



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:55 AM UTC

PDB ID : 4NZ2 / pdb_00004nz2
Title : Crystal structure of CYP2C9 in complex with an inhibitor
Authors : Branden, G.; Sjogren, T.; Xue, Y.
Deposited on : 2013-12-11
Resolution : 2.45 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

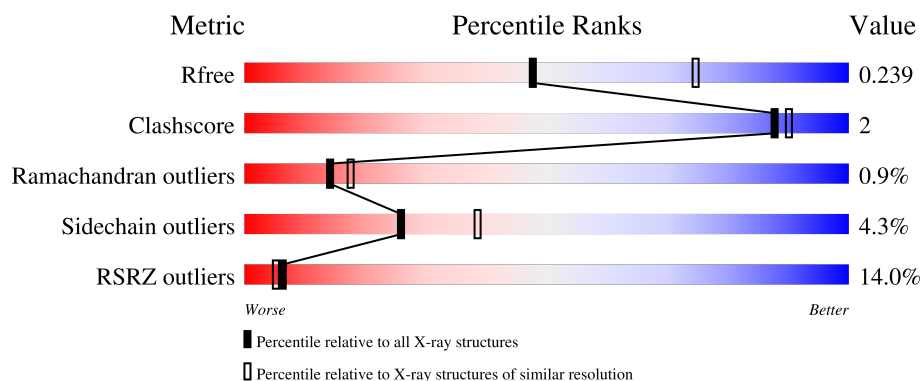
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	475	14% 88% 8% ..
1	B	475	13% 87% 9% ..

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
4	SO4	B	503	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7922 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 2C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3716	2398	623	672	23			
1	B	464	Total	C	N	O	S	0	0	0
			3716	2398	623	672	23			

There are 42 discrepancies between the modelled and reference sequences:

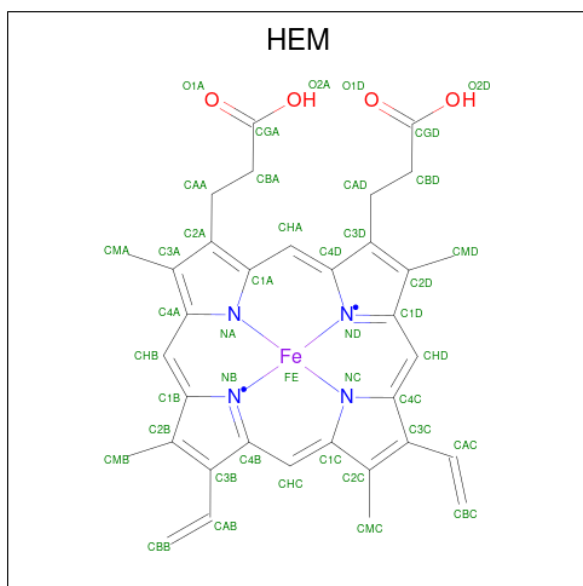
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	insertion	UNP P11712
A	21	ALA	-	insertion	UNP P11712
A	22	LYS	-	insertion	UNP P11712
A	23	LYS	-	insertion	UNP P11712
A	24	THR	-	insertion	UNP P11712
A	25	SER	-	insertion	UNP P11712
A	26	SER	-	insertion	UNP P11712
A	27	LYS	-	insertion	UNP P11712
A	28	GLY	-	insertion	UNP P11712
A	29	ARG	-	insertion	UNP P11712
A	206	GLU	LYS	engineered mutation	UNP P11712
A	215	VAL	ILE	engineered mutation	UNP P11712
A	216	TYR	CYS	engineered mutation	UNP P11712
A	220	PRO	SER	engineered mutation	UNP P11712
A	221	ALA	PRO	engineered mutation	UNP P11712
A	222	LEU	ILE	engineered mutation	UNP P11712
A	223	LEU	ILE	engineered mutation	UNP P11712
A	491	HIS	-	expression tag	UNP P11712
A	492	HIS	-	expression tag	UNP P11712
A	493	HIS	-	expression tag	UNP P11712
A	494	HIS	-	expression tag	UNP P11712
B	20	MET	-	insertion	UNP P11712
B	21	ALA	-	insertion	UNP P11712
B	22	LYS	-	insertion	UNP P11712
B	23	LYS	-	insertion	UNP P11712

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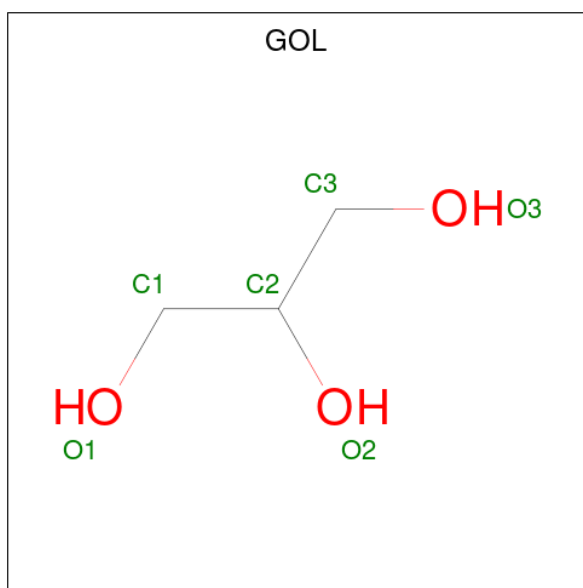
Chain	Residue	Modelled	Actual	Comment	Reference
B	24	THR	-	insertion	UNP P11712
B	25	SER	-	insertion	UNP P11712
B	26	SER	-	insertion	UNP P11712
B	27	LYS	-	insertion	UNP P11712
B	28	GLY	-	insertion	UNP P11712
B	29	ARG	-	insertion	UNP P11712
B	206	GLU	LYS	engineered mutation	UNP P11712
B	215	VAL	ILE	engineered mutation	UNP P11712
B	216	TYR	CYS	engineered mutation	UNP P11712
B	220	PRO	SER	engineered mutation	UNP P11712
B	221	ALA	PRO	engineered mutation	UNP P11712
B	222	LEU	ILE	engineered mutation	UNP P11712
B	223	LEU	ILE	engineered mutation	UNP P11712
B	491	HIS	-	expression tag	UNP P11712
B	492	HIS	-	expression tag	UNP P11712
B	493	HIS	-	expression tag	UNP P11712
B	494	HIS	-	expression tag	UNP P11712

