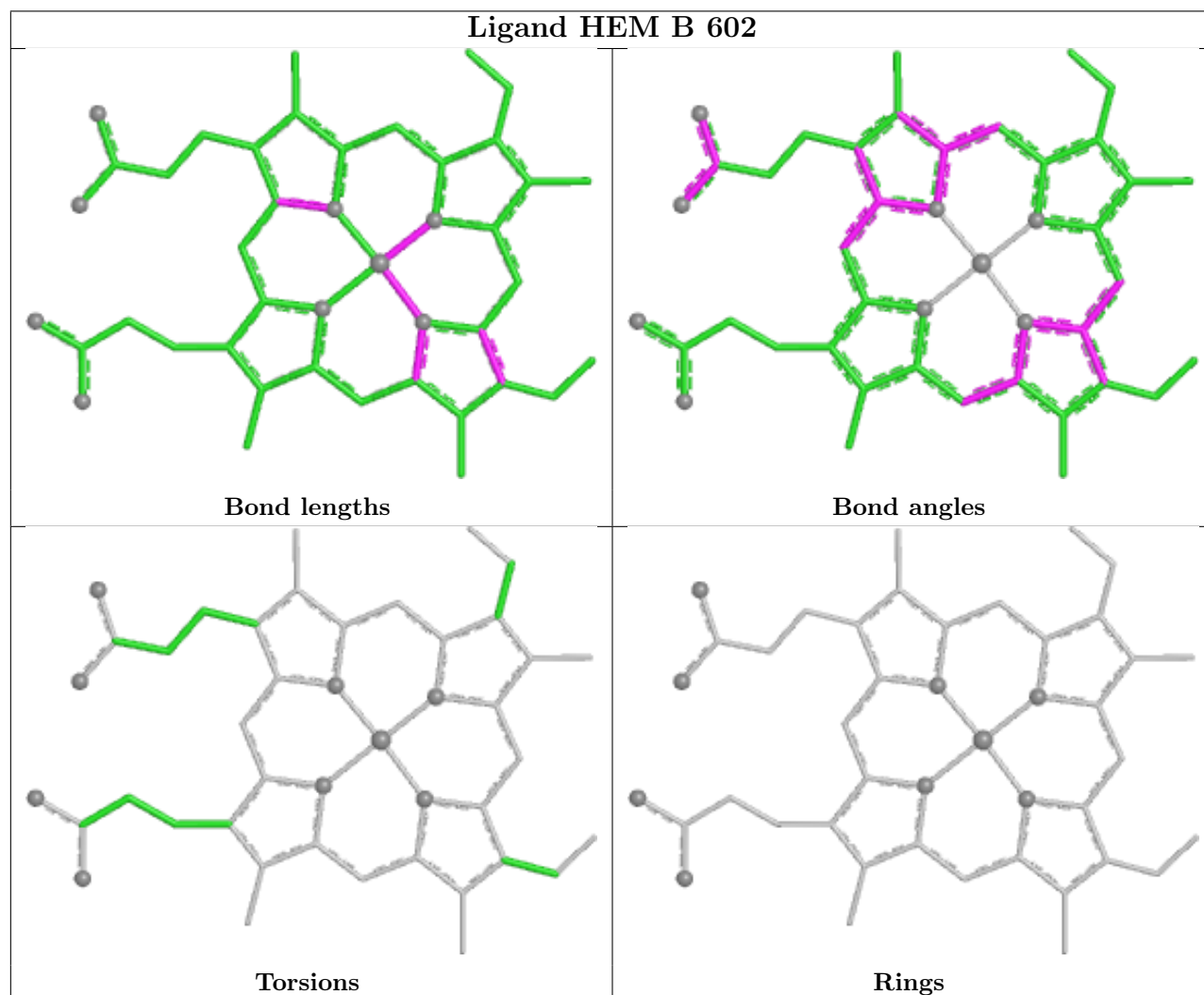
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	HEM	1	0
3	C	602	HEM	2	0
4	B	603	STR	1	0
4	A	604	STR	1	0

