Comment regarding 9F4I validation report

Please note that there is a discrepancy between the R values given in Table 1 of the manuscript and those in this PDB validation report:

R/Rfree quoted in the manuscript: 0.191 / 0.231

R/Rfree quoted by the DCC: 0.325 / 0.347

The discrepancy is due to the fact that the 9F4I entry represents the “pure triggered state” extracted from the structure, which was refined as the mixed state (dark + triggered state mixture). After the final round of refinement as a mixed state, the “pure triggered state” was extracted and then deposited. The validation software, however, calculates R-factors from the mixed state data, resulting in these high values. We have contacted PDB in this regard but not been able to obtain a validation for the correct procedure.

The 9ER4 structure corresponds to the dark state structure which was fixed and not moved during the final refinement with Phenix.

Please also note that links to the raw image data collected during the experiment are given in the manuscript.

Full wwPDB X-ray Structure Validation Report (i)

Jul 19, 2024 – 05:21 pm BST

PDB ID	:	9F4I
Title	:	Room temperature structure of Glycine max phyA in Pfr
Deposited on	:	2024-04-28
Resolution	:	2.20 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

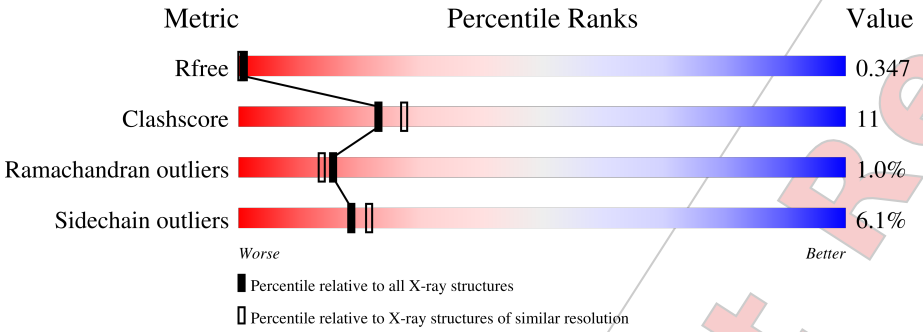
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	359	64% 18% • 17%
1	B	359	55% 26% • 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4866 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.

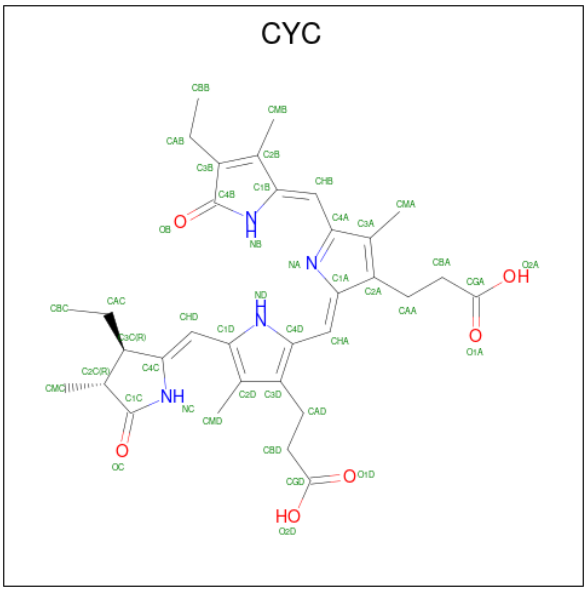
- Molecule 1 is a protein called Phytochrome A-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2315	1494	389	410	22			
1	B	299	Total	C	N	O	S	0	0	0
			2333	1505	392	414	22			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	initiating methionine	UNP B4YB07
A	403	HIS	-	expression tag	UNP B4YB07
A	404	HIS	-	expression tag	UNP B4YB07
A	405	HIS	-	expression tag	UNP B4YB07
A	406	HIS	-	expression tag	UNP B4YB07
A	407	HIS	-	expression tag	UNP B4YB07
A	408	HIS	-	expression tag	UNP B4YB07
B	50	MET	-	initiating methionine	UNP B4YB07
B	403	HIS	-	expression tag	UNP B4YB07
B	404	HIS	-	expression tag	UNP B4YB07
B	405	HIS	-	expression tag	UNP B4YB07
B	406	HIS	-	expression tag	UNP B4YB07
B	407	HIS	-	expression tag	UNP B4YB07
B	408	HIS	-	expression tag	UNP B4YB07

- Molecule 2 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 43 33 4 6	0	0
2	B	1	Total C N O 43 33 4 6	0	0

- Molecule 3 is water.

