



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:49 PM EDT

PDB ID : 4JLT / pdb_00004jlt
Title : Crystal structure of P450 2B4(H226Y) in complex with paroxetine
Authors : Shah, M.B.; Pascual, J.; Stout, C.D.; Halpert, J.R.
Deposited on : 2013-03-13
Resolution : 2.14 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

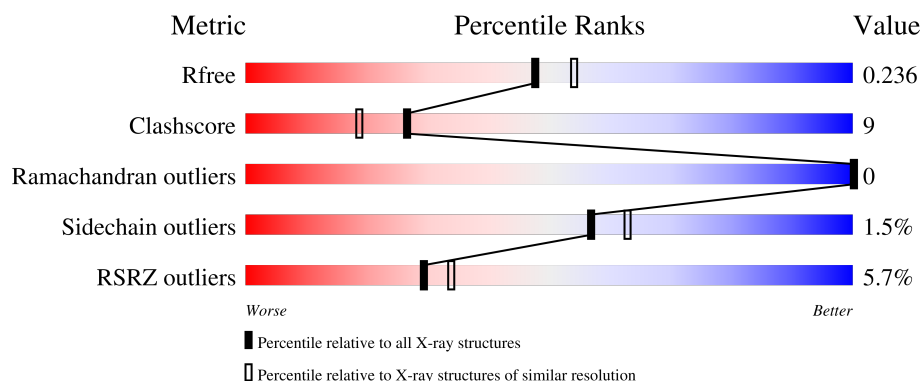
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	476	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	510	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4056 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3654	2360	624	660	10			

There are 33 discrepancies between the modelled and reference sequences:

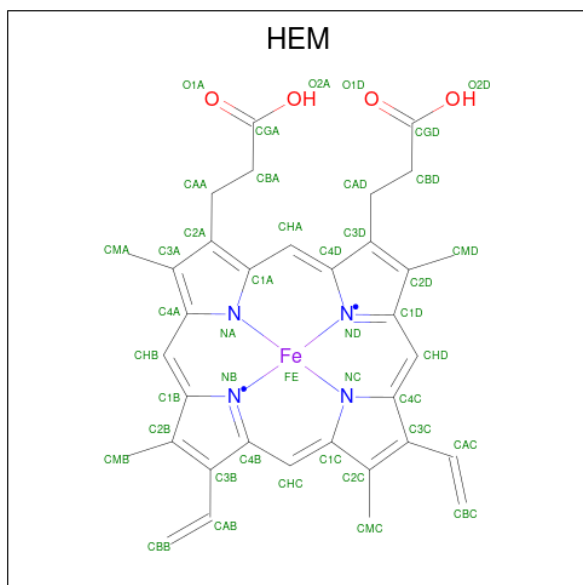
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178

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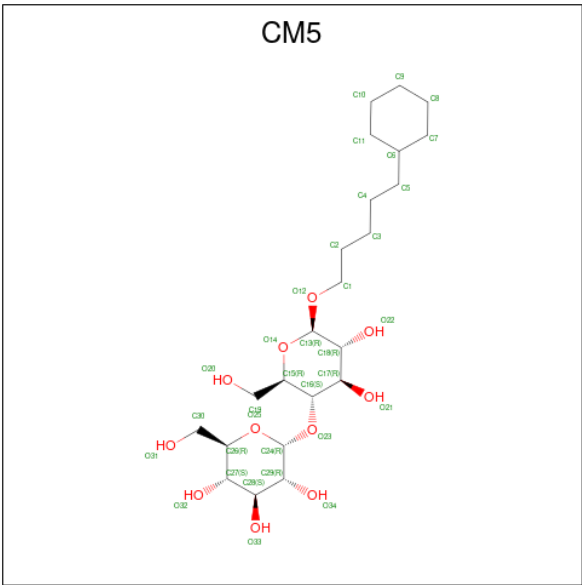
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	engineered mutation	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178

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



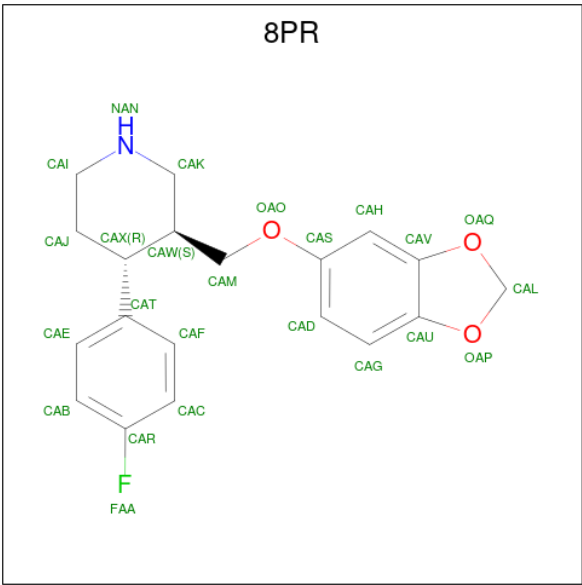
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (CCD ID: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			34	23	11		
3	A	1	Total	C	O	0	0
			34	23	11		
3	A	1	Total	C	O	0	0
			12	11	1		

- Molecule 4 is Paroxetine (CCD ID: 8PR) (formula: C₁₉H₂₀FNO₃).



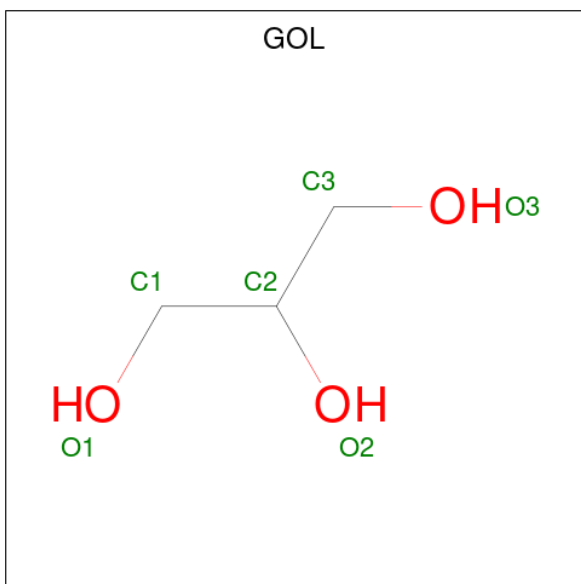
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			24	19	1	1	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