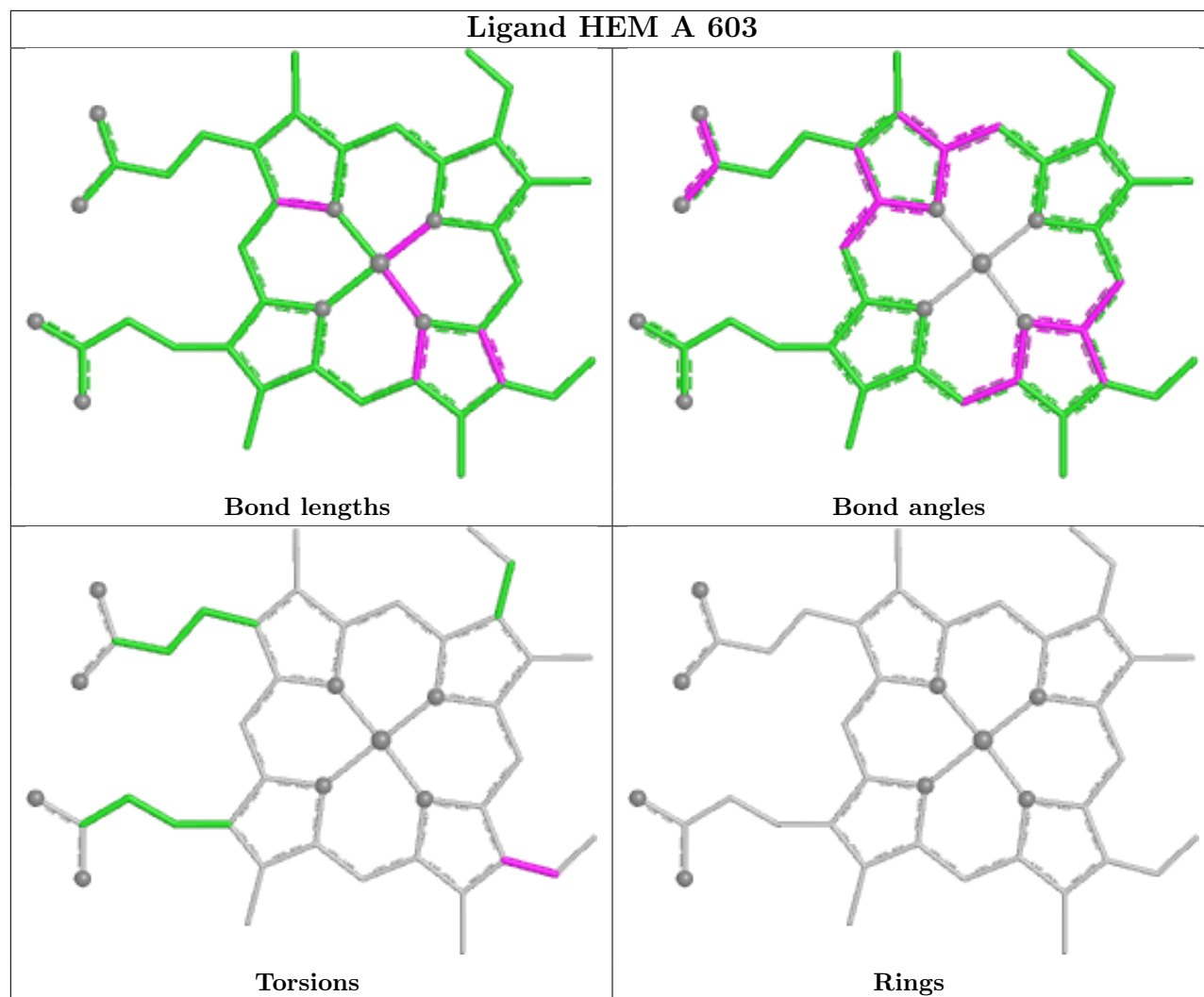
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