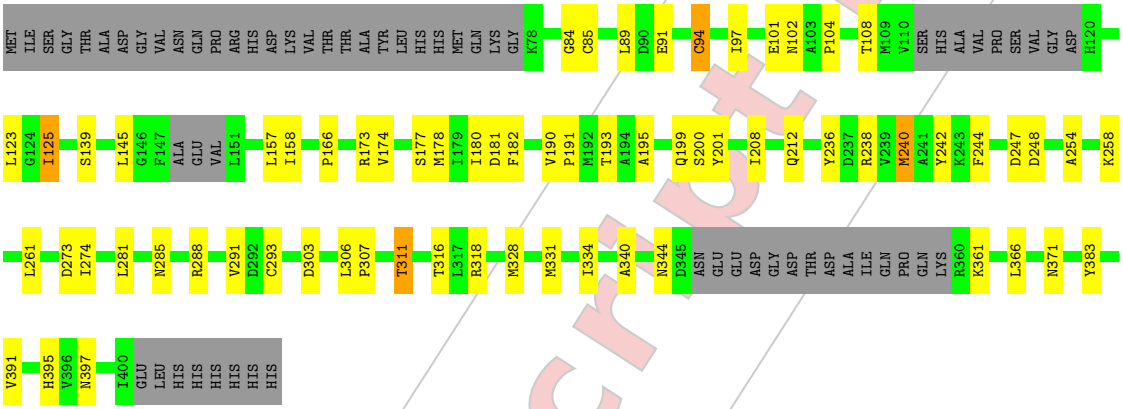
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	60	Total O 60 60	0	0
3	B	72	Total O 72 72	0	0

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. 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. 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.

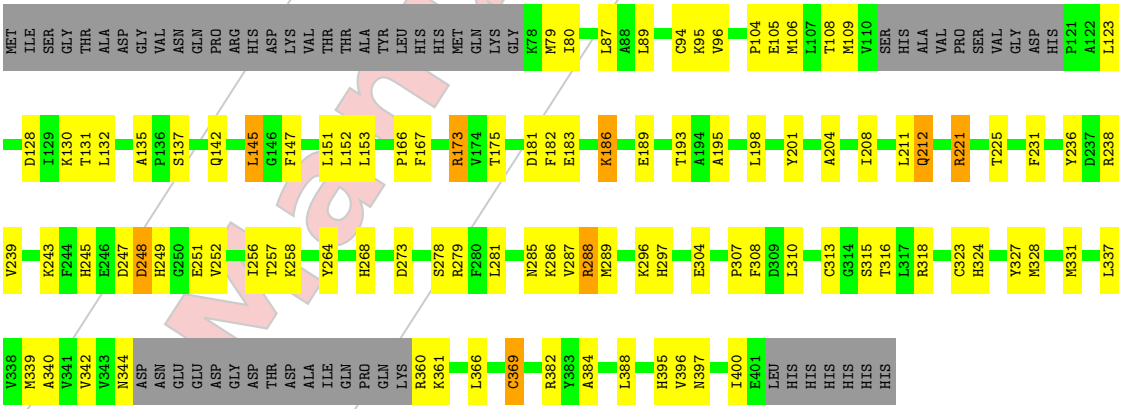
• Molecule 1: Phytochrome A-2

Chain A:



• Molecule 1: Phytochrome A-2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.45Å 115.05Å 69.80Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	20.48 – 2.20 20.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.48-2.20) 99.9 (20.91-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.21rc_5156	Depositor
R, R_{free}	0.191 , 0.231 0.325 , 0.347	Depositor DCC
R_{free} test set	2310 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4866	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 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CYC

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	0.37	0/2368	0.61	0/3209
1	B	0.59	1/2386 (0.0%)	0.79	2/3233 (0.1%)
All	All	0.49	1/4754 (0.0%)	0.70	2/6442 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	CYS	CB-SG	-6.52	1.71	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	145	LEU	CB-CG-CD1	-8.40	96.73	111.00
1	B	310	LEU	CA-CB-CG	5.20	127.25	115.30

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	2315	0	2352	46	0
1	B	2333	0	2380	65	0
2	A	43	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	36	3	0
3	A	60	0	0	10	0
3	B	72	0	0	14	0
All	All	4866	0	4804	109	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 11.

