



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 11:00 AM UTC

PDB ID : 3NXU / pdb_00003nxu
Title : Crystal structure of human cytochrome P4503A4 bound to an inhibitor ritonavir
Authors : Sevrioukova, I.F.; Poulos, T.L.
Deposited on : 2010-07-14
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

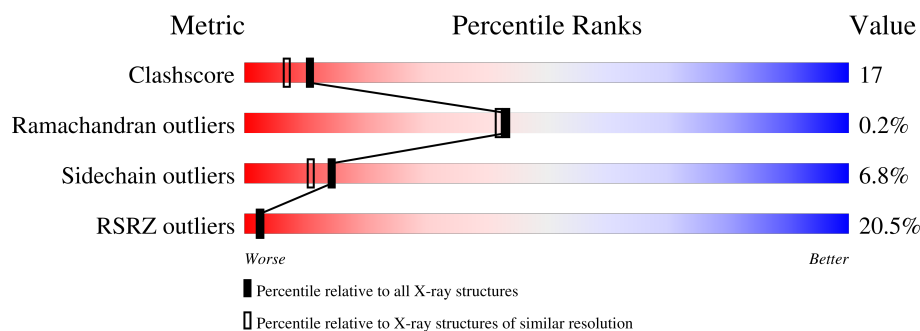
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	485	
1	B	485	

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	RIT	A	600	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7955 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 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3678	2394	603	657	24			
1	B	457	Total	C	N	O	S	0	0	0
			3678	2394	603	657	24			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	SEE REMARK 999	UNP P08684
A	24	ALA	-	SEE REMARK 999	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684
B	23	MET	-	SEE REMARK 999	UNP P08684
B	24	ALA	-	SEE REMARK 999	UNP P08684
B	504	HIS	-	expression tag	UNP P08684
B	505	HIS	-	expression tag	UNP P08684
B	506	HIS	-	expression tag	UNP P08684
B	507	HIS	-	expression tag	UNP P08684

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



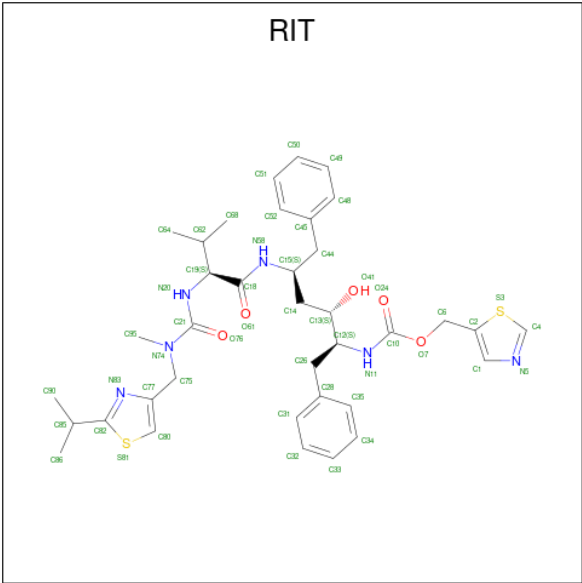
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

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



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

- Molecule 4 is RITONAVIR (CCD ID: RIT) (formula: C₃₇H₄₈N₆O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
4	B	1	Total	C	N	O	S	0	0
			50	37	6	5	2		

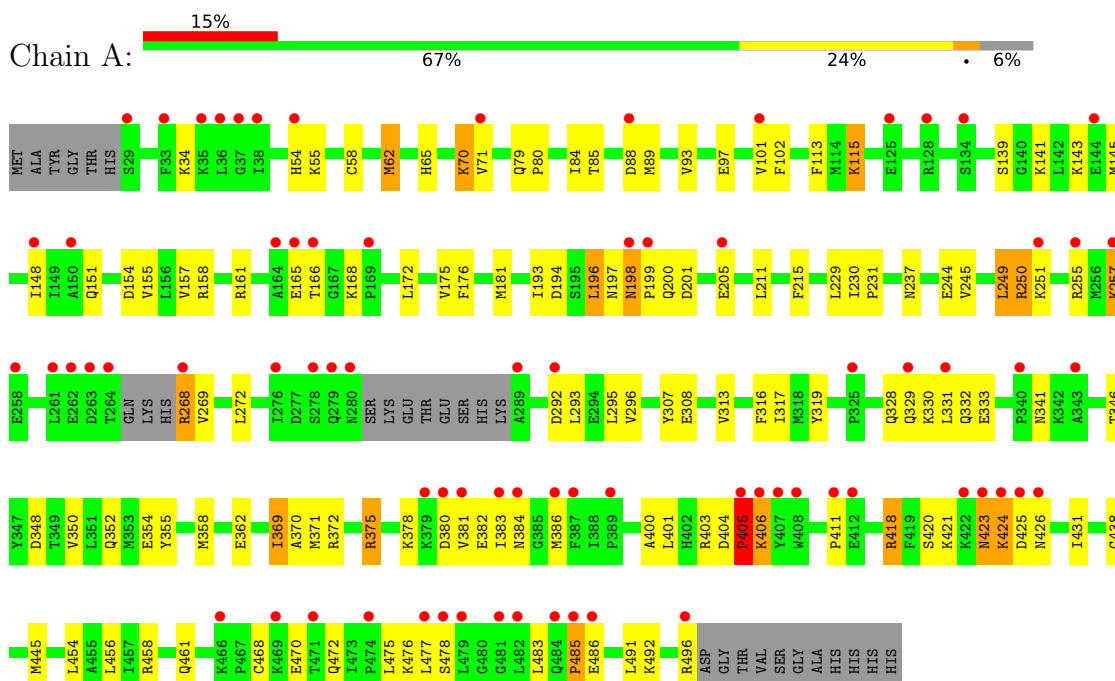
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total 217	O 217	0	0
5	B	172	Total 172	O 172	0	0