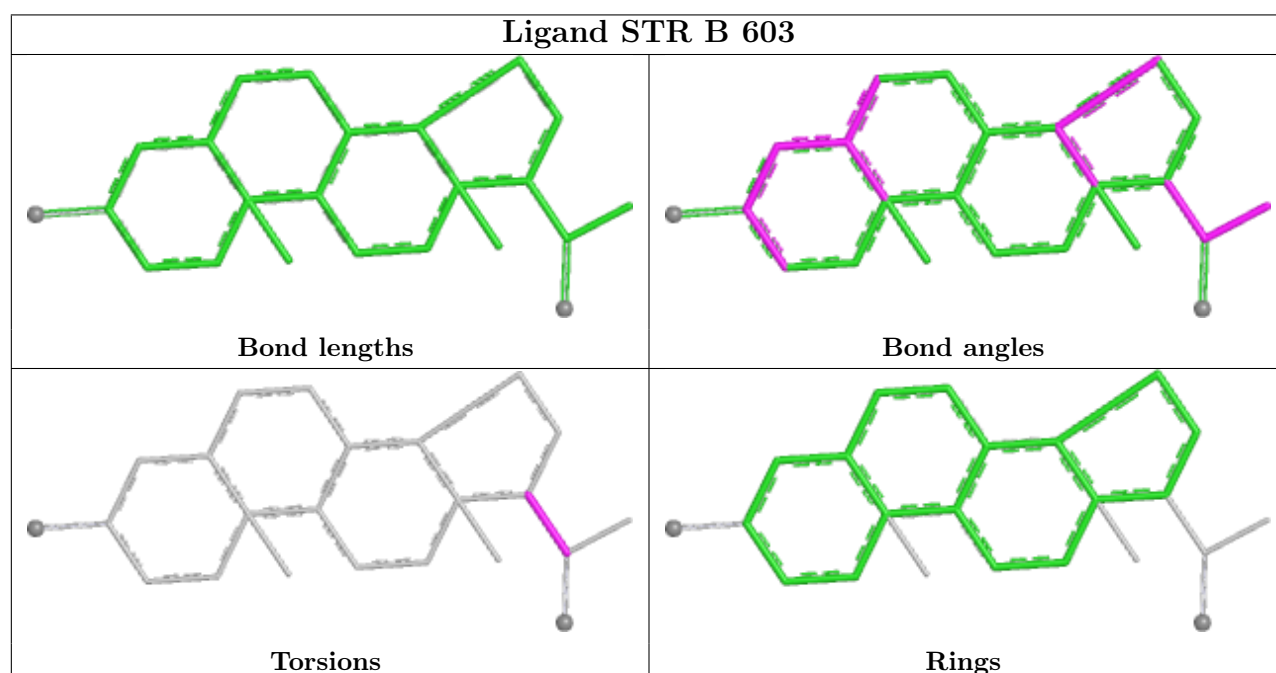