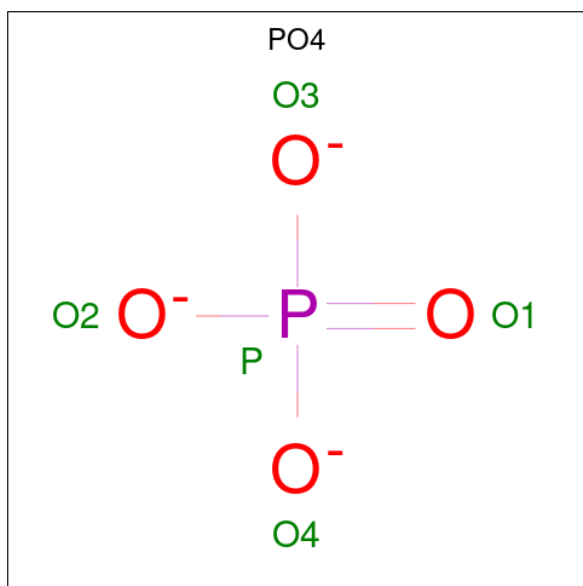
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		

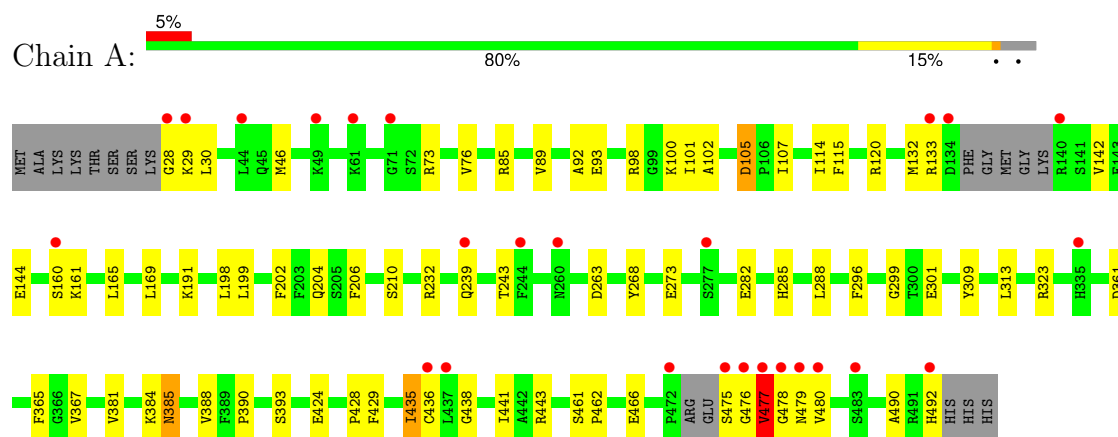
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	219	Total	O	0	0
			219	219		

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 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 2B4



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.76Å 90.76Å 153.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	78.60 – 2.14 78.60 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.3 (78.60-2.14) 99.3 (78.60-2.14)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.229 0.209 , 0.236	Depositor DCC
R_{free} test set	2066 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4056	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: SO4, HEM, PO4, CM5, 8PR, GOL

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	1.37	13/3745 (0.3%)	1.11	7/5074 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	VAL	CA-CB	-6.31	1.48	1.54
1	A	114	ILE	C-N	-5.79	1.25	1.33
1	A	243	THR	CA-CB	5.76	1.62	1.53
1	A	435	ILE	C-O	-5.61	1.17	1.24
1	A	263	ASP	C-O	-5.38	1.19	1.24
1	A	169	LEU	C-O	-5.37	1.18	1.24
1	A	144	GLU	C-O	-5.18	1.18	1.24
1	A	198	LEU	C-O	-5.16	1.18	1.24
1	A	443	ARG	C-O	-5.13	1.18	1.24
1	A	367	VAL	CA-C	5.11	1.57	1.52
1	A	490	ALA	C-O	-5.06	1.17	1.23
1	A	114	ILE	C-O	-5.06	1.18	1.24
1	A	428	PRO	C-O	-5.01	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	VAL	N-CA-C	-8.49	101.96	113.00
1	A	385	ASN	CB-CA-C	-5.89	99.17	110.65
1	A	105	ASP	CA-C-N	-5.82	113.62	119.56
1	A	105	ASP	C-N-CA	-5.82	113.62	119.56
1	A	390	PRO	CB-CA-C	-5.47	107.27	111.87
1	A	206	PHE	N-CA-C	5.07	116.49	111.07
1	A	89	VAL	N-CA-C	-5.06	106.87	111.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3654	0	3636	63	0
2	A	43	0	30	4	0
3	A	80	0	105	14	0
4	A	24	0	20	0	0
5	A	20	0	0	1	0
6	A	6	0	8	5	0
7	A	10	0	0	0	0
8	A	219	0	0	5	0
All	All	4056	0	3799	71	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 9.