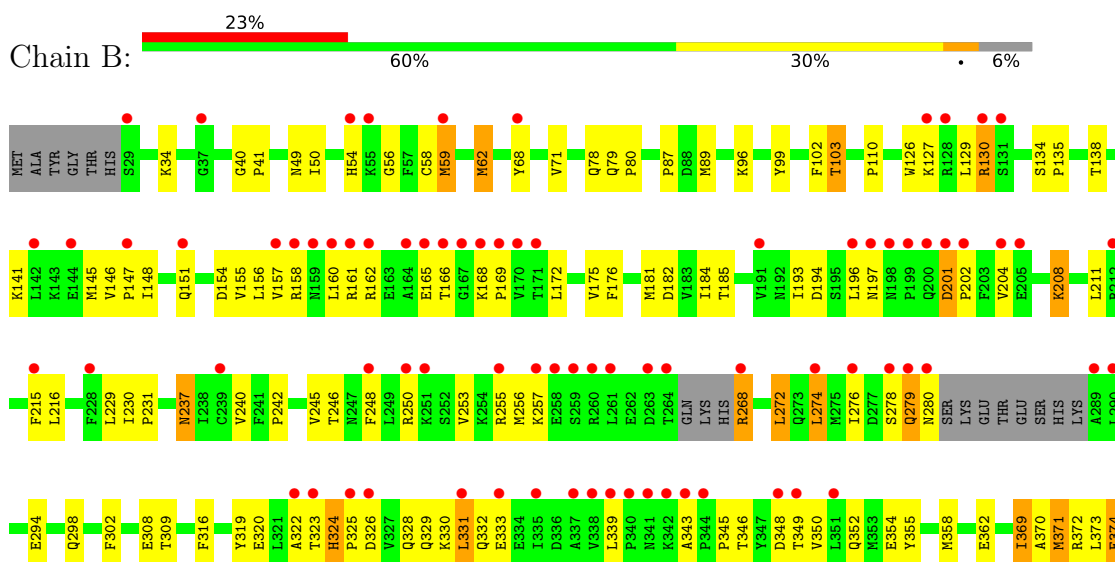
3 Residue-property plots

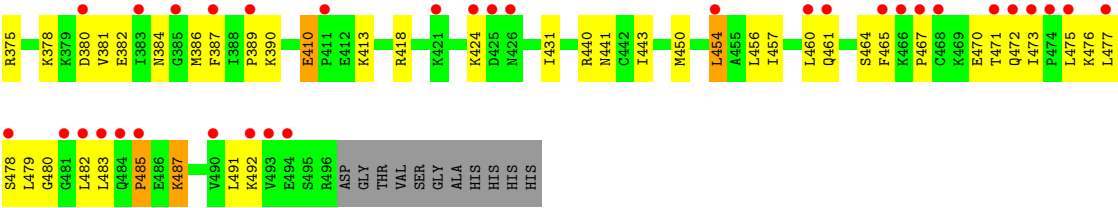
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 3A4



• Molecule 1: Cytochrome P450 3A4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.12Å 94.69Å 93.13Å 90.00° 124.25° 90.00°	Depositor
Resolution (Å)	40.40 – 2.00 40.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.40-2.00) 97.5 (40.40-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.262 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -1/2*h+3/2*k-l,1/2*h+1/2*k+1,1/2*h-1/2*k 0.003 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.009 for -h-k-l,l,k 0.016 for -h+k-l,-l,-k 0.003 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.005 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.010 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.016 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.012 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.015 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.018 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7955	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, RIT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	1/3766 (0.0%)	0.96	9/5094 (0.2%)
1	B	0.44	1/3766 (0.0%)	0.96	13/5094 (0.3%)
All	All	0.46	2/7532 (0.0%)	0.96	22/10188 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	VAL	C-O	-7.27	1.17	1.24
1	B	371	MET	SD-CE	-6.51	1.63	1.79

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	ILE	N-CA-C	-9.80	103.38	111.81
1	B	96	LYS	N-CA-C	8.04	119.67	111.07
1	A	406	LYS	N-CA-C	-6.78	104.89	113.43
1	A	198	ASN	CA-C-N	6.53	128.01	119.84
1	A	198	ASN	C-N-CA	6.53	128.01	119.84

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	3678	0	3764	107	0
1	B	3678	0	3764	139	0
2	A	16	0	24	3	0
2	B	8	0	12	2	0
3	A	43	0	30	7	0
3	B	43	0	30	6	0
4	A	50	0	47	6	0
4	B	50	0	46	4	0
5	A	217	0	0	13	0
5	B	172	0	0	14	0
All	All	7955	0	7717	253	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 17.