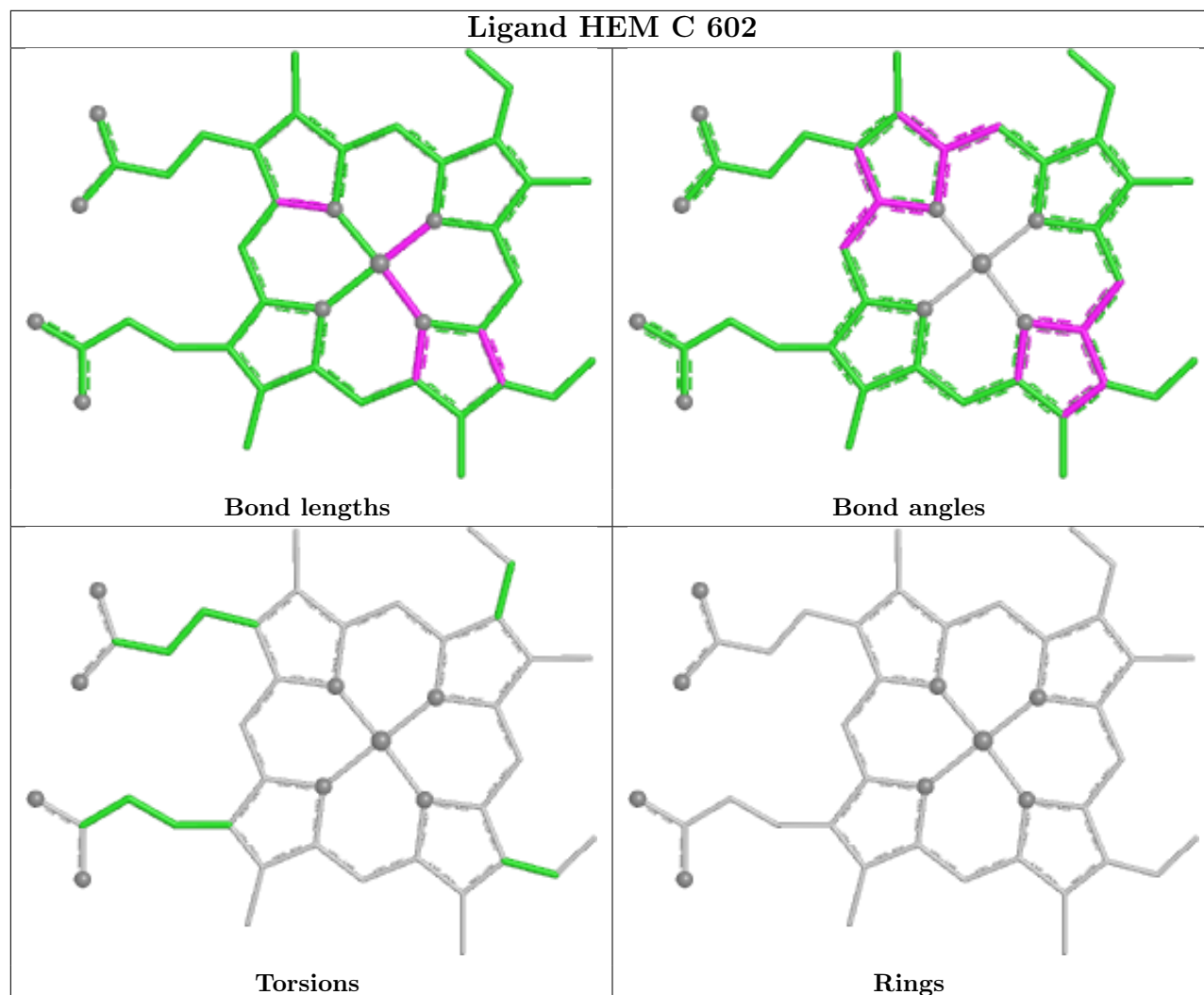
Ligand STR C 603

