



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 12:45 PM JST

PDB ID : 9KA8 / pdb\_00009ka8  
Title : Structure of the recombinant structure of the subunit of allophycocyanin (APC) and the formate dehydrogenase (FDH)  
Authors : Duan, M.P.; Zhang, T.  
Deposited on : 2024-10-28  
Resolution : 2.19 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](mailto: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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

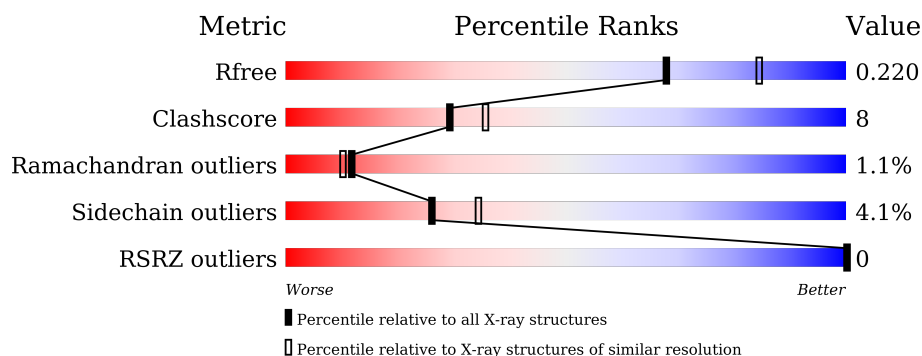
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.19 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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  $\geq 3$ , 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	355	 86% 13% .
1	B	355	 83% 15% .
2	C	160	 74% 11% . 11%
2	F	160	 76% 9% 6% 10%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8852 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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	355	Total	C	N	O	S	0	0	0
			2770	1767	474	522	7			
1	A	355	Total	C	N	O	S	0	0	0
			2770	1767	474	522	7			

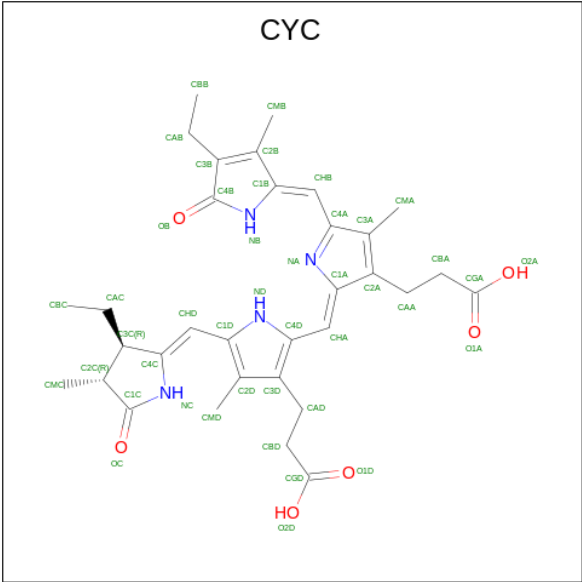
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	251	PRO	ALA	conflict	UNP A0A0A1EQY0
B	256	PRO	THR	conflict	UNP A0A0A1EQY0
B	354	VAL	ILE	conflict	UNP A0A0A1EQY0
A	251	PRO	ALA	conflict	UNP A0A0A1EQY0
A	256	PRO	THR	conflict	UNP A0A0A1EQY0
A	354	VAL	ILE	conflict	UNP A0A0A1EQY0

- Molecule 2 is a protein called Allophycocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	144	Total	C	N	O	S	0	0	0
			1079	673	182	216	8			
2	C	143	Total	C	N	O	S	0	0	0
			1071	667	181	215	8			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		

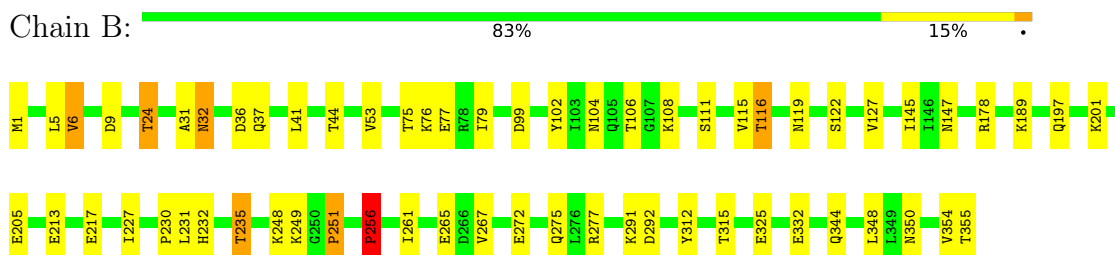
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	363	Total	O	0	0
			363	363		
4	F	171	Total	O	0	0
			171	171		
4	A	362	Total	O	0	0
			362	362		
4	C	180	Total	O	0	0
			180	180		