The worst 5 of 253 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:251:LYS:HG2	1:A:255:ARG:HH21	1.21	1.06
1:B:354:GLU:HG2	1:B:358:MET:HE2	1.40	1.02
1:B:355:TYR:HA	1:B:358:MET:HE3	1.42	0.99
1:A:70:LYS:HD2	1:A:71:VAL:HG23	1.41	0.98
1:A:369:ILE:HG12	3:A:508:HEM:HMB1	1.52	0.90

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	451/485 (93%)	433 (96%)	17 (4%)	1 (0%)	43	42
1	B	451/485 (93%)	426 (94%)	24 (5%)	1 (0%)	43	42
All	All	902/970 (93%)	859 (95%)	41 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	424	LYS
1	A	405	PRO

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	418/441 (95%)	389 (93%)	29 (7%)	14	11
1	B	418/441 (95%)	390 (93%)	28 (7%)	15	11
All	All	836/882 (95%)	779 (93%)	57 (7%)	14	11

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	486	GLU
1	B	487	LYS
1	B	168	LYS
1	B	485	PRO
1	B	369	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	352	GLN
1	B	426	ASN
1	A	451	ASN
1	A	461	GLN
1	A	472	GLN

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](#)

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	DMS	A	700	-	3,3,3	1.01	0	3,3,3	0.90	0
4	RIT	B	600	3	52,53,53	4.92	35 (67%)	62,71,71	3.27	26 (41%)
3	HEM	B	508	4,1	50,50,50	1.21	4 (8%)	67,82,82	0.75	0
2	DMS	A	703	-	3,3,3	0.79	0	3,3,3	0.90	0
3	HEM	A	508	4,1	50,50,50	1.35	4 (8%)	67,82,82	1.09	4 (5%)
2	DMS	A	701	-	3,3,3	0.88	0	3,3,3	0.99	0
4	RIT	A	600	3	52,53,53	4.97	36 (69%)	62,71,71	3.71	33 (53%)
2	DMS	A	702	-	3,3,3	0.80	0	3,3,3	0.98	0
2	DMS	B	705	-	3,3,3	1.85	1 (33%)	3,3,3	1.02	0
2	DMS	B	704	-	3,3,3	2.26	2 (66%)	3,3,3	0.82	0

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
3	HEM	B	508	4,1	-	0/14/54/54	-
4	RIT	B	600	3	-	8/53/53/53	0/4/4/4
3	HEM	A	508	4,1	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RIT	A	600	3	-	12/53/53/53	0/4/4/4

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	RIT	O24-C10	11.90	1.43	1.21
4	B	600	RIT	C6-C2	-10.19	1.19	1.49
4	B	600	RIT	C31-C28	10.11	1.58	1.38
4	B	600	RIT	O24-C10	9.64	1.39	1.21
4	B	600	RIT	C49-C48	9.19	1.54	1.38

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	RIT	S81-C82-N83	-10.26	100.78	114.19
4	B	600	RIT	S81-C82-N83	-9.78	101.42	114.19
4	A	600	RIT	C44-C15-N58	9.17	127.80	110.34
4	B	600	RIT	C44-C15-N58	8.61	126.73	110.34
4	A	600	RIT	C77-C80-S81	-8.55	99.16	110.59