All (109) 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:279:ARG:NH2	3:B:601:HOH:O	1.93	1.00
1:A:311:THR:O	3:A:601:HOH:O	1.90	0.90
1:B:285:ASN:HD21	1:B:318:ARG:HH21	1.25	0.84
1:A:101:GLU:O	3:A:602:HOH:O	2.00	0.78
1:A:344:ASN:OD1	1:A:397:ASN:ND2	2.13	0.76
1:B:251:GLU:OE1	1:B:268:HIS:NE2	2.23	0.72
1:B:186:LYS:NZ	3:B:602:HOH:O	2.06	0.71
1:A:212:GLN:OE1	1:B:212:GLN:NE2	2.25	0.69
1:A:208:ILE:HG23	1:A:391:VAL:HG11	1.73	0.68
1:B:285:ASN:ND2	1:B:318:ARG:HH21	1.93	0.66
1:B:186:LYS:HE3	1:B:186:LYS:H	1.61	0.66
1:A:173:ARG:NH2	1:A:174:VAL:O	2.29	0.66
1:A:288:ARG:HG2	3:A:625:HOH:O	1.97	0.64
3:A:619:HOH:O	1:B:195:ALA:HB1	1.98	0.63
1:A:244:PHE:O	3:A:603:HOH:O	2.15	0.63
1:A:285:ASN:HD21	1:A:318:ARG:HH12	1.49	0.60
1:B:183:GLU:CD	1:B:382:ARG:HH22	2.05	0.60
1:B:327:TYR:O	1:B:331:MET:HG2	2.02	0.60
1:B:324:HIS:ND1	3:B:611:HOH:O	2.32	0.59
1:B:135:ALA:N	3:B:604:HOH:O	2.17	0.58
1:A:212:GLN:HG2	1:A:395:HIS:NE2	2.19	0.58
1:B:247:ASP:O	1:B:248:ASP:HB2	2.03	0.57
1:A:101:GLU:OE1	3:A:604:HOH:O	2.18	0.57
1:B:243:LYS:HE2	1:B:245:HIS:HD2	1.69	0.56
1:B:95:LYS:HE3	1:B:128:ASP:HB2	1.89	0.55
1:B:297:HIS:NE2	3:B:605:HOH:O	2.17	0.55
1:A:85:CYS:SG	1:A:182:PHE:HB2	2.46	0.55
1:B:264:TYR:CE2	2:B:500:CYC:HBB1	2.43	0.54
2:B:500:CYC:NA	3:B:611:HOH:O	2.33	0.54
1:B:183:GLU:OE1	1:B:382:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:MET:HG2	3:B:649:HOH:O	2.08	0.53
1:B:318:ARG:HA	3:B:623:HOH:O	2.09	0.53
1:B:342:VAL:HG12	3:B:644:HOH:O	2.08	0.53
1:A:84:GLY:O	1:A:102:ASN:ND2	2.39	0.53
1:B:208:ILE:O	1:B:212:GLN:HG2	2.09	0.53
1:B:231:PHE:HD1	1:B:239:VAL:HG23	1.73	0.52
1:A:258:LYS:NZ	3:A:612:HOH:O	2.42	0.52
1:A:274:ILE:HD11	2:A:500:CYC:HMA3	1.91	0.52
1:A:273:ASP:HB3	2:A:500:CYC:HHB	1.93	0.51
1:B:208:ILE:HG13	1:B:388:LEU:HD13	1.92	0.51
1:A:177:SER:OG	1:A:178:MET:N	2.44	0.50
1:B:130:LYS:HG3	3:B:663:HOH:O	2.11	0.50
1:A:208:ILE:HD13	1:A:391:VAL:HG21	1.94	0.50
1:B:273:ASP:HB3	2:B:500:CYC:HHB	1.94	0.49
1:A:191:PRO:HG3	3:B:645:HOH:O	2.12	0.49
1:B:238:ARG:HG3	1:B:257:THR:HG22	1.95	0.49
1:B:189:GLU:O	1:B:193:THR:HG23	2.13	0.48
1:B:258:LYS:HA	1:B:258:LYS:HE2	1.95	0.48
1:B:212:GLN:HA	1:B:395:HIS:HE1	1.79	0.48
1:B:397:ASN:HA	1:B:400:ILE:HD12	1.95	0.48
1:A:331:MET:HE1	2:A:500:CYC:HMB2	1.96	0.48
1:A:97:ILE:HD11	1:A:177:SER:HB2	1.96	0.47
1:A:125:ILE:HG21	1:A:303:ASP:HB2	1.95	0.47
1:A:181:ASP:OD2	1:A:316:THR:N	2.42	0.47
1:B:204:ALA:HB2	1:B:384:ALA:HB1	1.96	0.47
1:B:147:PHE:HD2	1:B:151:LEU:HB3	1.81	0.46
1:B:152:LEU:HD21	3:B:670:HOH:O	2.16	0.46
1:A:104:PRO:O	1:A:108:THR:OG1	2.26	0.45