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



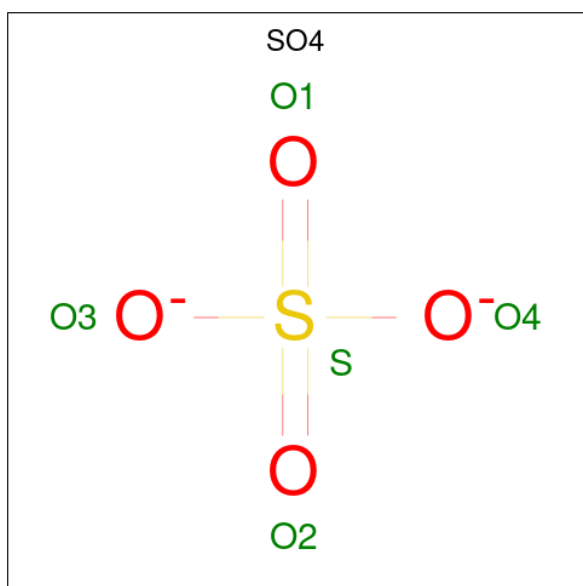
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



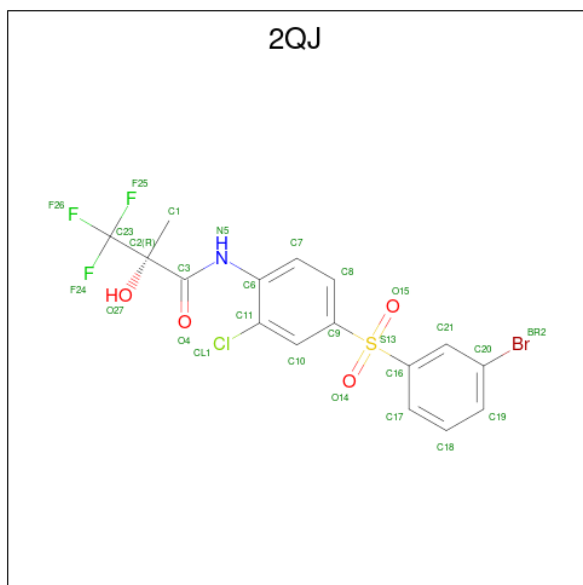
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is (2R)-N-{4-[(3-bromophenyl)sulfonyl]-2-chlorophenyl}-3,3,3-trifluoro-2-hydroxy-2-methylpropanamide (CCD ID: 2QJ) (formula: $C_{16}H_{12}BrClF_3NO_4S$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
5	A	1	Total	Br	C	Cl	F	N	O	S	0	0
			27	1	16	1	3	1	4	1		
5	B	1	Total	Br	C	Cl	F	N	O	S	0	0
			27	1	16	1	3	1	4	1		

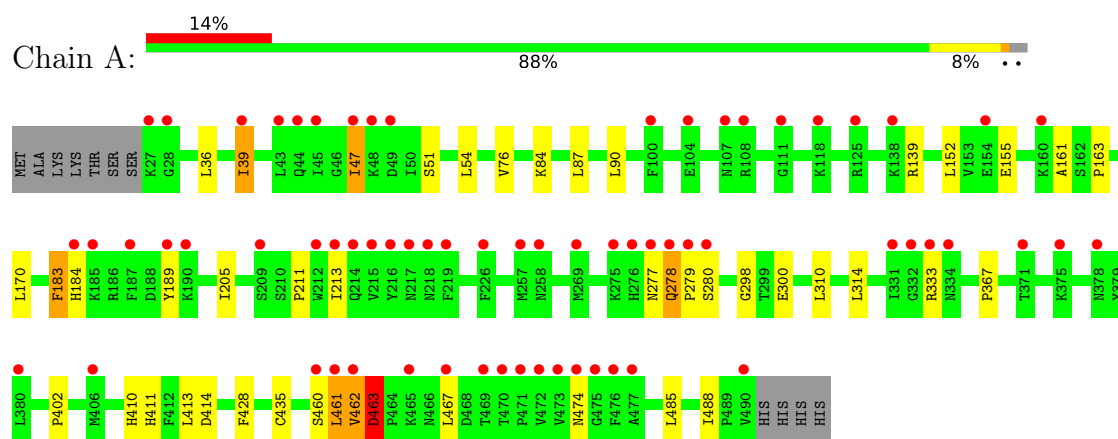
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	170	Total	O	0	0
			170	170		
6	B	158	Total	O	0	0
			158	158		

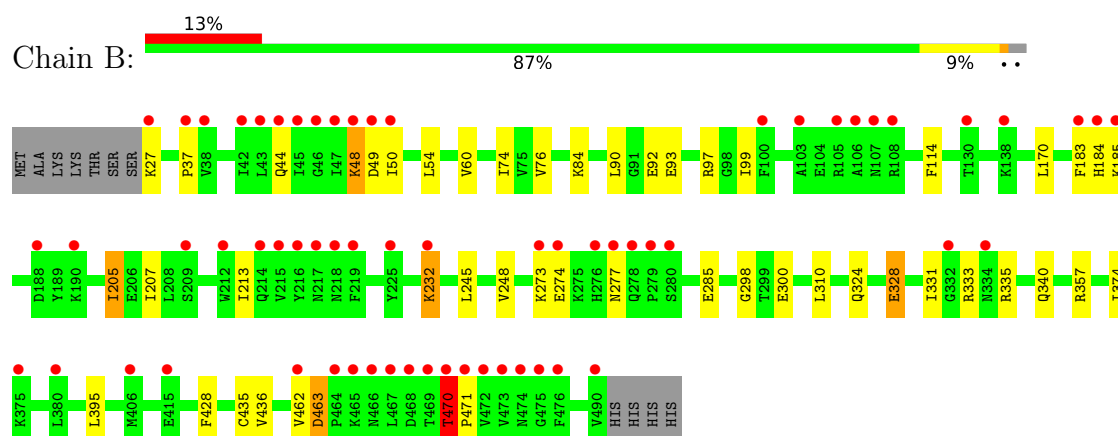
3 Residue-property plots [i](#)

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 2C9



• Molecule 1: Cytochrome P450 2C9



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.38Å 164.38Å 111.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 2.45 48.47 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.47-2.45) 99.6 (48.47-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.45Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.217 , 0.235 (Not available) , 0.239	Depositor DCC
R_{free} test set	3238 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	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	0.94	EDS
Total number of atoms	7922	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GOL, 2QJ, SO4

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	0.71	0/3807	1.34	8/5150 (0.2%)
1	B	0.70	0/3807	1.32	6/5150 (0.1%)
All	All	0.70	0/7614	1.33	14/10300 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	ARG	N-CA-C	-6.83	105.50	114.31
1	A	183	PHE	CA-CB-CG	5.88	119.68	113.80
1	B	90	LEU	CA-C-N	5.88	126.63	119.99
1	B	90	LEU	C-N-CA	5.88	126.63	119.99
1	A	333	ARG	N-CA-C	-5.84	105.92	114.39
1	A	90	LEU	CA-C-N	5.82	126.56	119.99
1	A	90	LEU	C-N-CA	5.82	126.56	119.99
1	B	183	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	470	THR	CB-CA-C	5.51	118.27	109.62
1	A	277	ASN	CA-C-N	5.50	127.84	120.58
1	A	277	ASN	C-N-CA	5.50	127.84	120.58
1	A	414	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	273	LYS	N-CA-C	-5.22	103.79	110.53
1	A	278	GLN	N-CA-C	5.17	120.64	113.45

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	3716	0	3748	17	0
1	B	3716	0	3748	14	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	170	0	0	0	0
6	B	158	0	0	0	0
All	All	7922	0	7596	31	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 2.