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

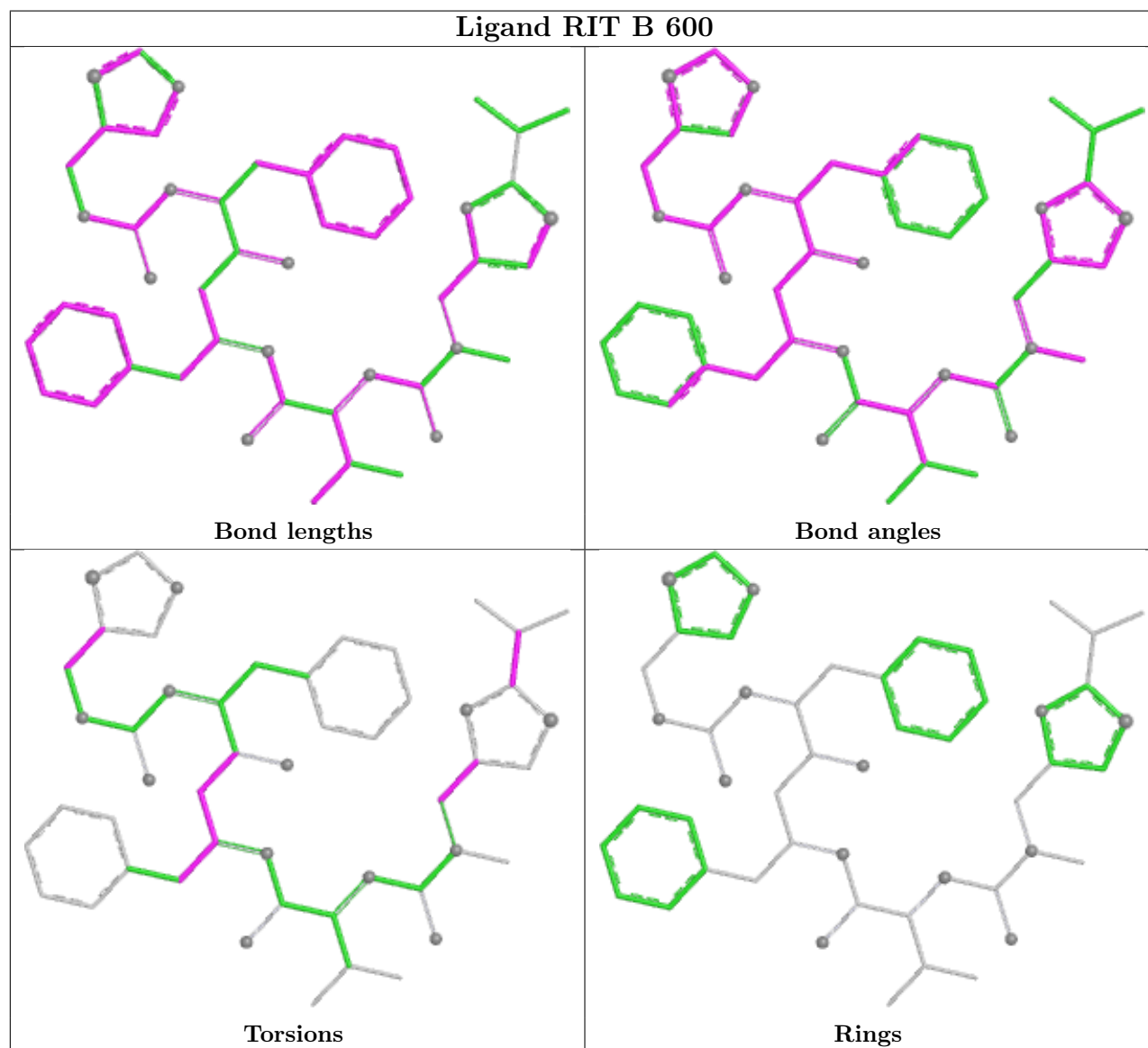
Mol	Chain	Res	Type	Atoms
4	A	600	RIT	C1-C2-C6-O7
4	A	600	RIT	C12-C13-C14-C15
4	A	600	RIT	C13-C14-C15-N58
4	B	600	RIT	C1-C2-C6-O7
4	B	600	RIT	S3-C2-C6-O7

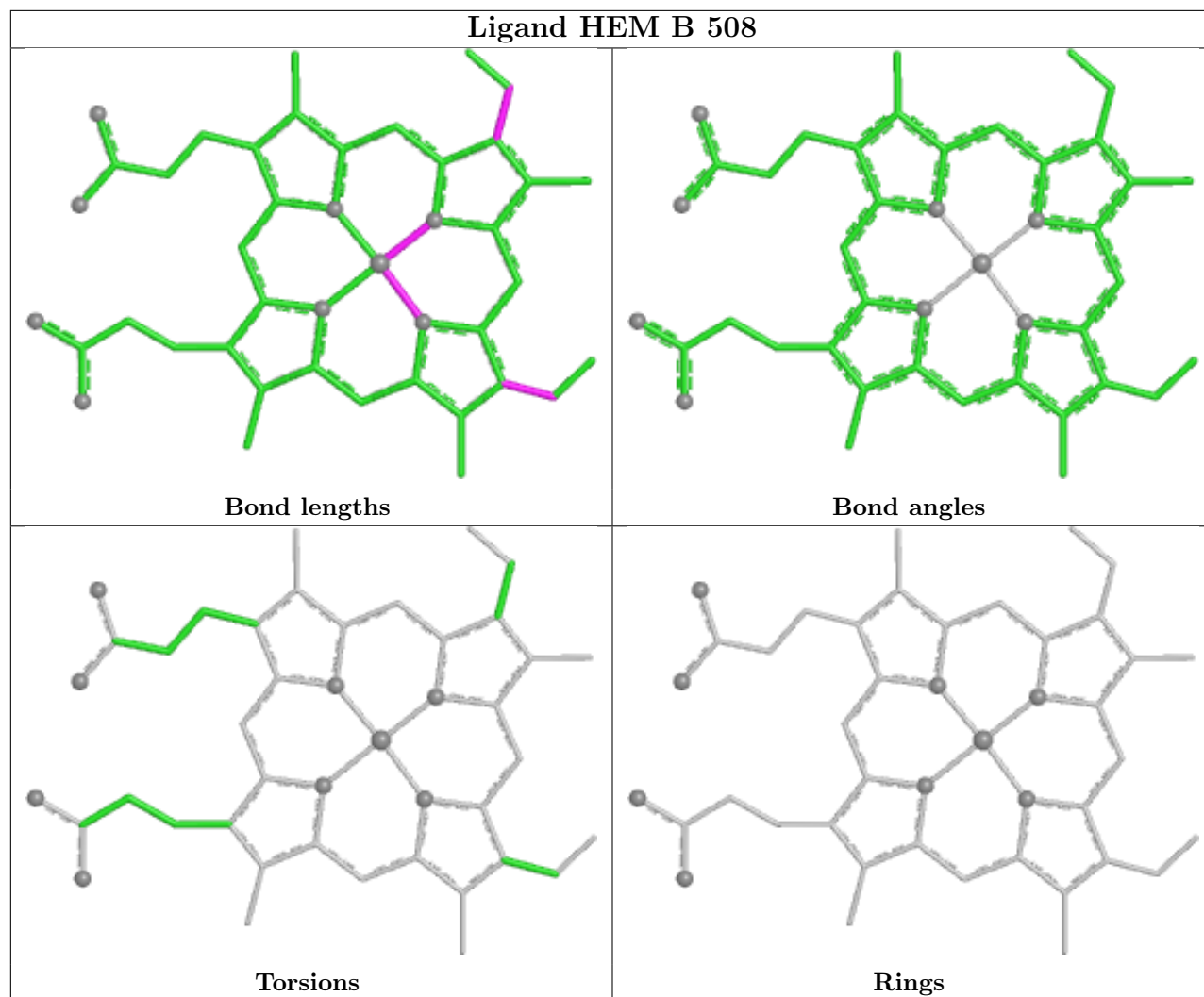
There are no ring outliers.