1:A:285:ASN:ND2	1:A:318:ARG:HH12	2.14	0.45
1:B:285:ASN:O	1:B:287:VAL:N	2.48	0.45
1:B:212:GLN:HG2	1:B:212:GLN:H	1.53	0.45
1:B:245:HIS:ND1	1:B:249:HIS:CE1	2.85	0.45
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.73	0.45
1:B:94:CYS:SG	1:B:145:LEU:HD11	2.56	0.45
1:B:89:LEU:HD23	1:B:96:VAL:HA	1.98	0.44
1:B:285:ASN:HD21	1:B:318:ARG:NH2	2.04	0.44
1:A:254:ALA:HA	3:A:605:HOH:O	2.16	0.44
1:A:281:LEU:HA	1:A:281:LEU:HD23	1.84	0.44
1:B:396:VAL:O	1:B:400:ILE:HG13	2.18	0.44
1:A:236:TYR:CD2	1:A:371:ASN:HB2	2.52	0.44
1:B:87:LEU:HD12	1:B:182:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ALA:HA	1:B:366:LEU:HD23	2.00	0.44
1:A:306:LEU:HA	1:A:307:PRO:HD3	1.87	0.44
1:B:288:ARG:HD3	1:B:289:MET:N	2.33	0.43
1:A:247:ASP:O	1:A:248:ASP:HB2	2.18	0.43
1:B:80:ILE:HG22	3:B:623:HOH:O	2.18	0.43
1:B:344:ASN:O	1:B:361:LYS:HE2	2.17	0.43
1:A:240:MET:HE3	1:A:240:MET:HB3	1.85	0.43
1:B:181:ASP:OD2	1:B:316:THR:OG1	2.29	0.43
1:A:242:TYR:HE2	2:A:500:CYC:O2A	2.02	0.43
1:B:145:LEU:HA	1:B:173:ARG:NH2	2.34	0.43
1:A:195:ALA:HB1	1:B:153:LEU:HB3	2.00	0.43
1:B:236:TYR:CB	1:B:369:CYS:HB3	2.49	0.42
1:A:94:CYS:SG	1:A:145:LEU:HD13	2.59	0.42
1:B:108:THR:HG22	1:B:132:LEU:HD22	2.01	0.42
1:B:104:PRO:HD2	3:B:619:HOH:O	2.18	0.42
1:A:293:CYS:SG	1:A:334:ILE:HA	2.60	0.42
1:B:281:LEU:HB3	1:B:318:ARG:NH2	2.34	0.42
1:A:306:LEU:HD12	1:A:307:PRO:CD	2.50	0.42
1:A:328:MET:HG2	3:A:653:HOH:O	2.19	0.42
1:B:243:LYS:HE2	1:B:245:HIS:CD2	2.52	0.42
1:A:89:LEU:HD11	1:A:180:ILE:HD11	2.01	0.41
1:A:190:VAL:O	1:A:193:THR:HG23	2.20	0.41
1:A:199:GLN:HG2	1:B:153:LEU:HD21	2.02	0.41
1:B:221:ARG:O	1:B:225:THR:OG1	2.35	0.41
1:A:91:GLU:O	1:A:145:LEU:HD11	2.20	0.41
2:A:500:CYC:HC	2:A:500:CYC:HD	1.69	0.41
1:A:157:LEU:HD11	1:A:166:PRO:HB2	2.03	0.41
1:B:256:ILE:HG13	1:B:257:THR:N	2.36	0.41
1:A:340:ALA:HA	1:A:366:LEU:HD23	2.03	0.41
1:B:106:MET:CE	1:B:167:PHE:HE2	2.34	0.41
1:B:288:ARG:HD3	1:B:288:ARG:C	2.42	0.41
1:B:307:PRO:HG2	1:B:308:PHE:CD2	2.56	0.41
1:B:123:LEU:HD13	1:B:132:LEU:HD11	2.04	0.40
1:B:236:TYR:CG	1:B:369:CYS:HB3	2.56	0.40
1:B:245:HIS:ND1	1:B:249:HIS:HE1	2.18	0.40
1:A:291:VAL:HB	3:A:618:HOH:O	2.21	0.40
1:A:383:TYR:CD2	1:B:198:LEU:HD13	2.57	0.40
1:A:238:ARG:NH2	1:A:261:LEU:HD12	2.36	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	289/359 (80%)	280 (97%)	8 (3%)	1 (0%)	41 46
1	B	293/359 (82%)	277 (94%)	11 (4%)	5 (2%)	9 6
All	All	582/718 (81%)	557 (96%)	19 (3%)	6 (1%)	15 14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	286	LYS
1	B	252	VAL
1	B	175	THR
1	B	248	ASP
1	B	166	PRO
1	A	125	ILE