All (71) 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:475:SER:HB2	1:A:476:GLY:CA	1.50	1.38
1:A:475:SER:HB2	1:A:476:GLY:HA2	1.06	1.06
1:A:475:SER:CB	1:A:476:GLY:HA2	1.79	1.04
1:A:475:SER:HB2	1:A:476:GLY:HA3	1.42	1.01
1:A:475:SER:CB	1:A:476:GLY:CA	2.36	0.98
1:A:475:SER:HB3	1:A:479:ASN:HA	1.47	0.93
1:A:46:MET:O	3:A:504:CM5:H12	1.74	0.87
1:A:29:LYS:HG3	1:A:30:LEU:H	1.48	0.78
3:A:503:CM5:H24	3:A:503:CM5:O21	1.83	0.78
1:A:133:ARG:CG	1:A:133:ARG:O	2.34	0.75
1:A:93:GLU:HB2	6:A:510:GOL:H12	1.66	0.75
1:A:29:LYS:HG3	1:A:30:LEU:N	2.01	0.74
1:A:93:GLU:CB	6:A:510:GOL:H12	2.22	0.69
1:A:384:LYS:O	1:A:385:ASN:HB2	1.93	0.68
1:A:133:ARG:O	1:A:133:ARG:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:CG	1:A:30:LEU:H	2.10	0.64
1:A:28:GLY:HA3	1:A:381:VAL:CG2	2.29	0.63
3:A:502:CM5:H20	3:A:502:CM5:C24	2.12	0.62
1:A:476:GLY:C	1:A:478:GLY:H	2.08	0.61
1:A:92:ALA:N	6:A:510:GOL:H2	2.15	0.60
3:A:502:CM5:C24	3:A:502:CM5:O20	2.50	0.60
1:A:476:GLY:C	1:A:478:GLY:N	2.58	0.60
3:A:503:CM5:O20	3:A:503:CM5:H26	2.01	0.60
1:A:73:ARG:HD3	8:A:605:HOH:O	2.02	0.58
1:A:475:SER:CB	1:A:479:ASN:HA	2.29	0.57
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.87	0.56
1:A:120:ARG:HA	1:A:282:GLU:HG3	1.86	0.56
1:A:299:GLY:HA2	2:A:501:HEM:C2C	2.41	0.56
1:A:93:GLU:H	6:A:510:GOL:H2	1.70	0.55
1:A:85:ARG:HD3	8:A:723:HOH:O	2.07	0.55
1:A:98:ARG:HG2	1:A:115:PHE:HA	1.89	0.54
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.37	0.54
1:A:273:GLU:HB2	3:A:503:CM5:C5	2.39	0.53
1:A:92:ALA:H	6:A:510:GOL:H2	1.74	0.53
1:A:210:SER:HA	1:A:477:VAL:HG13	1.91	0.53
1:A:28:GLY:HA3	1:A:381:VAL:HG23	1.90	0.52
1:A:100:LYS:HD2	1:A:105:ASP:CG	2.35	0.52
1:A:232:ARG:HD2	8:A:740:HOH:O	2.08	0.52
1:A:142:VAL:HG11	1:A:441:ILE:HG12	1.91	0.52
1:A:365:PHE:CE2	1:A:477:VAL:HA	2.45	0.52
1:A:210:SER:HA	1:A:477:VAL:CG1	2.40	0.51
1:A:29:LYS:O	1:A:381:VAL:N	2.34	0.51
1:A:133:ARG:O	1:A:133:ARG:HG3	2.11	0.51
1:A:309:TYR:CE2	1:A:313:LEU:HD11	2.46	0.50
1:A:429:PHE:HB3	1:A:436:CYS:HB3	1.93	0.50
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.47	0.49
1:A:28:GLY:HA3	1:A:381:VAL:HG21	1.94	0.48
1:A:202:PHE:CD1	3:A:502:CM5:H101	2.48	0.48
1:A:273:GLU:HB2	3:A:503:CM5:H51	1.95	0.48
1:A:85:ARG:NE	1:A:424:GLU:HG3	2.28	0.48
1:A:296:PHE:CD1	3:A:502:CM5:H102	2.50	0.47
1:A:365:PHE:CZ	1:A:477:VAL:HA	2.50	0.46
1:A:107:ILE:CD1	1:A:239:GLN:HG2	2.45	0.46
1:A:273:GLU:OE1	3:A:503:CM5:H52	2.16	0.46
1:A:199:LEU:C	1:A:199:LEU:HD23	2.41	0.45
1:A:204:GLN:HB2	8:A:766:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:CM5:O21	3:A:503:CM5:C24	2.60	0.45
3:A:502:CM5:O20	3:A:502:CM5:O25	2.35	0.45
1:A:477:VAL:O	1:A:477:VAL:HG23	2.16	0.45
1:A:435:ILE:O	1:A:436:CYS:C	2.59	0.44
1:A:438:GLY:HA3	2:A:501:HEM:C3C	2.53	0.44
1:A:273:GLU:HG2	3:A:503:CM5:H72	2.00	0.43
1:A:101:ILE:O	1:A:102:ALA:C	2.60	0.43
1:A:132:MET:HE3	1:A:132:MET:HB2	1.89	0.41
1:A:160:SER:O	1:A:161:LYS:HB2	2.20	0.41
1:A:285:HIS:HE1	8:A:651:HOH:O	2.03	0.41
1:A:273:GLU:HB2	3:A:503:CM5:H52	2.03	0.41
1:A:461:SER:OG	1:A:462:PRO:HD2	2.21	0.41
1:A:76:VAL:O	1:A:388:VAL:HA	2.20	0.40
1:A:323:ARG:NH2	5:A:507:SO4:O2	2.48	0.40
1:A:361:ASP:OD2	1:A:393:SER:OG	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/476 (95%)	439 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	400/421 (95%)	394 (98%)	6 (2%)	57 63

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	LEU
1	A	191	LYS
1	A	301	GLU
1	A	466	GLU
1	A	477	VAL
1	A	492	HIS

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

Mol	Chain	Res	Type
1	A	260	ASN
1	A	376	GLN
1	A	456	ASN
1	A	485	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 ⓘ

12 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
6	GOL	A	510	-	5,5,5	0.60	0	5,5,5	0.36	0
3	CM5	A	504	-	12,12,36	0.21	0	13,13,49	0.59	0
7	PO4	A	512	-	4,4,4	2.02	3 (75%)	6,6,6	0.80	0
5	SO4	A	508	-	4,4,4	0.64	0	6,6,6	0.24	0
5	SO4	A	509	-	4,4,4	1.46	0	6,6,6	0.66	0
4	8PR	A	505	-	27,27,27	3.58	10 (37%)	33,37,37	1.91	9 (27%)
3	CM5	A	502	-	36,36,36	0.40	0	49,49,49	0.75	1 (2%)
5	SO4	A	507	-	4,4,4	0.50	0	6,6,6	0.36	0
7	PO4	A	511	-	4,4,4	1.29	0	6,6,6	1.03	0
2	HEM	A	501	1	50,50,50	2.15	8 (16%)	67,82,82	1.69	15 (22%)
5	SO4	A	506	-	4,4,4	0.59	0	6,6,6	0.48	0
3	CM5	A	503	-	36,36,36	0.41	0	49,49,49	0.70	1 (2%)