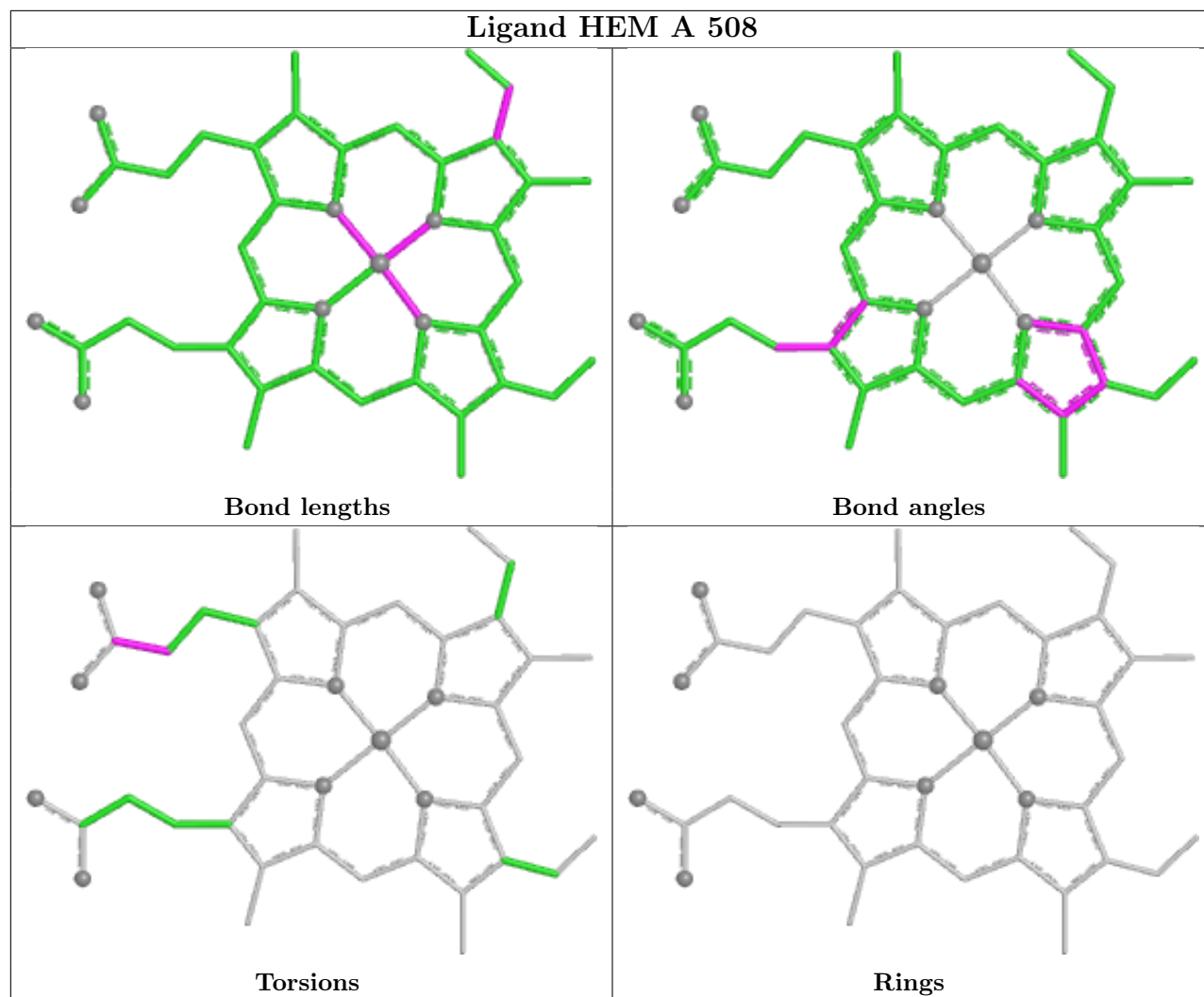
7 monomers are involved in 28 short contacts:

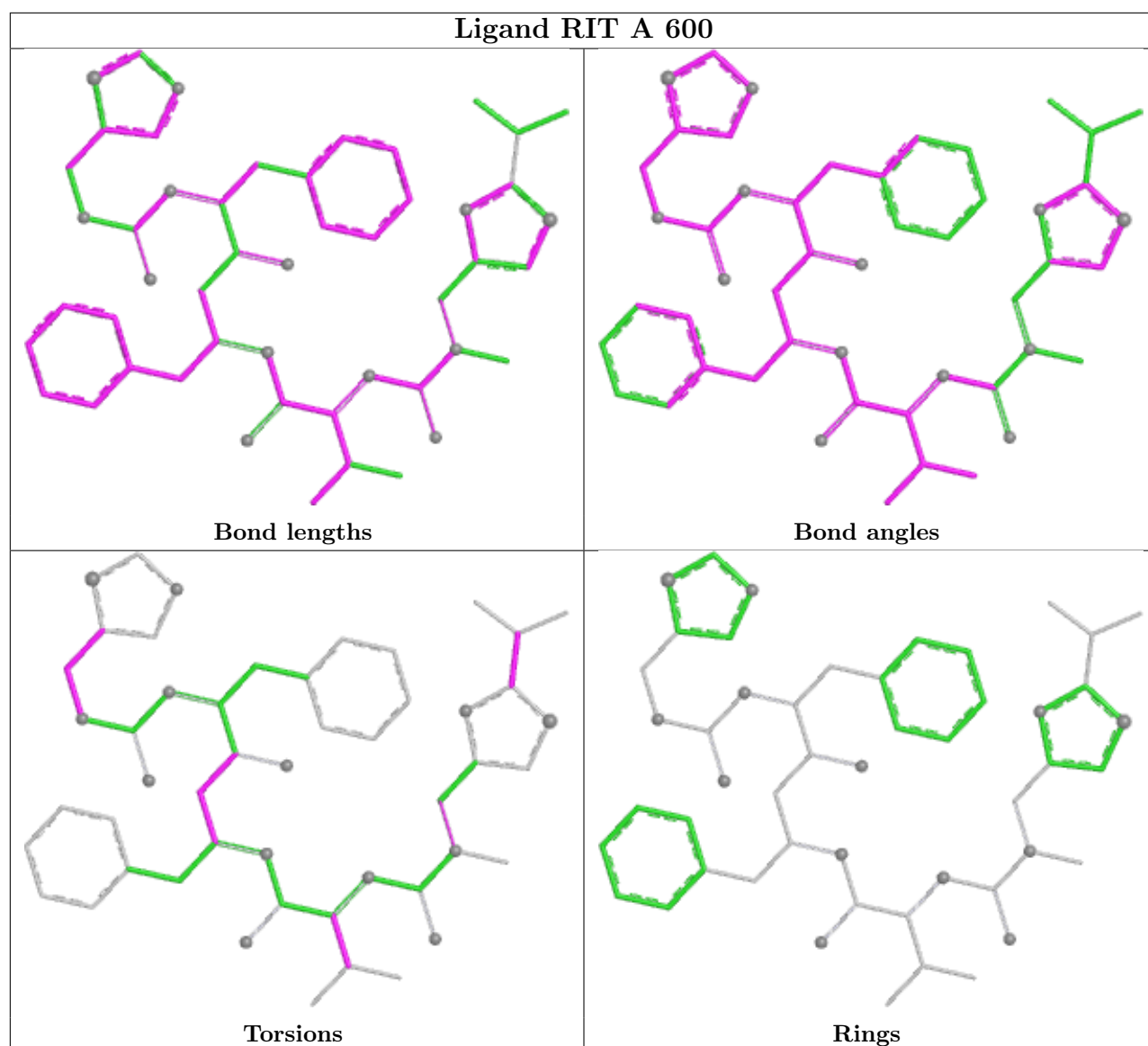
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	DMS	2	0
4	B	600	RIT	4	0
3	B	508	HEM	6	0
2	A	703	DMS	1	0
3	A	508	HEM	7	0
4	A	600	RIT	6	0
2	B	704	DMS	2	0

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/485 (94%)	0.95	75 (16%) 4 4	24, 38, 64, 75	0
1	B	457/485 (94%)	1.24	112 (24%) 2 1	26, 46, 70, 83	0
All	All	914/970 (94%)	1.10	187 (20%) 2 2	24, 42, 68, 83	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ASN	7.6
1	B	289	ALA	5.6
1	A	289	ALA	5.2
1	B	482	LEU	5.1
1	B	485	PRO	4.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