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	254/307 (83%)	245 (96%)	9 (4%)	36 46
1	B	256/307 (83%)	234 (91%)	22 (9%)	10 10
All	All	510/614 (83%)	479 (94%)	31 (6%)	18 21

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	CYS
1	A	123	LEU
1	A	139	SER
1	A	158	ILE
1	A	200	SER
1	A	201	TYR
1	A	240	MET
1	A	311	THR
1	A	361	LYS
1	B	79	MET
1	B	105	GLU
1	B	109	MET
1	B	131	THR
1	B	137	SER
1	B	142	GLN
1	B	173	ARG
1	B	186	LYS
1	B	201	TYR
1	B	211	LEU
1	B	212	GLN
1	B	221	ARG
1	B	278	SER
1	B	288	ARG
1	B	296	LYS
1	B	304	GLU
1	B	313	CYS
1	B	315	SER
1	B	323	CYS
1	B	337	LEU
1	B	339	MET
1	B	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	B	285	ASN
1	B	297	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	CYC	B	500	1	42,46,46	1.10	1 (2%)	50,67,67	1.08	3 (6%)
2	CYC	A	500	1	42,46,46	1.14	1 (2%)	50,67,67	1.13	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CYC	B	500	1	-	10/25/74/74	0/4/4/4
2	CYC	A	500	1	-	10/25/74/74	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	CYC	CHA-C1A	5.85	1.40	1.35
2	B	500	CYC	CHA-C1A	5.14	1.39	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	CYC	CMB-C2B-C1B	3.90	129.04	124.17
2	B	500	CYC	CMB-C2B-C1B	3.52	128.56	124.17
2	A	500	CYC	C1B-CHB-C4A	3.05	135.53	128.08
2	B	500	CYC	CHA-C1A-NA	-2.75	125.02	128.83
2	A	500	CYC	CHA-C1A-NA	-2.46	125.41	128.83
2	B	500	CYC	C2C-C3C-C4C	2.23	104.68	101.34
2	A	500	CYC	C2C-C3C-C4C	2.16	104.57	101.34

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	CYC	C3A-C4A-CHB-C1B
2	A	500	CYC	NB-C1B-CHB-C4A
2	A	500	CYC	C2B-C1B-CHB-C4A
2	A	500	CYC	C2C-C3C-CAC-CBC
2	A	500	CYC	C4C-C3C-CAC-CBC
2	B	500	CYC	C3A-C4A-CHB-C1B
2	B	500	CYC	NB-C1B-CHB-C4A
2	B	500	CYC	C2B-C1B-CHB-C4A
2	B	500	CYC	C2C-C3C-CAC-CBC
2	B	500	CYC	C4C-C3C-CAC-CBC
2	A	500	CYC	NA-C4A-CHB-C1B
2	B	500	CYC	NA-C4A-CHB-C1B
2	A	500	CYC	CAA-CBA-CGA-O1A
2	A	500	CYC	CAD-CBD-CGD-O1D
2	A	500	CYC	CAA-CBA-CGA-O2A
2	A	500	CYC	CAD-CBD-CGD-O2D
2	B	500	CYC	CAD-CBD-CGD-O2D
2	B	500	CYC	CAD-CBD-CGD-O1D
2	B	500	CYC	CAA-CBA-CGA-O2A
2	B	500	CYC	CAA-CBA-CGA-O1A

There are no ring outliers.

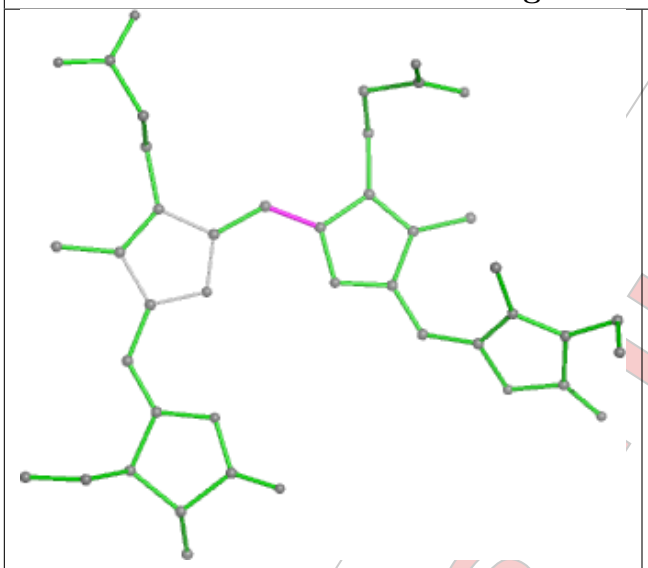
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	CYC	3	0
2	A	500	CYC	5	0

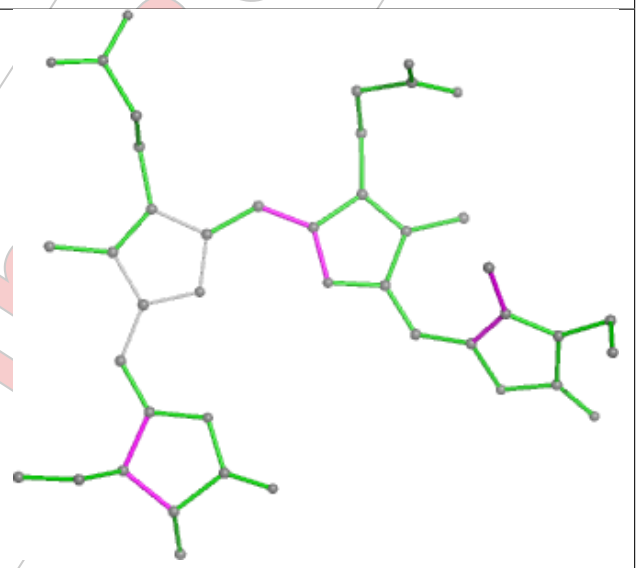
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