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
6	GOL	A	510	-	-	2/4/4/4	-
3	CM5	A	504	-	-	1/6/14/65	0/1/1/3
4	8PR	A	505	-	-	0/9/26/26	0/4/4/4
3	CM5	A	502	-	-	4/17/65/65	0/3/3/3
2	HEM	A	501	1	-	2/14/54/54	-
3	CM5	A	503	-	-	14/17/65/65	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	8PR	CAG-CAD	8.23	1.52	1.38
4	A	505	8PR	CAD-CAS	8.22	1.54	1.38
4	A	505	8PR	CAH-CAS	8.04	1.52	1.39
2	A	501	HEM	C3D-C2D	7.12	1.52	1.36
2	A	501	HEM	FE-NB	7.10	2.16	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	8PR	OAP-CAU	-7.07	1.26	1.38
2	A	501	HEM	FE-ND	6.37	2.14	1.94
4	A	505	8PR	OAQ-CAV	-4.84	1.30	1.38
4	A	505	8PR	CAV-CAU	3.79	1.48	1.39
2	A	501	HEM	CAB-C3B	3.47	1.56	1.47
4	A	505	8PR	CAH-CAV	-3.21	1.33	1.38
2	A	501	HEM	C1B-NB	-3.10	1.34	1.40
4	A	505	8PR	CAK-CAW	3.03	1.55	1.52
4	A	505	8PR	CAG-CAU	-2.82	1.33	1.39
2	A	501	HEM	CAC-C3C	2.73	1.54	1.47
4	A	505	8PR	OAQ-CAS	2.46	1.43	1.37
2	A	501	HEM	CMB-C2B	2.20	1.55	1.50
7	A	512	PO4	P-O3	-2.14	1.48	1.54
2	A	501	HEM	CAA-C2A	2.05	1.56	1.51
7	A	512	PO4	P-O2	-2.03	1.48	1.54
7	A	512	PO4	P-O4	-2.03	1.48	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	8PR	CAG-CAD-CAS	-5.23	113.76	119.73
4	A	505	8PR	CAJ-CAX-CAT	-4.38	104.49	112.54
2	A	501	HEM	C4D-ND-C1D	4.19	110.17	105.21
2	A	501	HEM	CHD-C4C-NC	4.18	129.01	124.45
4	A	505	8PR	CAC-CAF-CAT	-3.92	117.27	121.18
2	A	501	HEM	C1B-NB-C4B	3.82	109.73	105.21
2	A	501	HEM	CBD-CAD-C3D	-3.70	102.30	112.53
2	A	501	HEM	C3B-C2B-C1B	3.62	109.13	106.41
2	A	501	HEM	CMB-C2B-C1B	-3.47	119.61	125.03
2	A	501	HEM	CAA-CBA-CGA	-3.34	104.79	113.67
2	A	501	HEM	C2B-C1B-NB	-3.12	106.25	109.84
4	A	505	8PR	CAF-CAT-CAE	3.00	122.02	118.30
3	A	503	CM5	C24-O23-C16	-2.61	111.80	117.98
4	A	505	8PR	CAJ-CAI-NAN	2.46	115.45	110.81
4	A	505	8PR	CAG-CAU-CAV	-2.35	118.59	121.50
2	A	501	HEM	CHA-C1A-NA	2.32	128.07	123.86
2	A	501	HEM	C1A-CHA-C4D	-2.30	120.84	126.25
4	A	505	8PR	CAD-CAG-CAU	2.28	124.37	120.06
2	A	501	HEM	O2A-CGA-CBA	2.20	120.97	114.00
3	A	502	CM5	O14-C15-C16	2.19	114.25	109.72
2	A	501	HEM	CHD-C4C-C3C	-2.17	121.55	125.21
2	A	501	HEM	CHB-C4A-NA	2.15	127.76	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	8PR	CAD-CAS-CAH	-2.13	117.63	120.50
2	A	501	HEM	CHC-C1C-NC	2.09	126.73	124.45
4	A	505	8PR	CAF-CAT-CAX	-2.03	117.18	121.08
2	A	501	HEM	CHD-C1D-ND	2.01	126.58	124.42

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	CM5	C1-C2-C3-C4
3	A	503	CM5	O14-C13-O12-C1
3	A	503	CM5	O25-C26-C30-O31
3	A	503	CM5	O14-C15-C19-O20
3	A	503	CM5	C18-C13-O12-C1
3	A	503	CM5	C27-C26-C30-O31
6	A	510	GOL	O2-C2-C3-O3
3	A	502	CM5	O25-C26-C30-O31
3	A	503	CM5	C15-C16-O23-C24
3	A	503	CM5	C17-C16-O23-C24
6	A	510	GOL	C1-C2-C3-O3
3	A	504	CM5	C1-C2-C3-C4
3	A	502	CM5	C1-C2-C3-C4
3	A	502	CM5	O14-C15-C19-O20
3	A	503	CM5	C3-C4-C5-C6
3	A	503	CM5	C2-C3-C4-C5
3	A	503	CM5	C4-C5-C6-C7
3	A	503	CM5	C4-C5-C6-C11
3	A	503	CM5	C16-C15-C19-O20
3	A	503	CM5	C2-C1-O12-C13
3	A	502	CM5	C27-C26-C30-O31
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

6 monomers are involved in 24 short contacts:

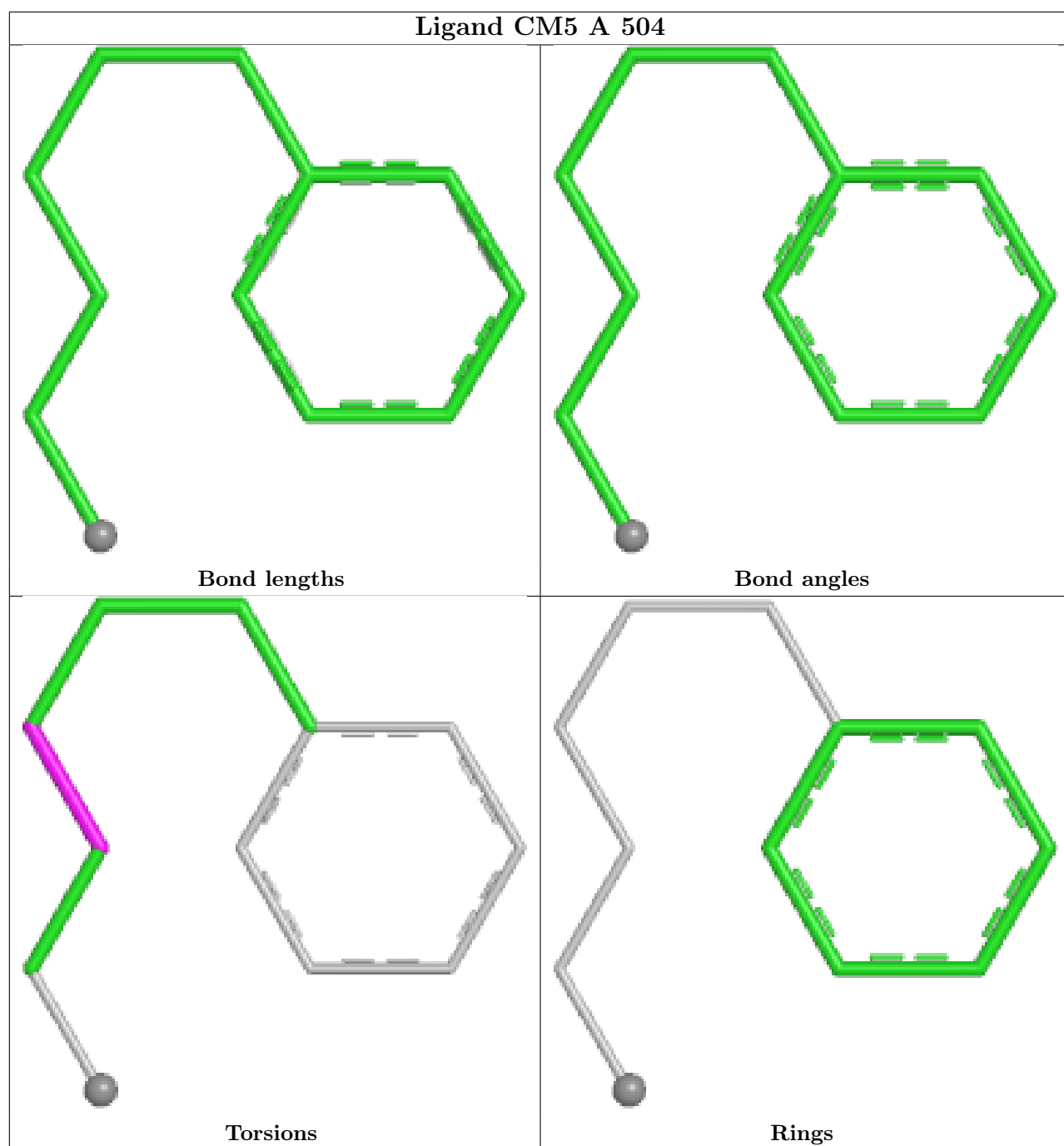
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	510	GOL	5	0
3	A	504	CM5	1	0
3	A	502	CM5	5	0
5	A	507	SO4	1	0