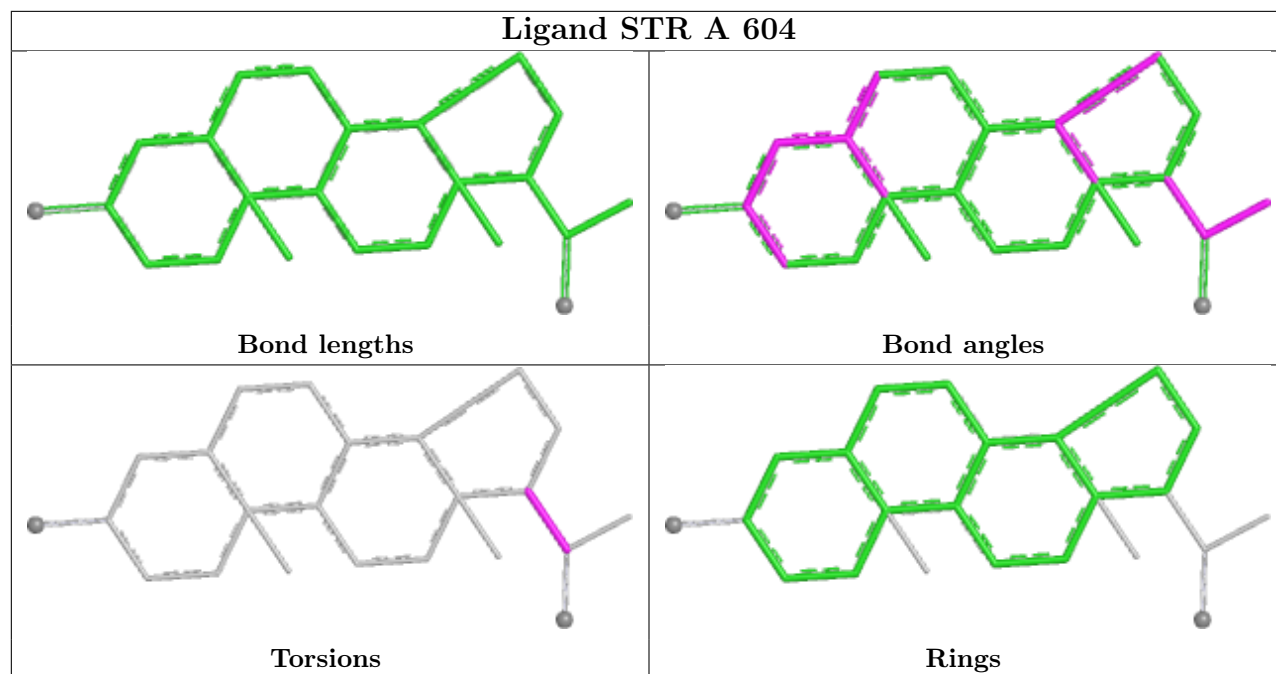


Ligand HEM B 602









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 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	440/482 (91%)	0.34	10 (2%) 61 57	25, 41, 58, 81	0
1	B	440/482 (91%)	0.34	9 (2%) 65 61	28, 41, 63, 82	0
1	C	442/482 (91%)	0.28	6 (1%) 73 70	27, 43, 60, 73	0
All	All	1322/1446 (91%)	0.32	25 (1%) 66 62	25, 42, 61, 82	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	TYR	3.3
1	B	182	ILE	3.1
1	B	466	PRO	3.0
1	A	449	ALA	2.8
1	A	183	LYS	2.8
1	C	183	LYS	2.8
1	C	401	ARG	2.7
1	C	66	LEU	2.4
1	B	183	LYS	2.4
1	B	467	HIS	2.4
1	A	406	TRP	2.4
1	A	414	GLY	2.4
1	A	334	ARG	2.4
1	A	323	ASP	2.3
1	A	223	GLY	2.3
1	A	266	ALA	2.2
1	B	324	HIS	2.2
1	A	66	LEU	2.2
1	B	186	ASN	2.2
1	B	414	GLY	2.2
1	B	267	GLN	2.1
1	B	482	GLN	2.1
1	C	406	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	54	GLN	2.0
1	C	266	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

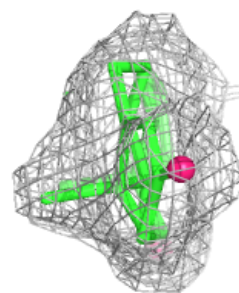
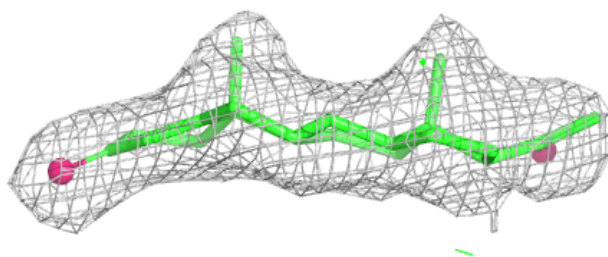
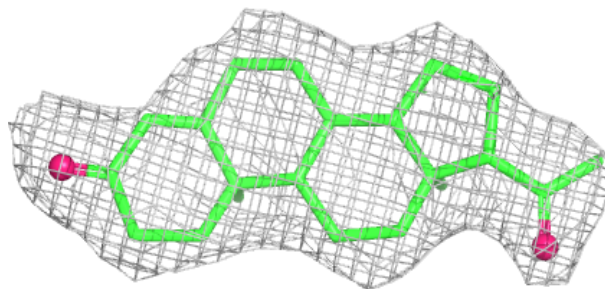
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	STR	A	604	23/23	0.90	0.10	30,30,31,32	0
4	STR	B	603	23/23	0.92	0.09	30,30,33,35	0
4	STR	C	603	23/23	0.92	0.09	34,35,36,38	0
3	HEM	A	603	43/43	0.95	0.08	24,25,26,26	0
3	HEM	C	602	43/43	0.96	0.08	24,25,26,26	0
2	SO4	A	602	5/5	0.96	0.06	36,36,36,37	5
2	SO4	A	601	5/5	0.96	0.06	30,30,30,30	5
3	HEM	B	602	43/43	0.96	0.08	26,27,29,29	0
2	SO4	B	601	5/5	0.98	0.07	41,41,42,42	0
2	SO4	C	601	5/5	0.98	0.09	31,31,32,32	0