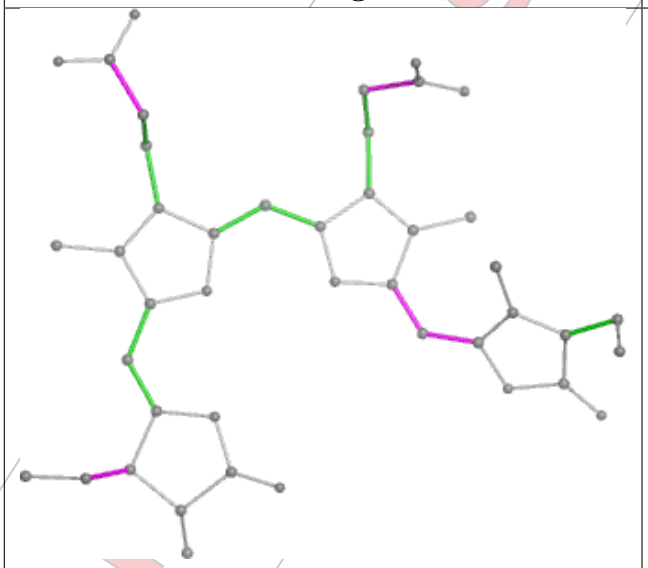
Ligand CYC B 500



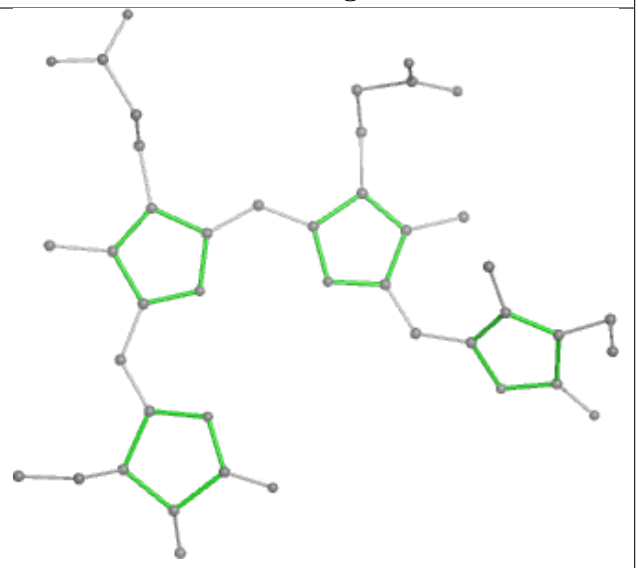
Bond lengths



Bond angles

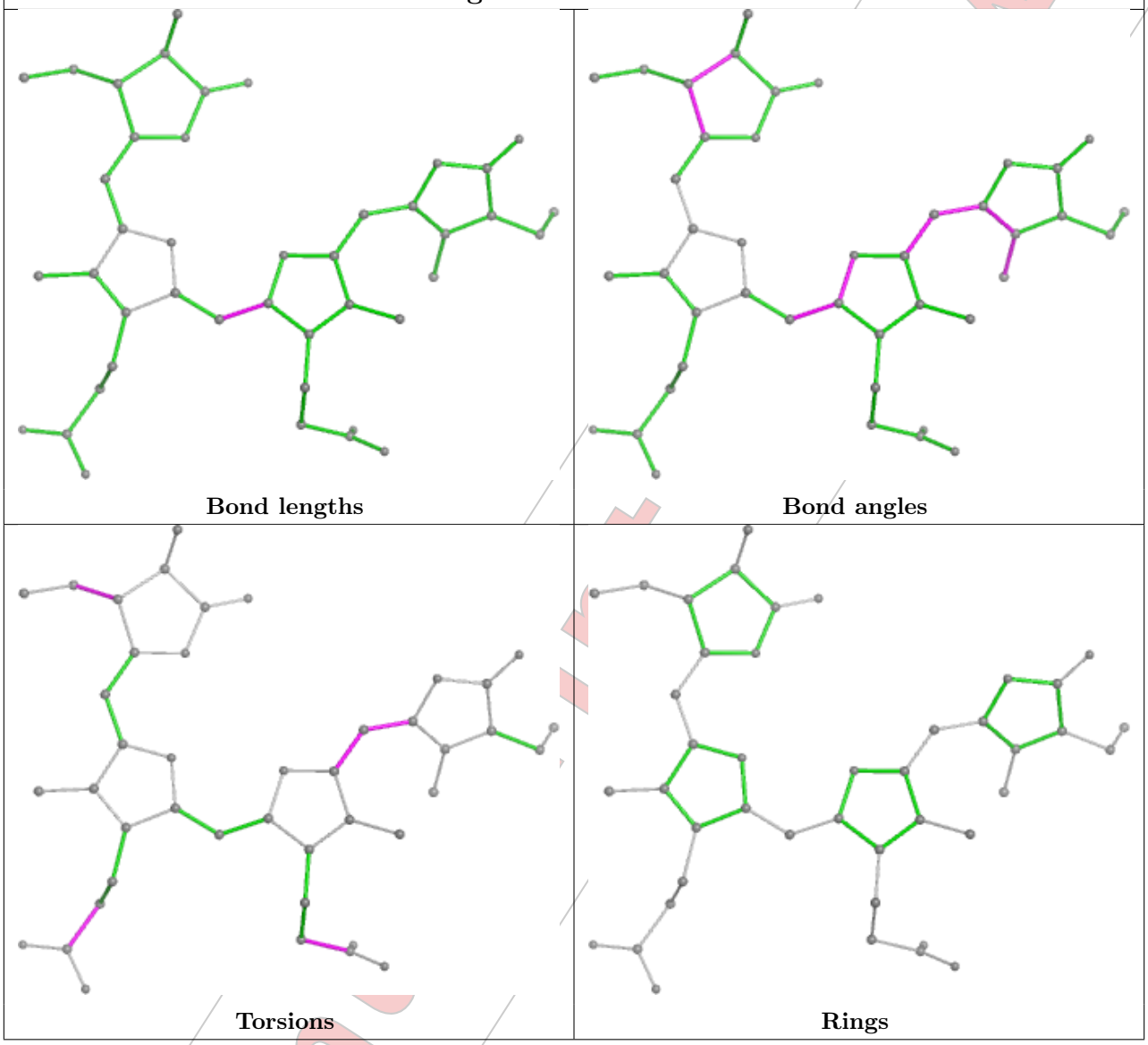


Torsions



Rings

Ligand CYC A 500