All (31) 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:B:205:ILE:HG12	1:B:300:GLU:HG2	1.80	0.64
1:A:205:ILE:HG13	1:A:300:GLU:HG3	1.82	0.60
1:A:314:LEU:HD22	1:A:460:SER:HB3	1.89	0.55
1:A:367:PRO:HG3	3:A:502:GOL:H11	1.91	0.53
1:B:207:ILE:HD11	1:B:232:LYS:HD2	1.91	0.53
1:A:170:LEU:HD11	1:A:310:LEU:HD12	1.90	0.52
1:A:155:GLU:HG3	1:A:189:TYR:CD2	2.46	0.50
1:B:170:LEU:HD11	1:B:310:LEU:HD12	1.94	0.50
1:B:436:VAL:HG23	2:B:501:HEM:HBD2	1.93	0.50
1:A:428:PHE:HB3	1:A:435:CYS:HB3	1.95	0.48
1:B:324:GLN:O	1:B:328:GLU:HG2	2.15	0.47
1:B:357:ARG:HA	1:B:395:LEU:HD22	1.98	0.45
1:B:428:PHE:HB3	1:B:435:CYS:HB3	1.97	0.45
1:B:93:GLU:HG2	1:B:374:ILE:HD13	2.00	0.44
1:A:54:LEU:HD22	1:A:76:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HD3	3:A:502:GOL:H32	2.00	0.43
1:A:36:LEU:HB2	1:A:39:ILE:HG22	2.00	0.43
1:A:161:ALA:HB1	1:A:488:ILE:HG13	2.01	0.43
1:B:298:GLY:HA2	2:B:501:HEM:C2C	2.54	0.43
1:A:163:PRO:HB3	1:A:461:LEU:HD22	2.01	0.43
1:B:54:LEU:HD22	1:B:76:VAL:HG11	2.01	0.43
1:B:470:THR:HA	1:B:471:PRO:HD3	1.93	0.43
1:A:278:GLN:O	1:A:279:PRO:C	2.61	0.42
1:B:97:ARG:HG2	1:B:114:PHE:HA	2.01	0.42
1:A:402:PRO:O	1:A:411:HIS:HE1	2.03	0.42
1:A:462:VAL:O	1:A:463:ASP:HB3	2.19	0.41
1:B:48:LYS:HB2	1:B:49:ASP:H	1.60	0.41
1:A:211:PRO:HG3	1:A:474:ASN:HB3	2.04	0.40
1:A:298:GLY:HA2	2:A:501:HEM:C2C	2.55	0.40
1:A:410:HIS:HA	1:A:413:LEU:HB2	2.03	0.40
1:B:245:LEU:HA	1:B:248:VAL:HG22	2.02	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	462/475 (97%)	442 (96%)	16 (4%)	4 (1%)	14	17
1	B	462/475 (97%)	441 (96%)	17 (4%)	4 (1%)	14	17
All	All	924/950 (97%)	883 (96%)	33 (4%)	8 (1%)	14	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	SER
1	B	48	LYS

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Mol	Chain	Res	Type
1	B	463	ASP
1	A	184	HIS
1	B	37	PRO
1	B	184	HIS
1	A	463	ASP
1	A	47	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	418/428 (98%)	404 (97%)	14 (3%)	33	48
1	B	418/428 (98%)	396 (95%)	22 (5%)	20	30
All	All	836/856 (98%)	800 (96%)	36 (4%)	26	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	47	ILE
1	A	51	SER
1	A	84	LYS
1	A	87	LEU
1	A	139	ARG
1	A	152	LEU
1	A	183	PHE
1	A	213	ILE
1	A	461	LEU
1	A	462	VAL
1	A	463	ASP
1	A	467	LEU
1	A	485	LEU
1	B	27	LYS
1	B	44	GLN
1	B	50	ILE

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Mol	Chain	Res	Type
1	B	60	VAL
1	B	74	ILE
1	B	84	LYS
1	B	92	GLU
1	B	99	ILE
1	B	185	LYS
1	B	205	ILE
1	B	213	ILE
1	B	232	LYS
1	B	274	GLU
1	B	277	ASN
1	B	285	GLU
1	B	328	GLU
1	B	331	ILE
1	B	335	ARG
1	B	340	GLN
1	B	462	VAL
1	B	463	ASP
1	B	470	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	192	GLN
1	A	196	ASN
1	A	202	ASN
1	A	218	ASN
1	A	324	GLN
1	A	396	HIS
1	A	398	ASN
1	A	411	HIS
1	A	418	ASN
1	A	454	GLN
1	A	457	ASN
1	A	466	ASN
1	B	44	GLN
1	B	107	ASN
1	B	192	GLN
1	B	196	ASN
1	B	202	ASN
1	B	214	GLN

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Mol	Chain	Res	Type
1	B	218	ASN
1	B	278	GLN
1	B	324	GLN
1	B	474	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	2QJ	B	504	-	27,28,28	0.55	0	40,44,44	1.17	3 (7%)
4	SO4	A	503	-	4,4,4	0.21	0	6,6,6	0.09	0
4	SO4	B	503	-	4,4,4	0.26	0	6,6,6	0.07	0
2	HEM	B	501	6,1	50,50,50	1.19	6 (12%)	67,82,82	1.37	6 (8%)
3	GOL	B	502	-	5,5,5	0.05	0	5,5,5	0.17	0
2	HEM	A	501	6,1	50,50,50	1.20	5 (10%)	67,82,82	1.31	7 (10%)
3	GOL	A	502	-	5,5,5	0.05	0	5,5,5	0.14	0
5	2QJ	A	504	-	27,28,28	0.57	0	40,44,44	1.19	3 (7%)