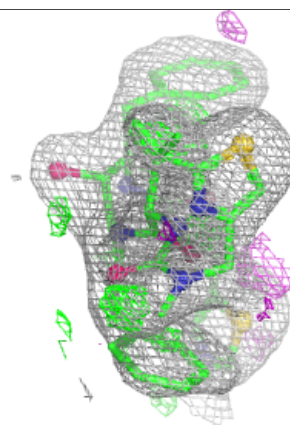
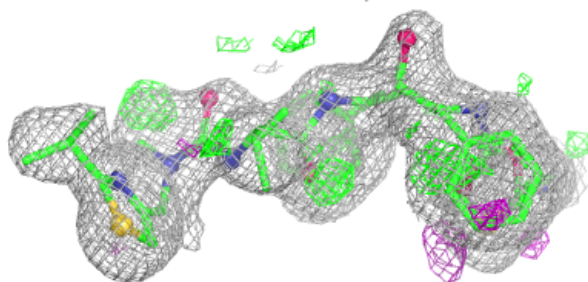
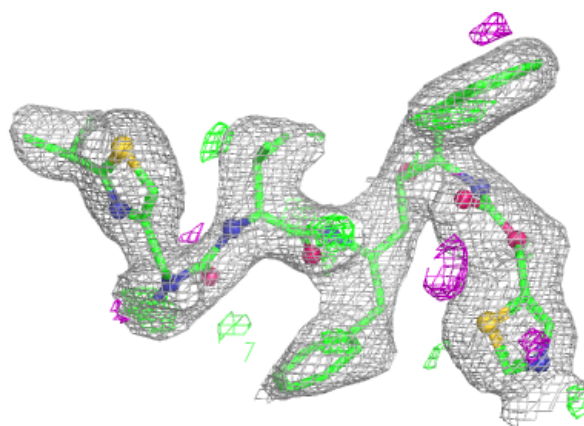
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
2	DMS	B	705	4/4	0.70	0.25	60,60,61,65	0
2	DMS	A	703	4/4	0.87	0.18	71,71,72,74	0
4	RIT	B	600	50/50	0.88	0.17	41,53,58,59	0
2	DMS	A	701	4/4	0.89	0.19	71,71,71,73	0
4	RIT	A	600	50/50	0.90	0.13	33,40,45,46	0
2	DMS	A	702	4/4	0.91	0.16	71,71,72,74	0
2	DMS	B	704	4/4	0.92	0.15	51,53,54,56	0
2	DMS	A	700	4/4	0.96	0.10	38,39,39,43	0
3	HEM	A	508	43/43	0.97	0.07	23,26,29,31	0
3	HEM	B	508	43/43	0.97	0.07	30,32,34,36	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.

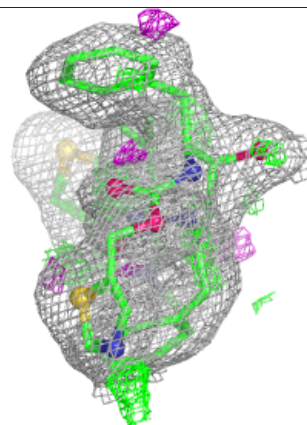
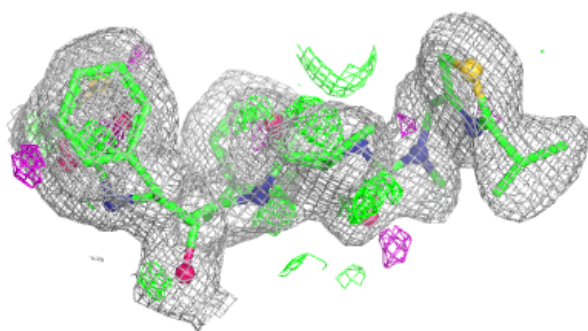
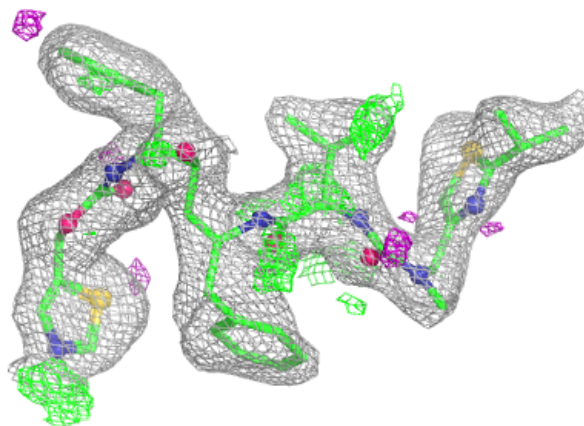
Electron density around RIT B 600:

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



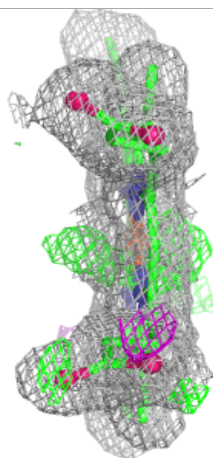
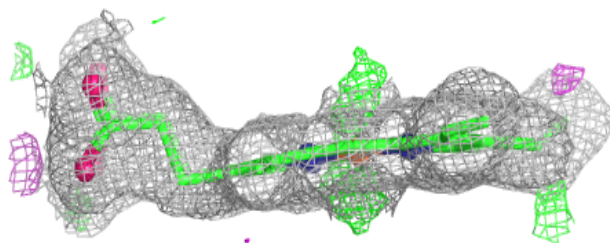
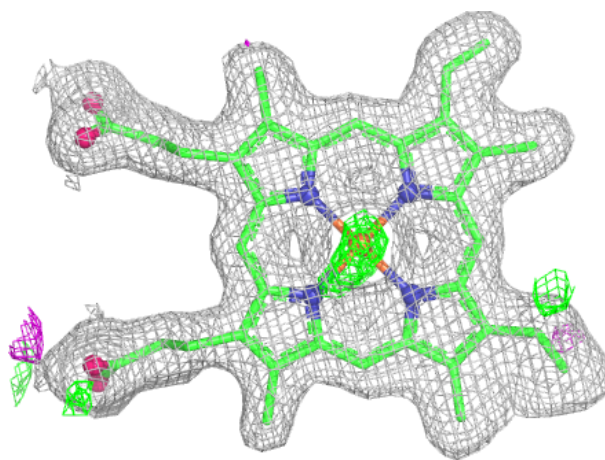
Electron density around RIT A 600:

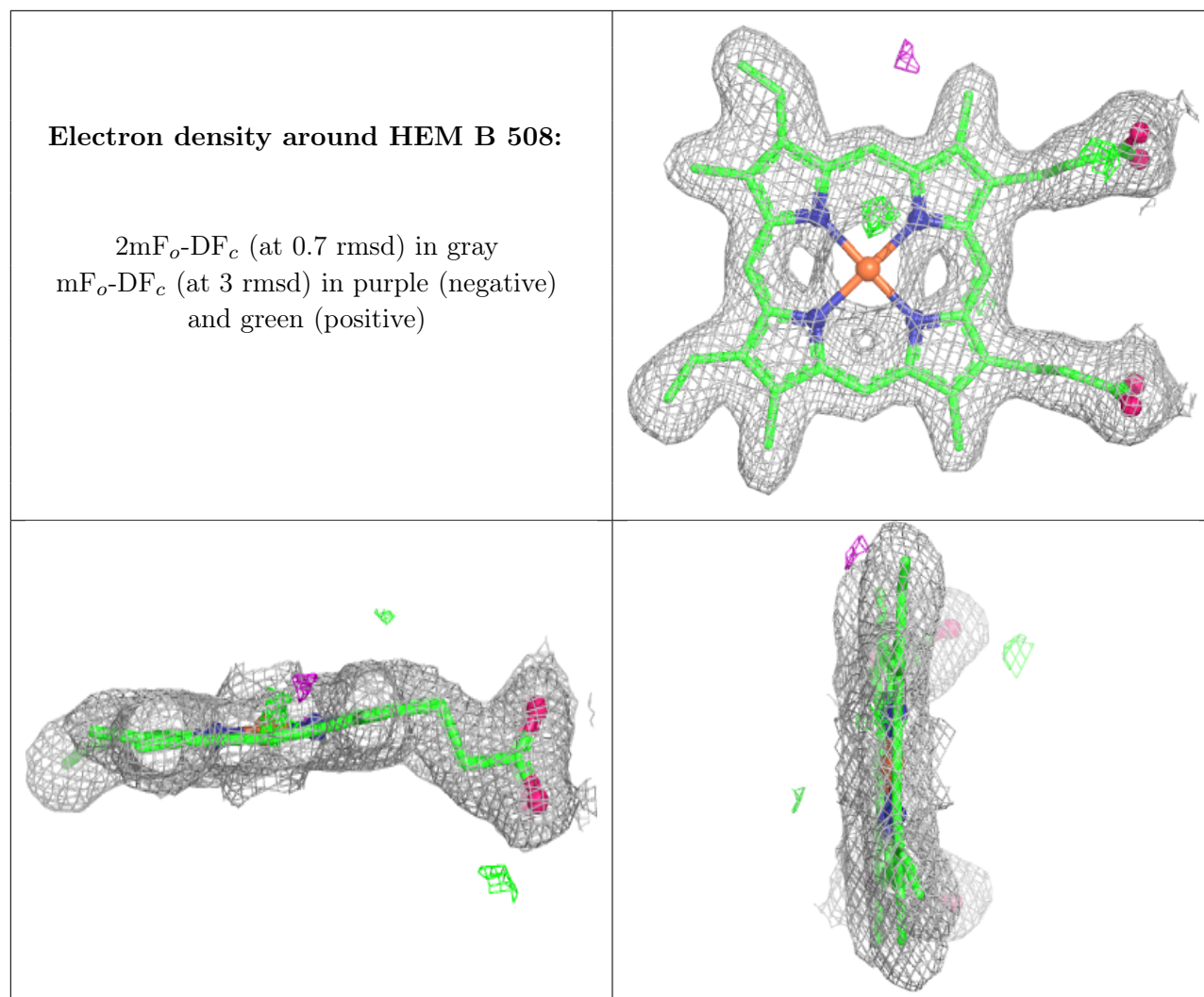
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 508:

$2mF_o-DF_c$ (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.