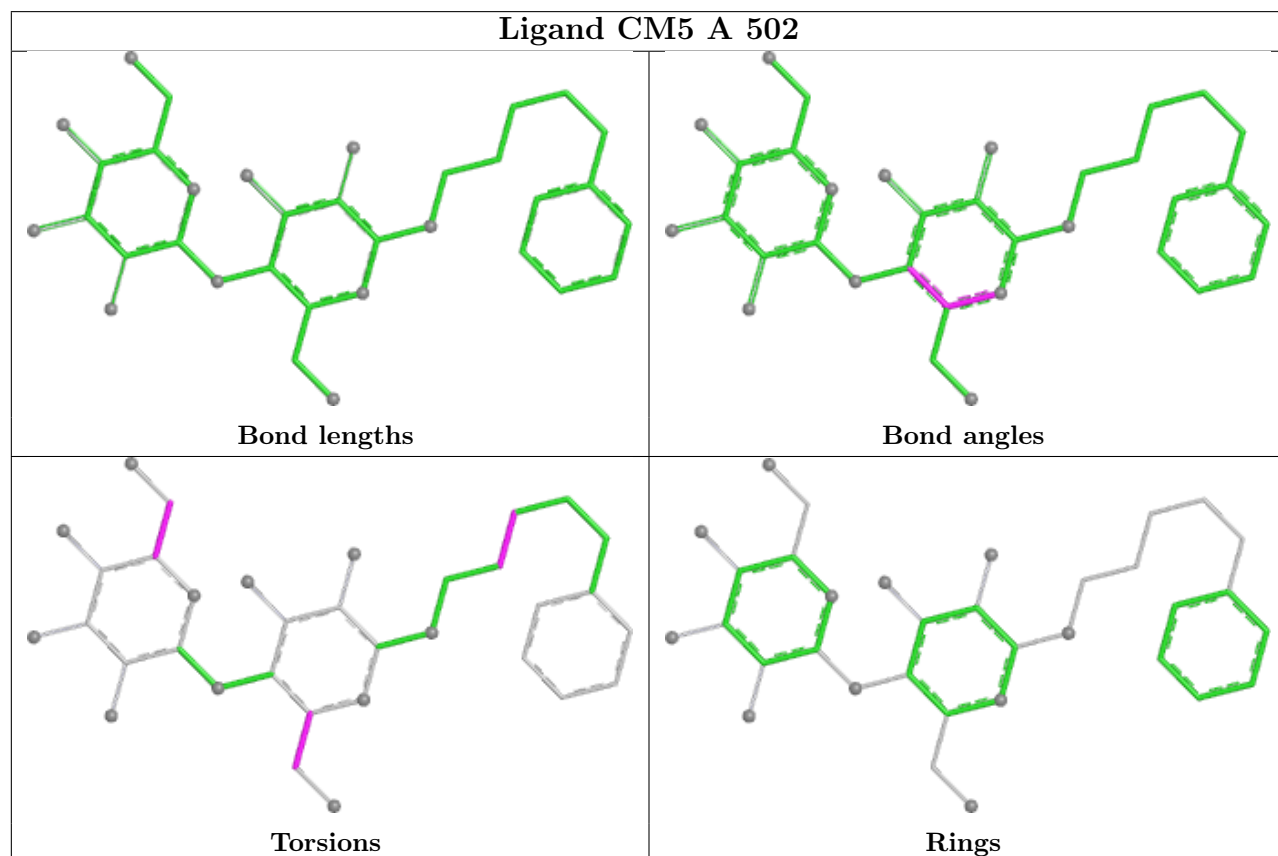
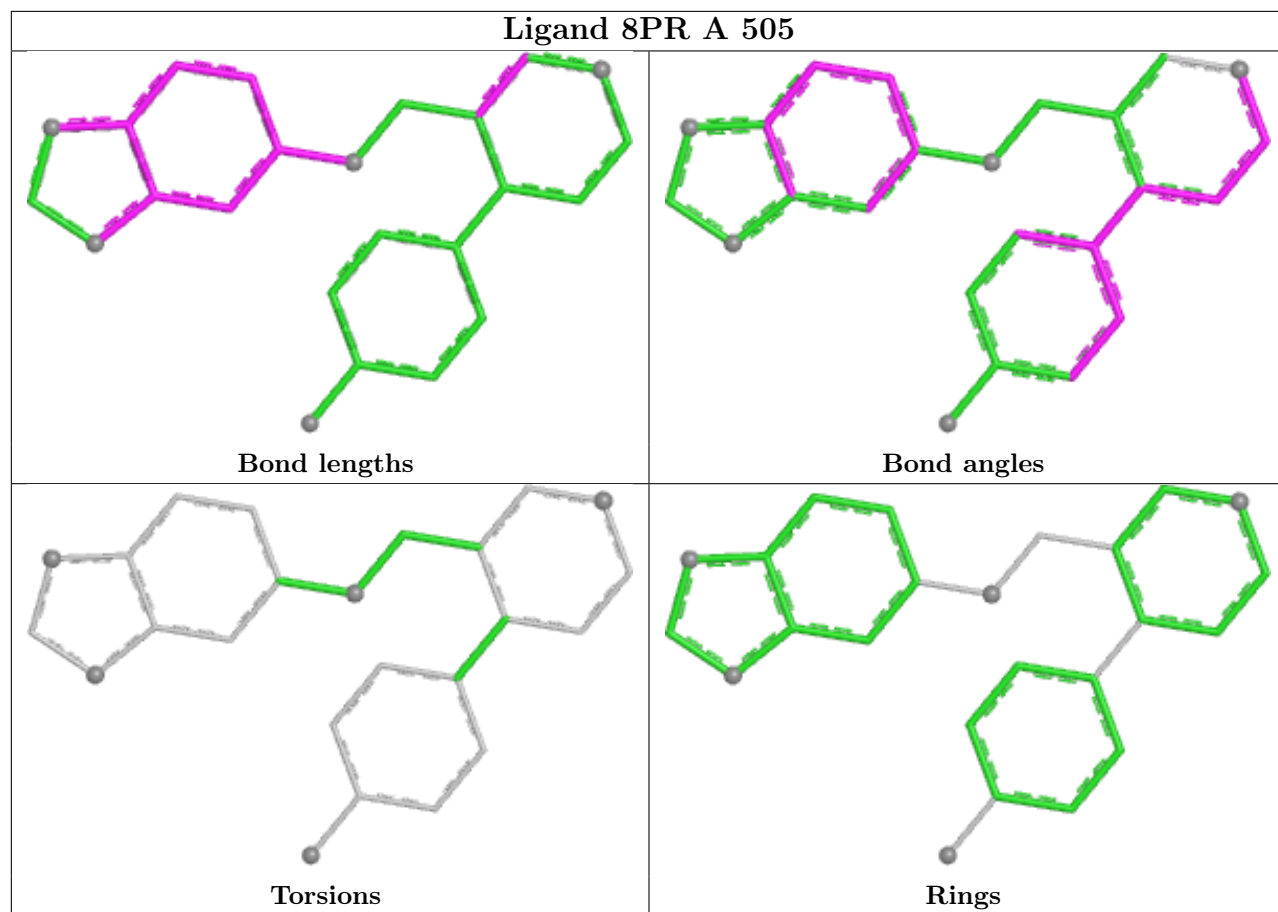
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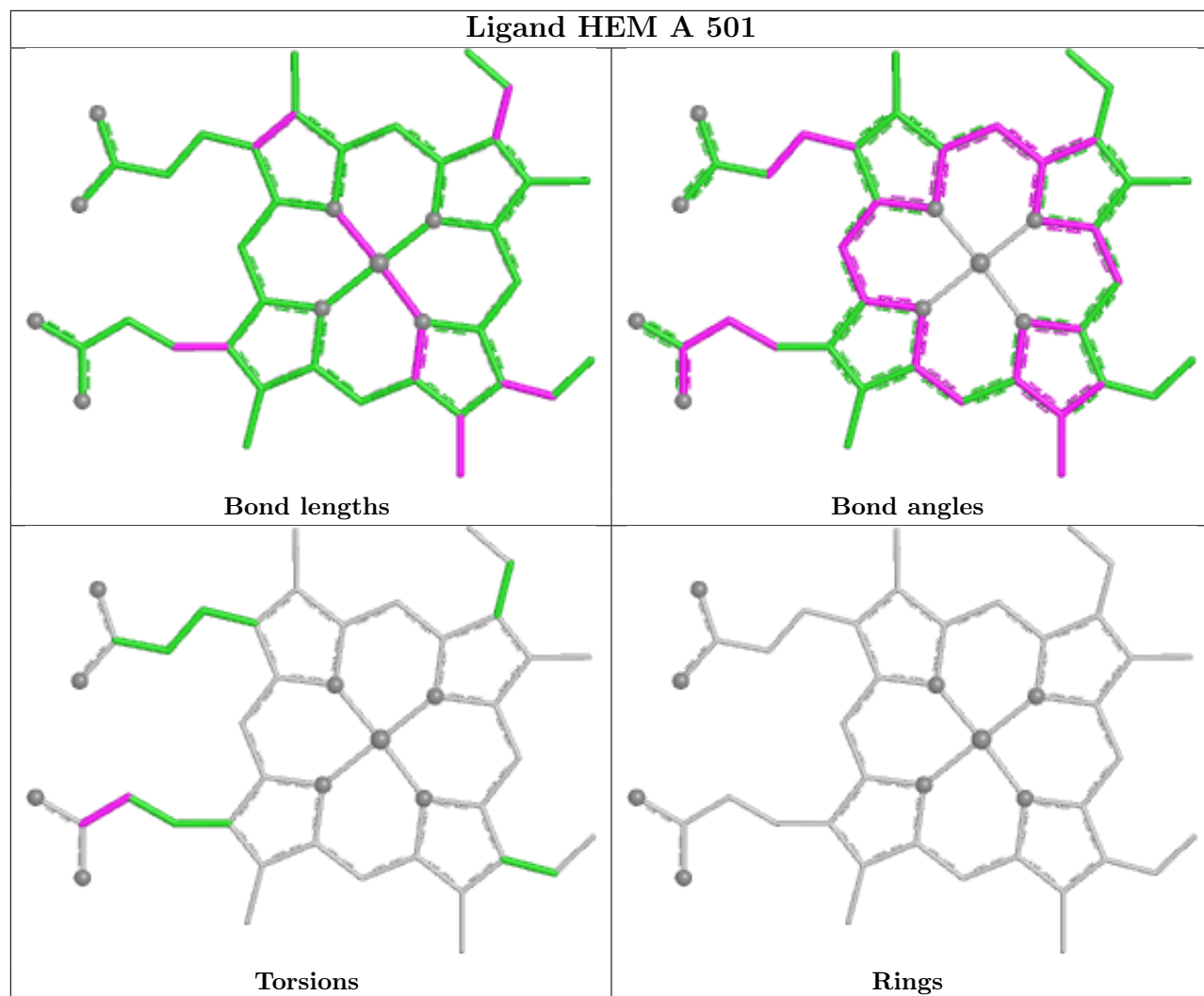
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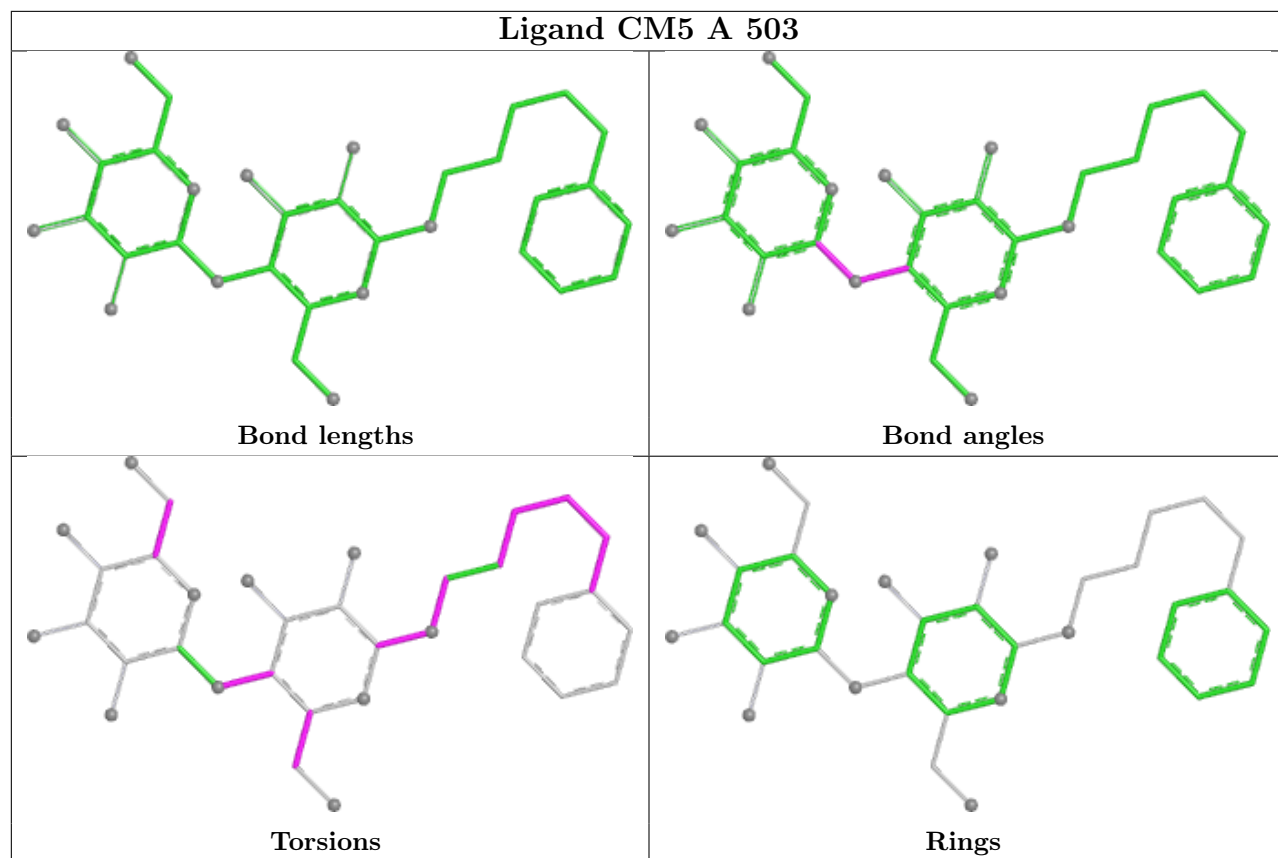
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
3	A	503	CM5	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	458/476 (96%)	0.41	26 (5%)	29 34	16, 36, 55, 81	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	GLY	9.0
1	A	476	GLY	8.6
1	A	477	VAL	7.8
1	A	28	GLY	6.3
1	A	492	HIS	4.9
1	A	140	ARG	4.6
1	A	472	PRO	3.9
1	A	29	LYS	3.8
1	A	475	SER	3.5
1	A	335	HIS	3.3
1	A	160	SER	3.3
1	A	134	ASP	3.3
1	A	49	LYS	3.2
1	A	480	VAL	3.0
1	A	483	SER	3.0
1	A	133	ARG	3.0
1	A	239	GLN	2.9
1	A	479	ASN	2.8
1	A	71	GLY	2.8
1	A	61	LYS	2.8
1	A	437	LEU	2.7
1	A	436	CYS	2.6
1	A	244	PHE	2.5
1	A	277	SER	2.4
1	A	260	ASN	2.3
1	A	44	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