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
5	2QJ	B	504	-	-	4/31/31/31	0/2/2/2
2	HEM	B	501	6,1	-	4/14/54/54	-
3	GOL	B	502	-	-	0/4/4/4	-
2	HEM	A	501	6,1	-	6/14/54/54	-
3	GOL	A	502	-	-	0/4/4/4	-
5	2QJ	A	504	-	-	6/31/31/31	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1B-NB	-3.46	1.34	1.40
2	A	501	HEM	C4D-ND	-2.99	1.35	1.40
2	A	501	HEM	C1B-NB	-2.92	1.35	1.40
2	B	501	HEM	C4D-ND	-2.88	1.35	1.40
2	A	501	HEM	C4B-NB	-2.76	1.33	1.38
2	B	501	HEM	C4B-NB	-2.41	1.34	1.38
2	A	501	HEM	C1D-ND	-2.37	1.34	1.38
2	A	501	HEM	C3B-C4B	2.36	1.49	1.44
2	B	501	HEM	C1D-ND	-2.19	1.34	1.38
2	B	501	HEM	C1C-C2C	-2.05	1.41	1.45
2	B	501	HEM	C4D-C3D	2.03	1.48	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3B-C4B-NB	3.91	112.28	109.47
5	A	504	2QJ	C2-C3-N5	-3.46	111.21	114.55
2	A	501	HEM	C3B-C4B-NB	3.43	111.93	109.47
2	B	501	HEM	C4B-C3B-C2B	-3.40	104.15	107.28
5	A	504	2QJ	C1-C2-C23	3.35	113.48	109.04
5	B	504	2QJ	C2-C3-N5	-3.29	111.38	114.55
2	A	501	HEM	C2B-C1B-NB	3.13	113.44	109.84
5	B	504	2QJ	C1-C2-C23	2.99	113.01	109.04
2	B	501	HEM	C2B-C1B-NB	2.88	113.15	109.84
2	A	501	HEM	C4B-C3B-C2B	-2.87	104.64	107.28
2	B	501	HEM	CHD-C1D-C2D	-2.74	120.70	125.03
2	B	501	HEM	CHD-C1D-ND	2.65	127.27	124.42
2	A	501	HEM	CHD-C1D-C2D	-2.60	120.92	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	504	2QJ	O15-S13-C9	-2.46	104.93	107.96
2	B	501	HEM	O2D-CGD-CBD	2.35	121.42	114.00
2	A	501	HEM	O2D-CGD-CBD	2.31	121.31	114.00
2	A	501	HEM	CHD-C1D-ND	2.26	126.86	124.42
5	A	504	2QJ	O15-S13-C9	-2.21	105.24	107.96
2	A	501	HEM	O2A-CGA-CBA	2.01	120.35	114.00

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	C2C-C3C-CAC-CBC
5	B	504	2QJ	C17-C16-S13-O14
5	A	504	2QJ	C17-C16-S13-O14
5	B	504	2QJ	C21-C16-S13-O14
5	A	504	2QJ	C21-C16-S13-O14
2	A	501	HEM	C4C-C3C-CAC-CBC
5	B	504	2QJ	C17-C16-S13-C9
5	A	504	2QJ	C17-C16-S13-C9
2	B	501	HEM	C4C-C3C-CAC-CBC
5	B	504	2QJ	C21-C16-S13-C9
2	B	501	HEM	CAA-CBA-CGA-O1A
5	A	504	2QJ	C21-C16-S13-C9
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
5	A	504	2QJ	C23-C2-C3-O4
2	A	501	HEM	CAA-CBA-CGA-O1A
5	A	504	2QJ	C23-C2-C3-N5
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D

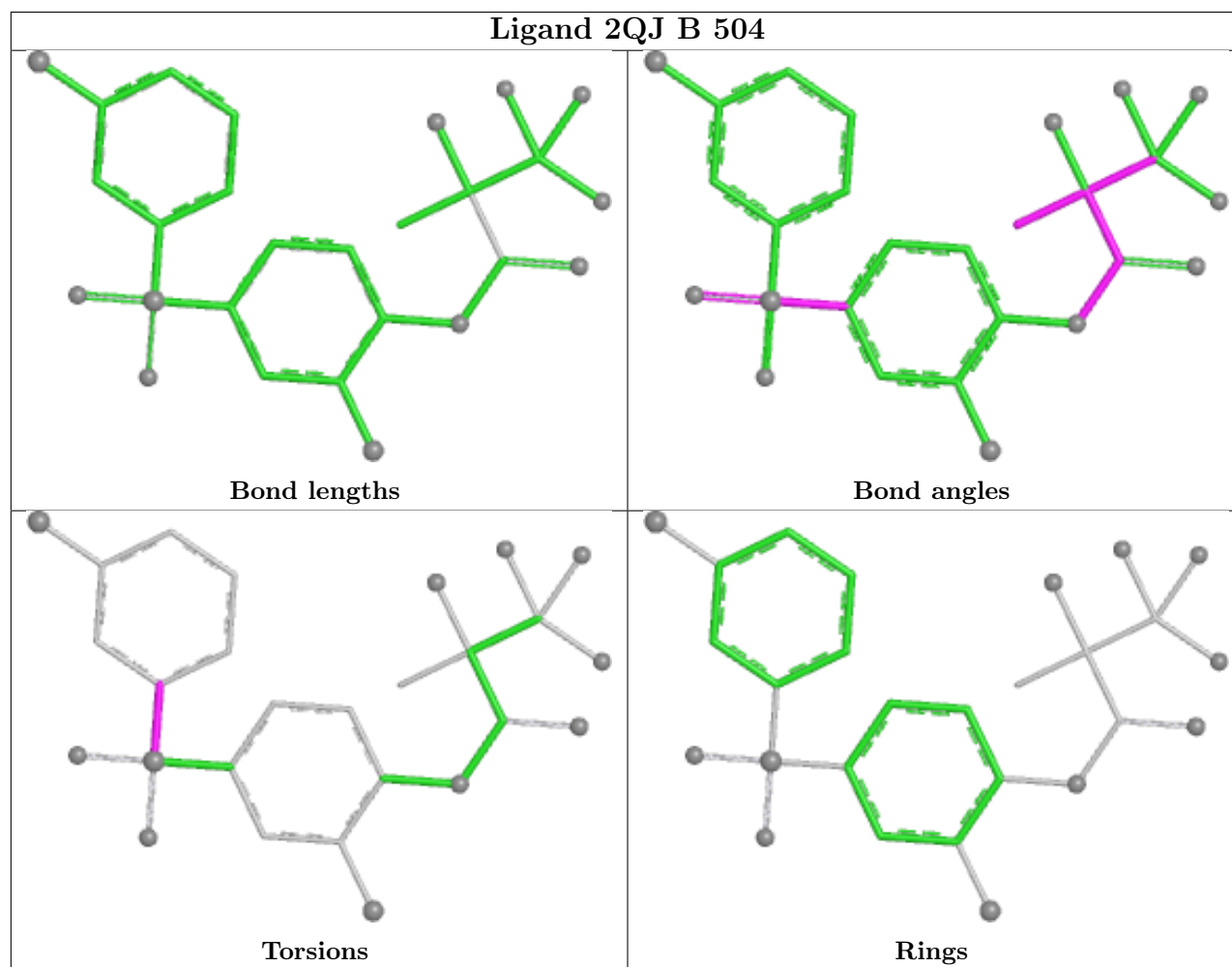
There are no ring outliers.