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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

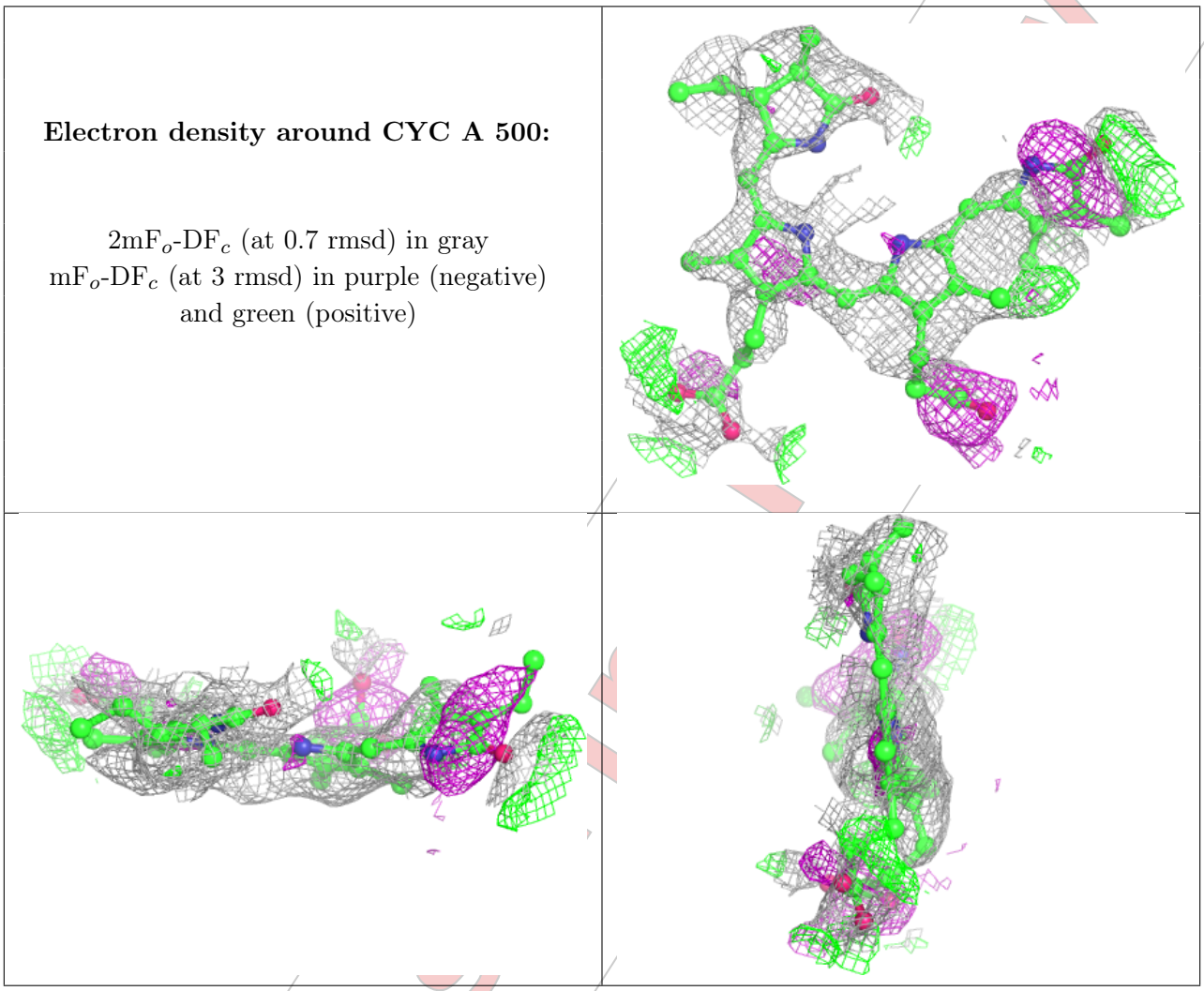
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