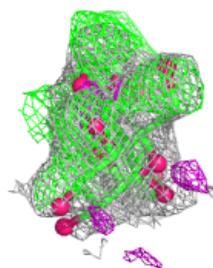
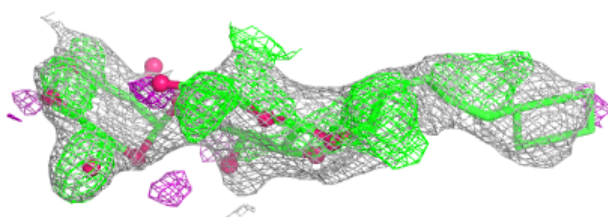
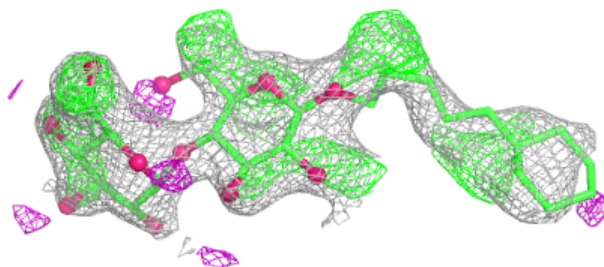
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PO4	A	511	5/5	0.66	0.13	71,74,76,79	0
5	SO4	A	507	5/5	0.67	0.12	81,81,83,83	0
3	CM5	A	503	34/34	0.67	0.38	89,144,167,172	0
7	PO4	A	512	5/5	0.69	0.19	69,70,71,72	0
5	SO4	A	506	5/5	0.75	0.13	85,86,87,88	0
3	CM5	A	502	34/34	0.76	0.35	89,144,167,172	0
6	GOL	A	510	6/6	0.76	0.17	50,58,59,59	0
5	SO4	A	508	5/5	0.82	0.12	71,72,72,72	0
3	CM5	A	504	12/34	0.88	0.45	89,95,114,116	0
4	8PR	A	505	24/24	0.92	0.10	39,43,48,49	0
5	SO4	A	509	5/5	0.95	0.11	46,50,51,53	0
2	HEM	A	501	43/43	0.98	0.06	23,27,29,32	0