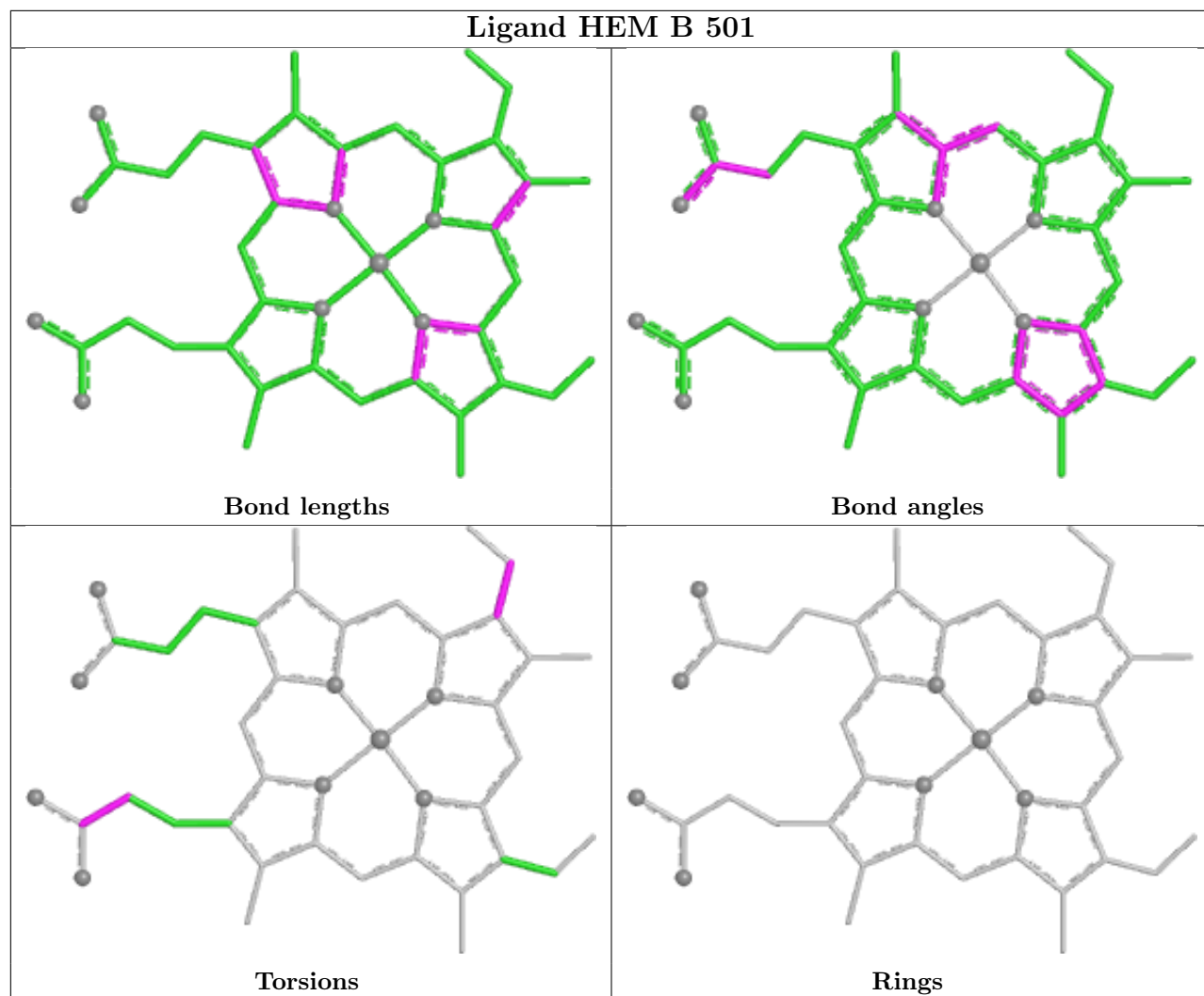
3 monomers are involved in 5 short contacts:

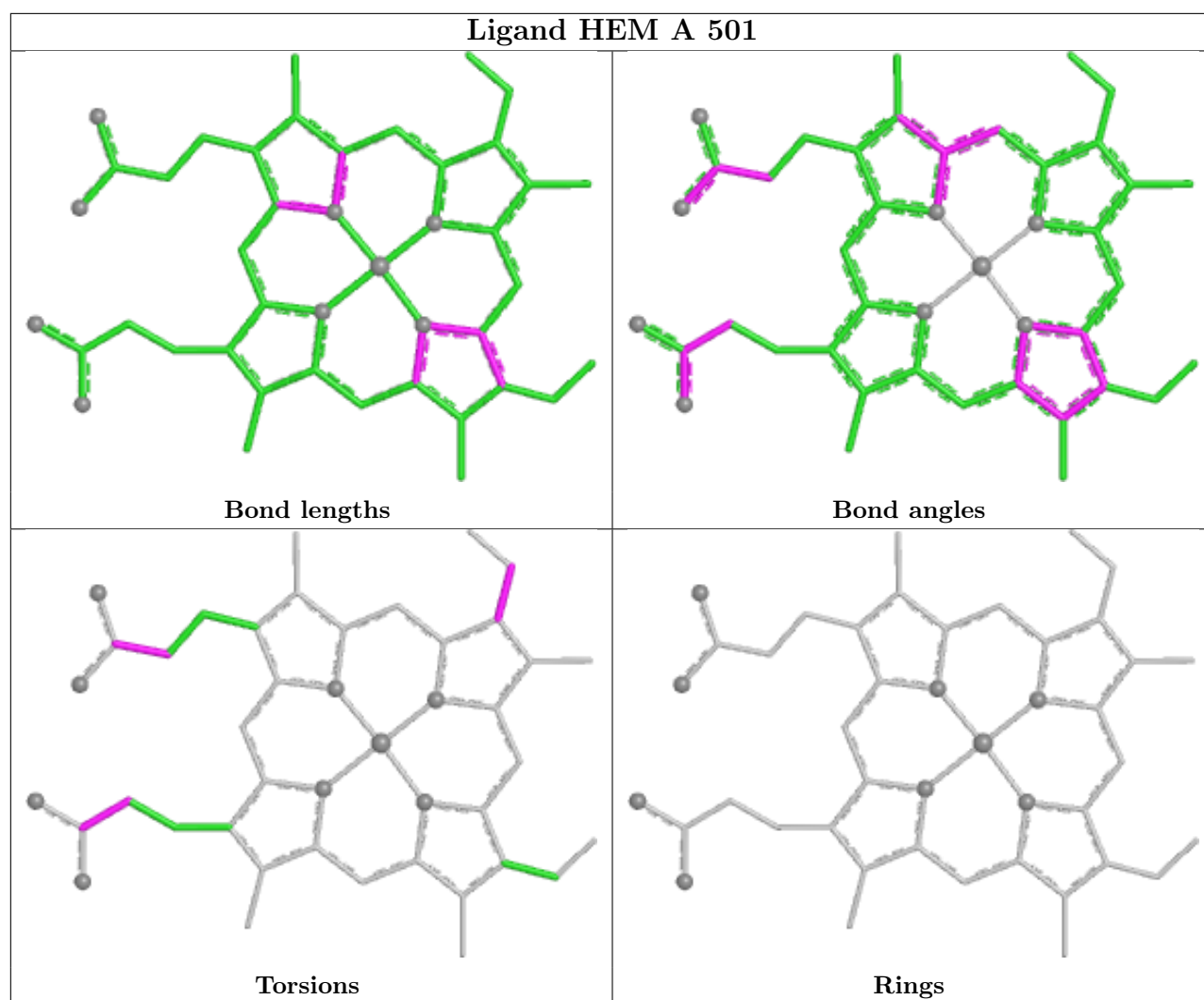
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	2	0
2	A	501	HEM	1	0
3	A	502	GOL	2	0