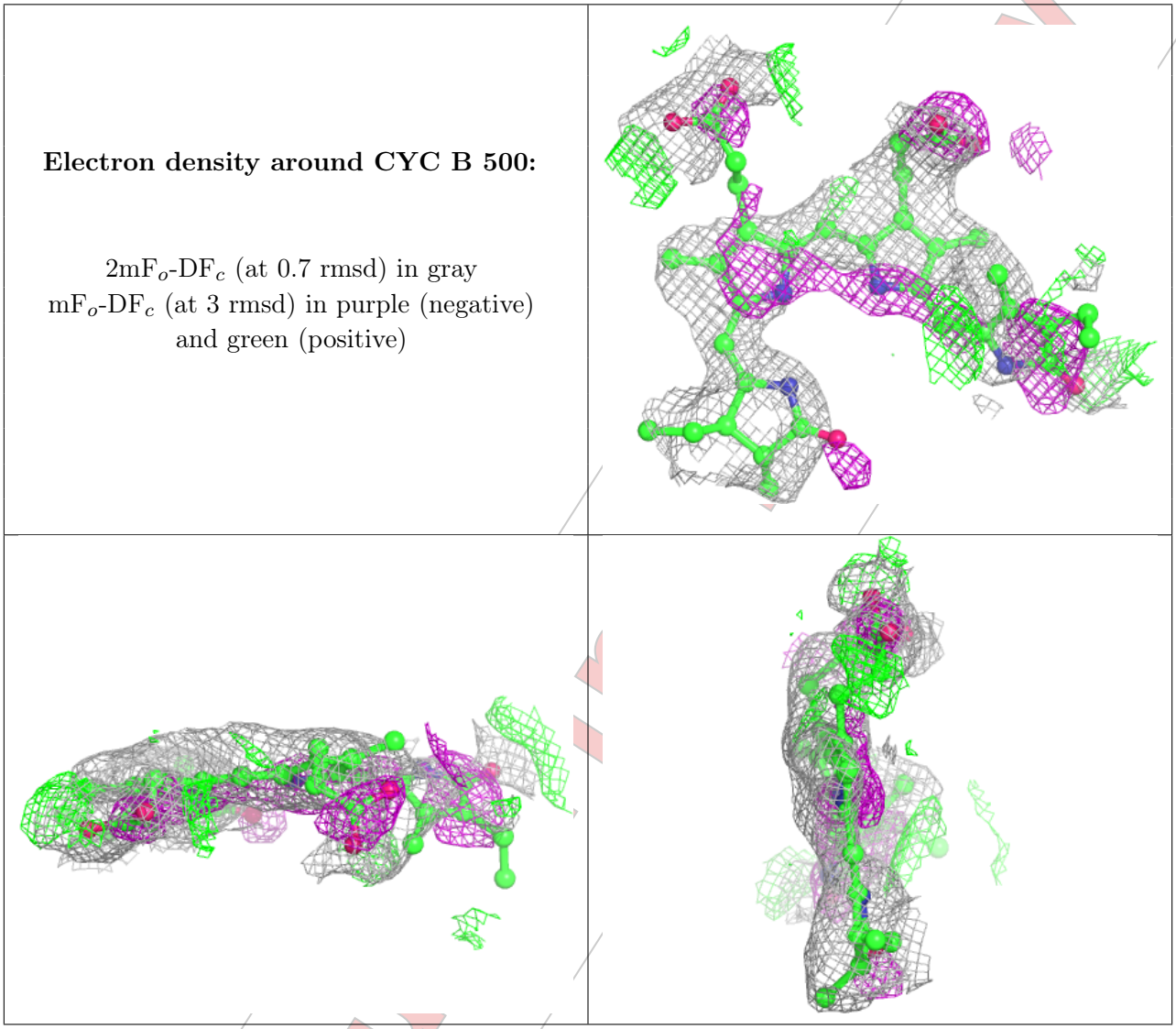
Electron density around CYC A 500:

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



Electron density around CYC B 500:

$2mF_o$-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

Unable to reproduce the depositors R factor - this section is therefore empty.