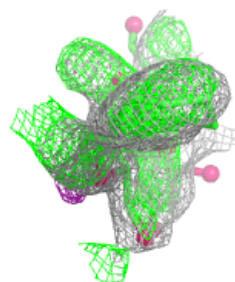
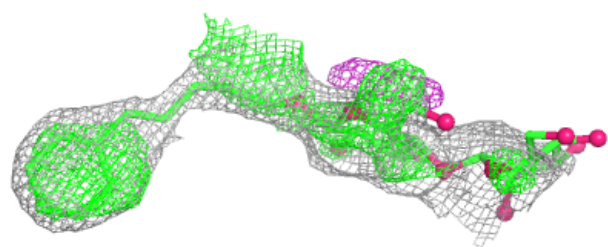
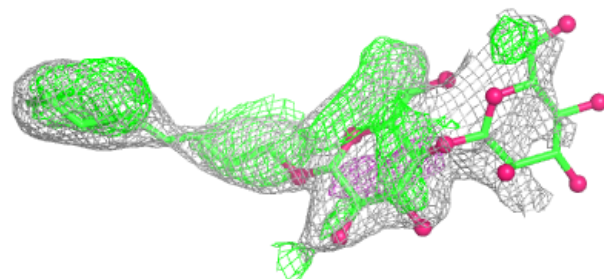
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CM5 A 503:

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

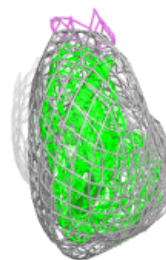
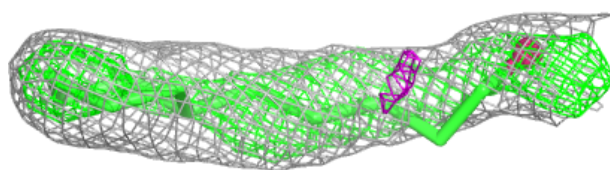
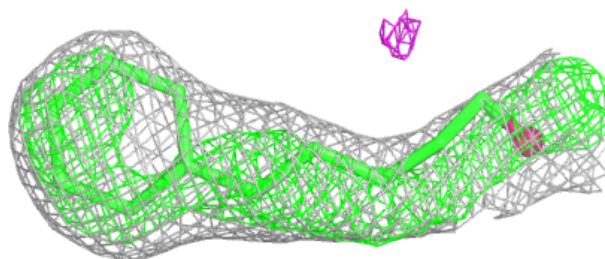
**Electron density around CM5 A 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



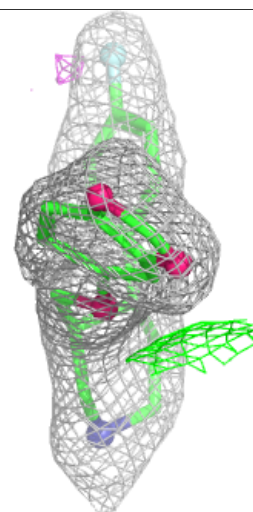
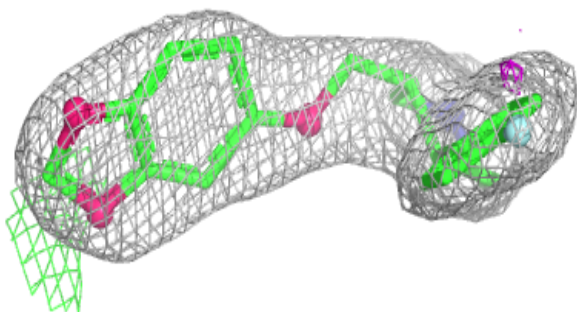
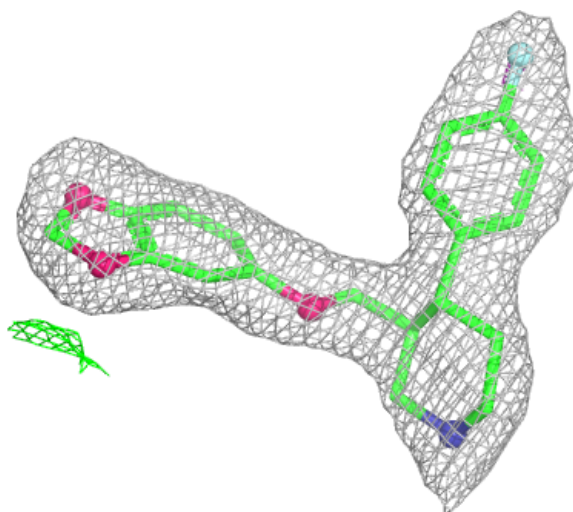
Electron density around CM5 A 504:

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and green (positive)



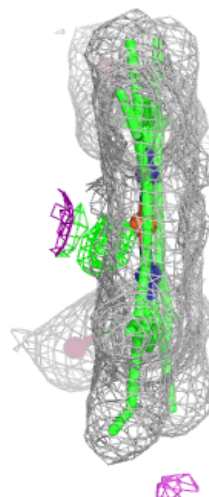
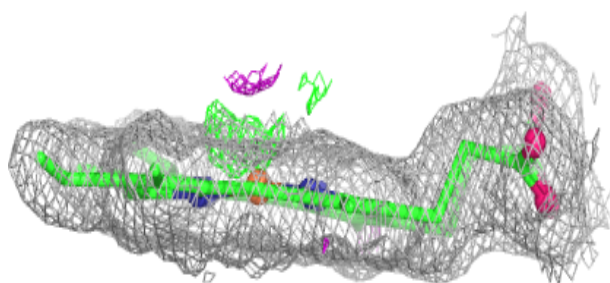
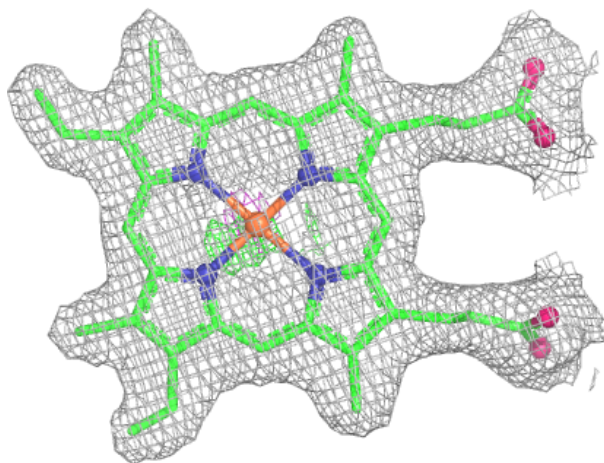
Electron density around 8PR A 505:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 501:

$2mF_o-DF_c$ (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.