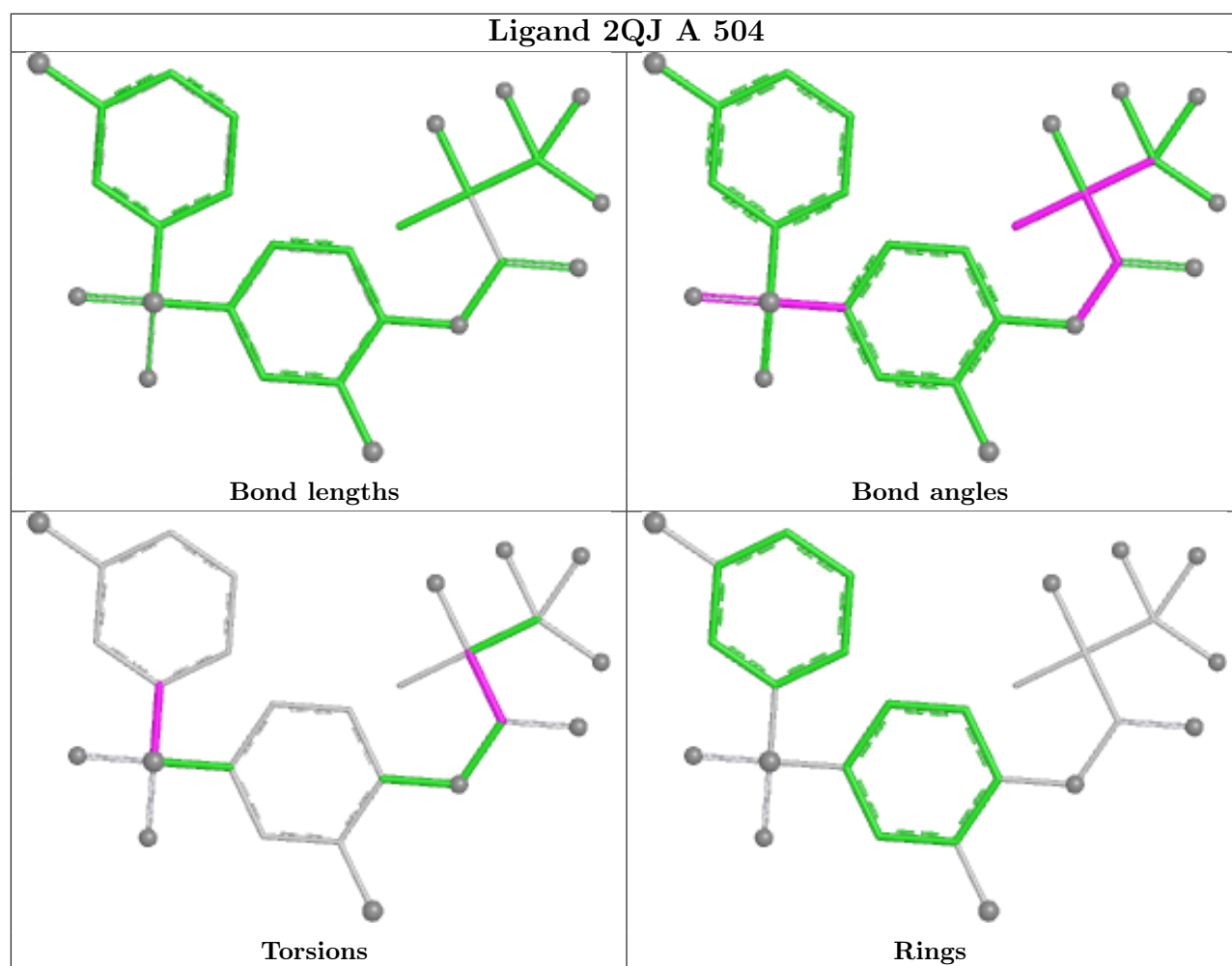
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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	464/475 (97%)	0.78	67 (14%) 6 4	31, 52, 82, 117	0
1	B	464/475 (97%)	0.74	63 (13%) 7 5	31, 51, 83, 112	0
All	All	928/950 (97%)	0.76	130 (14%) 6 5	31, 51, 83, 117	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	VAL	7.9
1	A	473	VAL	7.4
1	A	472	VAL	6.6
1	B	476	PHE	6.6
1	B	472	VAL	6.4
1	A	476	PHE	6.1
1	A	279	PRO	5.5
1	B	185	LYS	5.3
1	A	47	ILE	4.9
1	B	471	PRO	4.9
1	B	475	GLY	4.9
1	A	218	ASN	4.8
1	A	470	THR	4.8
1	A	257	MET	4.7
1	A	471	PRO	4.6
1	A	475	GLY	4.4
1	B	474	ASN	4.2
1	B	462	VAL	4.1
1	B	183	PHE	4.0
1	B	470	THR	3.9
1	B	108	ARG	3.9
1	B	218	ASN	3.9
1	B	48	LYS	3.9
1	B	47	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	100	PHE	3.8
1	A	258	ASN	3.8
1	A	490	VAL	3.7
1	A	216	TYR	3.6
1	B	490	VAL	3.6
1	A	214	GLN	3.6
1	B	278	GLN	3.5
1	A	474	ASN	3.5
1	B	217	ASN	3.5
1	A	108	ARG	3.5
1	B	466	ASN	3.4
1	A	138	LYS	3.4
1	A	215	VAL	3.4
1	A	185	LYS	3.4
1	B	103	ALA	3.3
1	A	107	ASN	3.3
1	B	279	PRO	3.3
1	A	277	ASN	3.3
1	B	43	LEU	3.3
1	B	214	GLN	3.2
1	A	100	PHE	3.1
1	A	28	GLY	3.1
1	B	27	LYS	3.1
1	A	465	LYS	3.1
1	A	48	LYS	3.1
1	B	212	TRP	3.1
1	A	332	GLY	3.1
1	A	27	LYS	3.0
1	B	465	LYS	3.0
1	A	189	TYR	3.0
1	B	190	LYS	3.0
1	B	50	ILE	3.0
1	A	187	PHE	3.0
1	A	44	GLN	3.0
1	B	45	ILE	2.9
1	A	43	LEU	2.9
1	A	276	HIS	2.9
1	A	219	PHE	2.9
1	A	275	LYS	2.8
1	B	105	ARG	2.8
1	A	212	TRP	2.7
1	A	469	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	49	ASP	2.7
1	A	334	ASN	2.7
1	A	467	LEU	2.7
1	B	216	TYR	2.7
1	B	273	LYS	2.7
1	B	46	GLY	2.7
1	B	42	ILE	2.7
1	B	467	LEU	2.7
1	A	45	ILE	2.6
1	B	219	PHE	2.6
1	B	469	THR	2.6
1	B	184	HIS	2.6
1	B	276	HIS	2.6
1	B	138	LYS	2.6
1	A	375	LYS	2.6
1	B	380	LEU	2.6
1	B	38	VAL	2.6
1	A	278	GLN	2.5
1	A	380	LEU	2.5
1	B	44	GLN	2.5
1	B	107	ASN	2.5
1	B	334	ASN	2.5
1	A	406	MET	2.5
1	B	188	ASP	2.5
1	A	39	ILE	2.5
1	B	274	GLU	2.5
1	B	332	GLY	2.4
1	B	225	TYR	2.4
1	B	106	ALA	2.4
1	A	460	SER	2.4
1	A	111	GLY	2.4
1	B	232	LYS	2.4
1	A	333	ARG	2.4
1	A	462	VAL	2.4
1	B	209	SER	2.4
1	A	461	LEU	2.4
1	B	37	PRO	2.4
1	A	160	LYS	2.3
1	A	209	SER	2.3
1	B	375	LYS	2.3
1	A	104	GLU	2.3
1	A	217	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	280	SER	2.3
1	A	269	MET	2.3
1	A	118	LYS	2.3
1	A	190	LYS	2.3
1	A	125	ARG	2.3
1	B	215	VAL	2.2
1	A	477	ALA	2.2
1	A	213	ILE	2.2
1	B	468	ASP	2.2
1	B	49	ASP	2.2
1	A	184	HIS	2.1
1	A	378	ASN	2.1
1	B	464	PRO	2.1
1	A	371	THR	2.1
1	A	331	ILE	2.1
1	A	226	PHE	2.1
1	A	154	GLU	2.1
1	B	130	THR	2.1
1	B	415	GLU	2.0
1	B	277	ASN	2.0
1	B	406	MET	2.0
1	A	280	SER	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	SO4	A	503	5/5	0.59	0.39	82,82,82,82	5