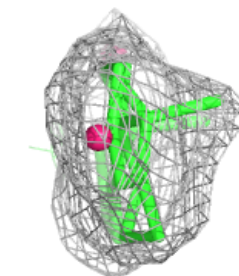
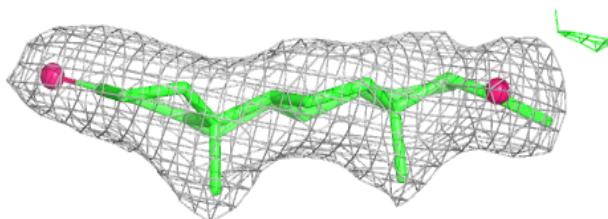
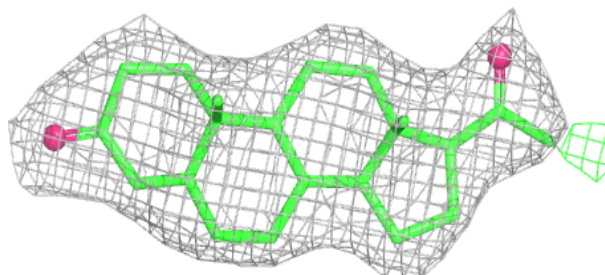
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STR A 604:

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

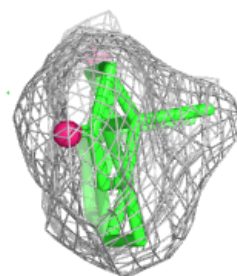
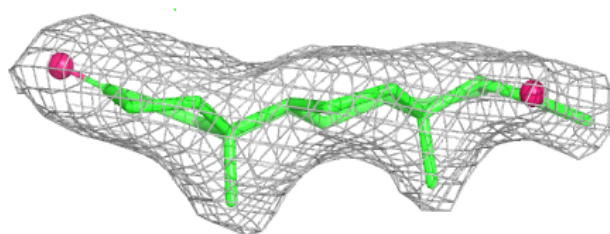
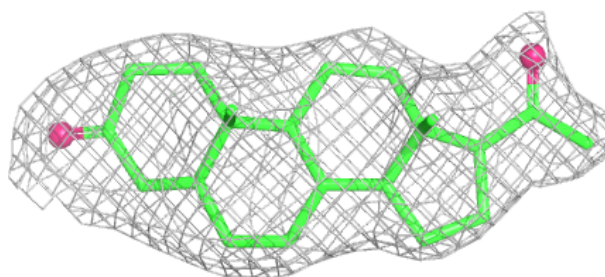
**Electron density around STR B 603:**

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



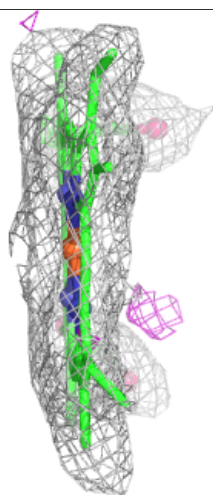
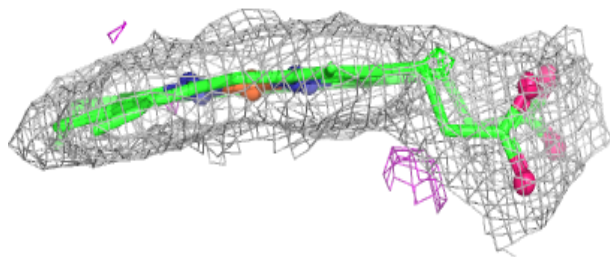
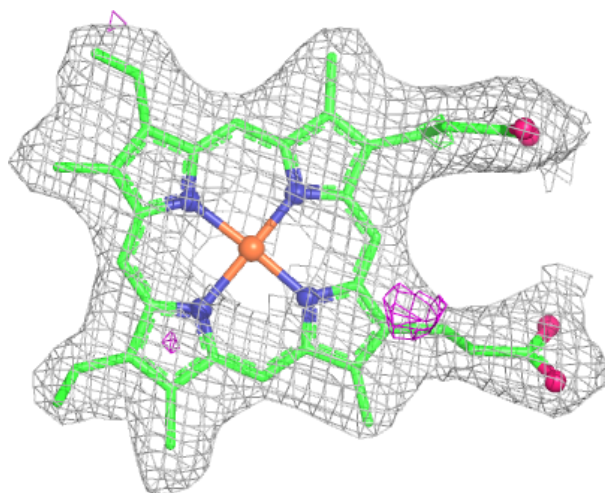
Electron density around STR C 603:

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



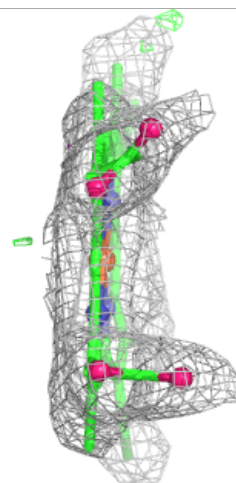
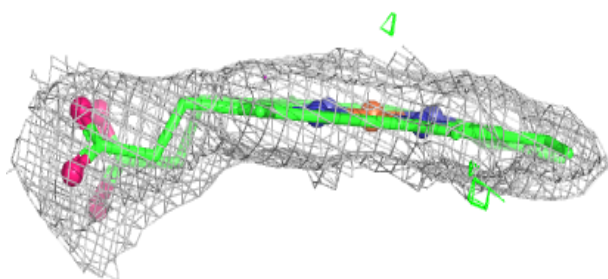
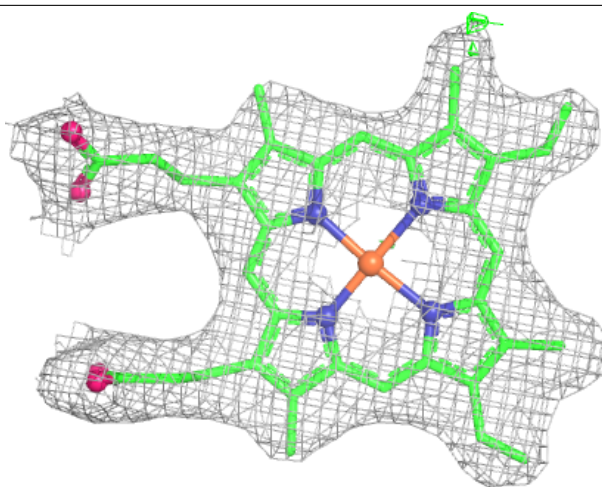
Electron density around HEM A 603:

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



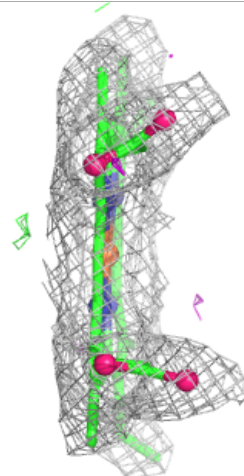
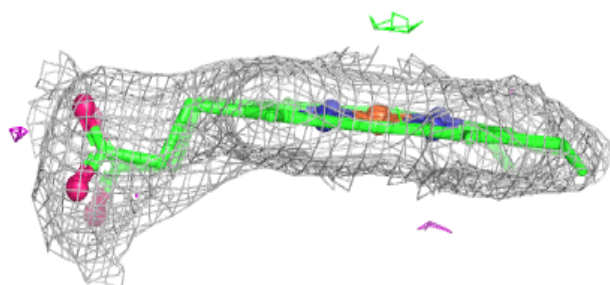
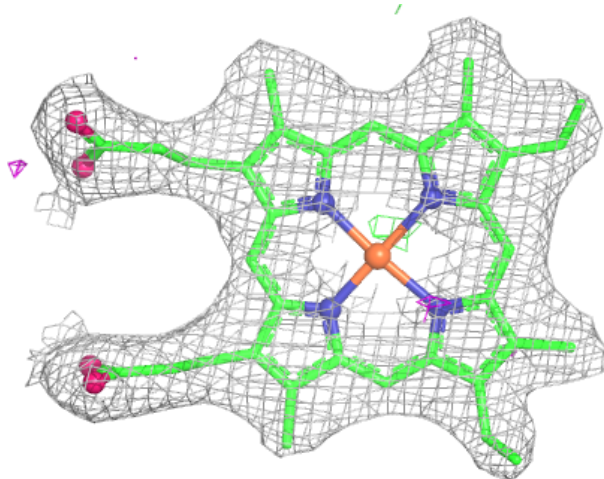
Electron density around HEM C 602:

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



Electron density around HEM B 602:

$2mF_o-DF_c$ (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.