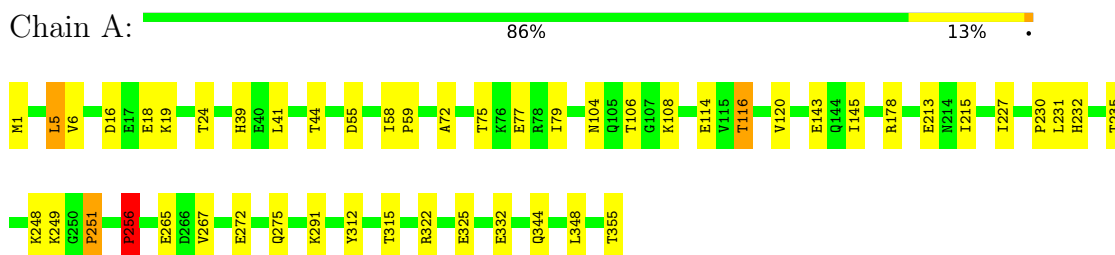
### 3 Residue-property plots [i](#)

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.

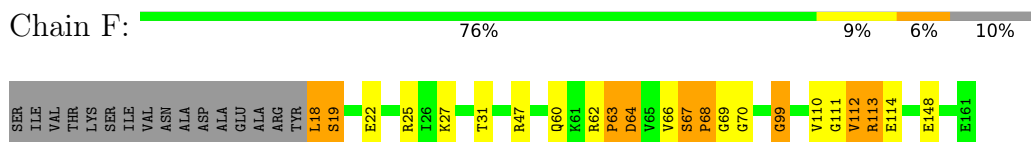
- Molecule 1: Formate dehydrogenase



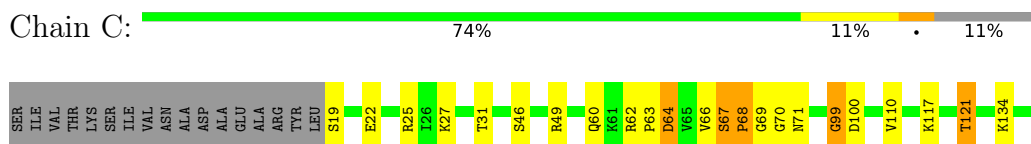
- Molecule 1: Formate dehydrogenase



- Molecule 2: Allophycocyanin



- Molecule 2: Allophycocyanin



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.78Å 189.78Å 153.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.40 – 2.19 29.40 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.40-2.19) 99.7 (29.40-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.188 , 0.217 0.189 , 0.220	Depositor DCC
$R_{free}$ test set	2003 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.47	1/2829 (0.0%)	0.59	2/3841 (0.1%)
1	B	0.48	1/2829 (0.0%)	0.59	0/3841
2	C	0.43	0/1085	0.64	0/1463
2	F	0.41	0/1093	0.62	0/1474
All	All	0.46	2/7836 (0.0%)	0.60	2/10619 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	F	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ILE	CG1-CD1	-5.21	1.31	1.51
1	B	145	ILE	CG1-CD1	-5.19	1.31	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ARG	CA-C-N	-6.90	109.22	122.06
1	A	322	ARG	C-N-CA	-6.90	109.22	122.06

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	64	ASP	Peptide
2	C	99	GLY	Peptide
2	F	64	ASP	Peptide
2	F	99	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2770	0	2776	42	0
1	B	2770	0	2776	52	0
2	C	1071	0	1060	18	0
2	F	1079	0	1071	22	0
3	C	43	0	37	0	0
3	F	43	0	37	0	0
4	A	362	0	0	17	1
4	B	363	0	0	28	3
4	C	180	0	0	7	0
4	F	171	0	0	8	1
All	All	8852	0	7757	132	3

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 8.