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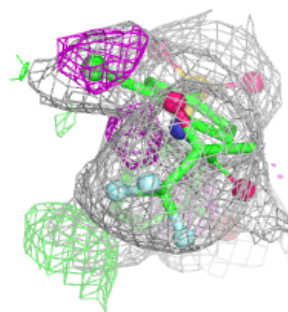
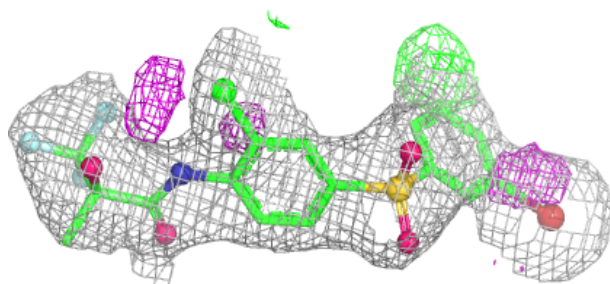
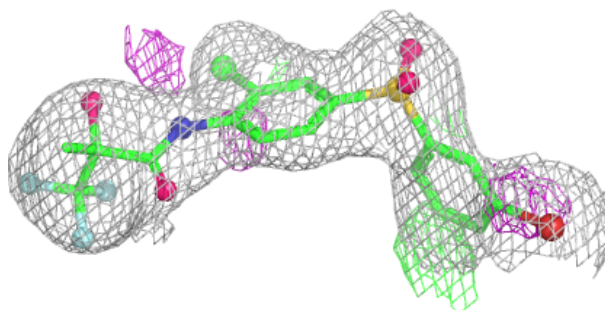
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	503	5/5	0.69	0.41	78,79,79,79	5
3	GOL	A	502	6/6	0.75	0.28	82,82,82,83	0
3	GOL	B	502	6/6	0.77	0.32	83,84,84,85	0
5	2QJ	B	504	27/27	0.92	0.15	77,78,78,79	0
5	2QJ	A	504	27/27	0.93	0.14	75,78,79,80	0
2	HEM	A	501	43/43	0.99	0.06	32,33,39,40	0
2	HEM	B	501	43/43	0.99	0.05	31,32,39,39	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.

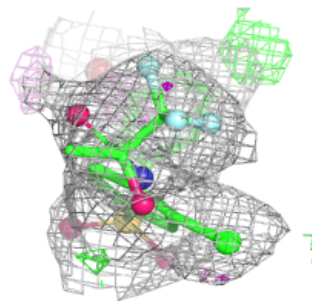
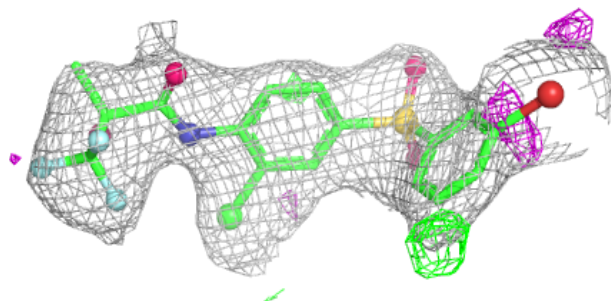
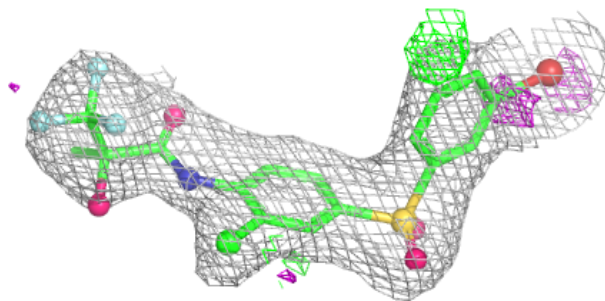
Electron density around 2QJ B 504:

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



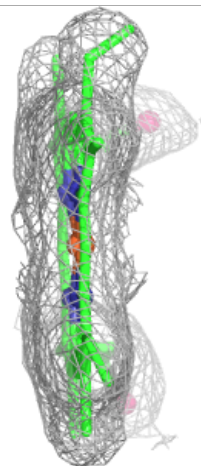
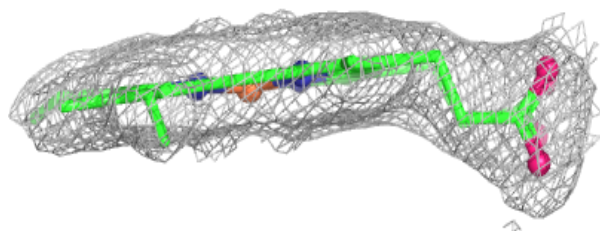
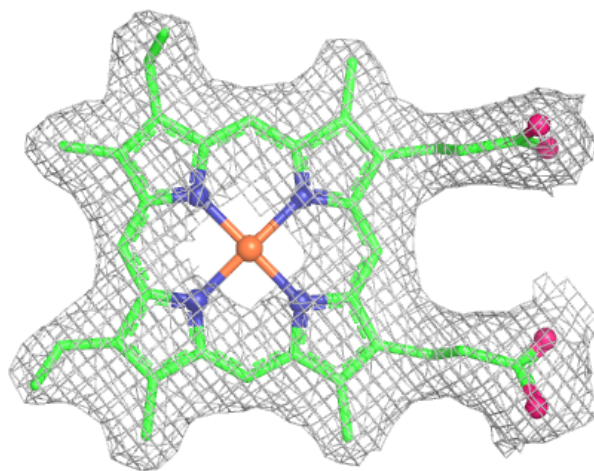
Electron density around 2QJ A 504:

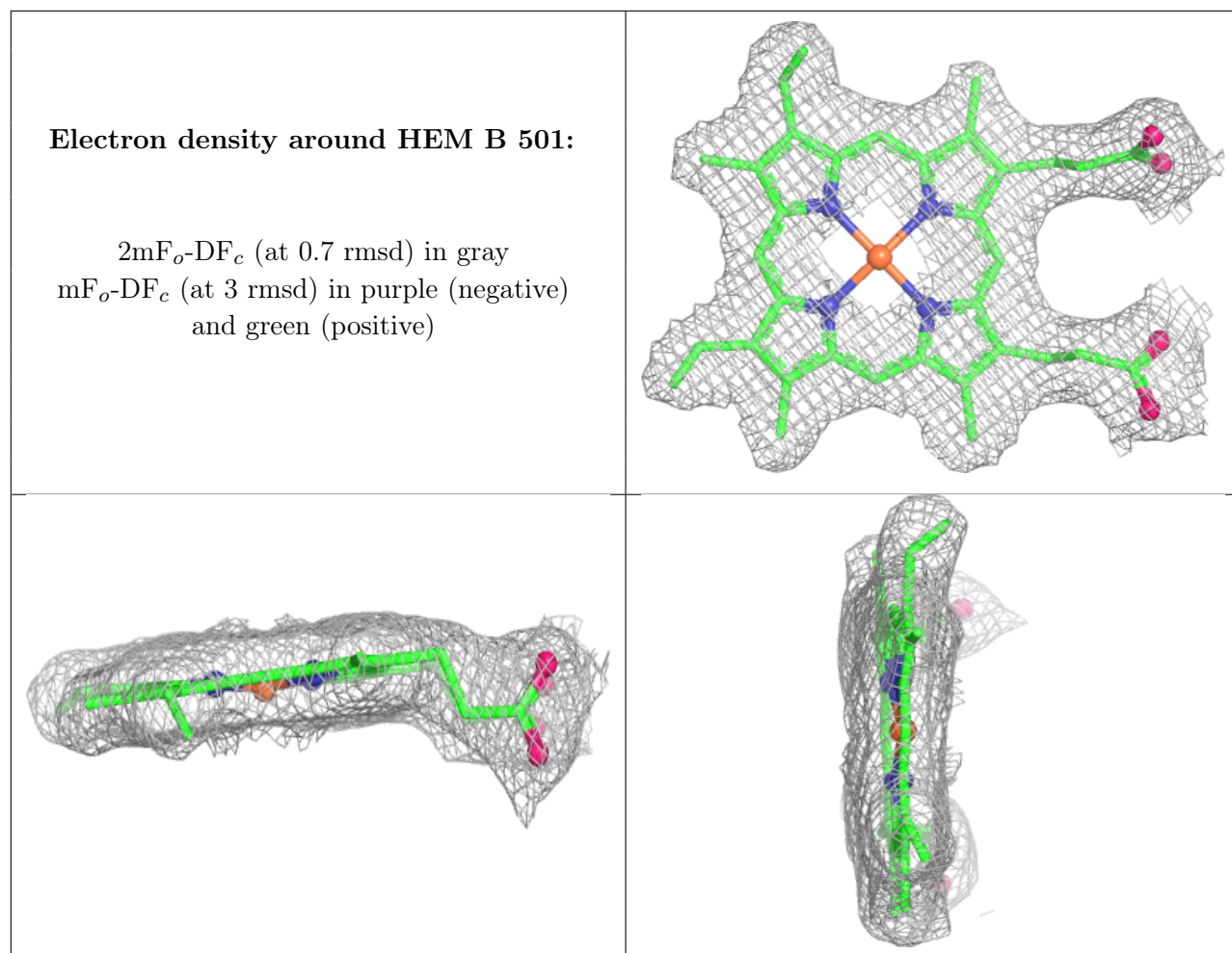
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 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 ⓘ

There are no such residues in this entry.