All (132) 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:272:GLU:OE1	4:A:401:HOH:O	1.68	1.09
1:B:178:ARG:NH1	4:B:403:HOH:O	2.00	0.94
1:B:31:ALA:O	4:B:401:HOH:O	1.88	0.91
1:B:291:LYS:HD2	1:B:291:LYS:H	1.34	0.91
1:B:36:ASP:OD1	4:B:402:HOH:O	1.89	0.90
1:A:291:LYS:NZ	4:A:404:HOH:O	2.08	0.85
1:A:325:GLU:OE1	4:A:402:HOH:O	1.96	0.84
1:A:332:GLU:OE2	4:A:403:HOH:O	1.99	0.80
1:B:291:LYS:NZ	4:B:409:HOH:O	2.16	0.79
1:A:232:HIS:H	1:A:235:THR:HG22	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:O	1:B:251:PRO:HD3	1.86	0.74
1:B:104:ASN:ND2	4:B:412:HOH:O	2.18	0.74
1:A:291:LYS:HD2	1:A:291:LYS:H	1.54	0.73
1:B:1:MET:SD	4:B:622:HOH:O	2.45	0.73
2:F:18:LEU:N	4:F:303:HOH:O	2.21	0.72
2:F:148:GLU:OE1	4:F:301:HOH:O	2.08	0.72
2:C:22:GLU:OE1	4:C:301:HOH:O	2.07	0.72
1:B:332:GLU:OE2	4:B:404:HOH:O	2.07	0.71
1:B:106:THR:HG21	1:B:108:LYS:HE2	1.72	0.70
1:B:217:GLU:OE2	4:B:405:HOH:O	2.09	0.70
1:A:248:LYS:O	1:A:251:PRO:HD3	1.90	0.70
1:A:106:THR:HG21	1:A:108:LYS:HE2	1.74	0.69
1:A:18:GLU:OE1	4:A:405:HOH:O	2.11	0.68
1:B:147:ASN:OD1	4:B:406:HOH:O	2.10	0.68
1:A:230:PRO:O	1:A:235:THR:HG21	1.94	0.67
2:C:62:ARG:O	2:C:64:ASP:N	2.27	0.67
1:A:272:GLU:OE2	4:A:406:HOH:O	2.14	0.66
1:B:99:ASP:OD2	4:B:407:HOH:O	2.13	0.66
1:A:6:VAL:HG21	1:A:72:ALA:HB2	1.79	0.64
1:A:16:ASP:OD1	4:A:407:HOH:O	2.15	0.64
1:A:19:LYS:NZ	4:A:408:HOH:O	2.19	0.64
1:A:104:ASN:ND2	4:A:418:HOH:O	2.31	0.64
2:C:49:ARG:NH1	4:C:302:HOH:O	2.20	0.64
1:B:232:HIS:HB2	2:F:111:GLY:HA3	1.79	0.64
2:F:25:ARG:HD2	2:F:99:GLY:HA3	1.80	0.64
1:A:291:LYS:NZ	4:A:420:HOH:O	2.31	0.63
2:F:60:GLN:NE2	4:F:305:HOH:O	2.27	0.63
1:B:272:GLU:OE2	4:B:408:HOH:O	2.16	0.61
1:A:5:LEU:HD22	1:A:41:LEU:HD11	1.83	0.60
1:B:189:LYS:NZ	4:B:419:HOH:O	2.28	0.60
1:B:275:GLN:OE1	4:B:410:HOH:O	2.16	0.60
2:C:60:GLN:NE2	4:C:306:HOH:O	2.34	0.60
1:B:230:PRO:O	1:B:235:THR:HG21	2.01	0.60
1:B:53:VAL:HG23	4:B:411:HOH:O	2.01	0.59
1:B:235:THR:HG23	1:B:261:ILE:HG12	1.85	0.58
1:B:312:TYR:O	1:B:315:THR:HG22	2.04	0.57
2:F:114:GLU:HB2	4:F:409:HOH:O	2.04	0.57
1:A:291:LYS:H	1:A:291:LYS:CD	2.17	0.56
2:F:64:ASP:O	4:F:302:HOH:O	2.18	0.55
1:A:249:LYS:NZ	4:A:422:HOH:O	2.38	0.55
2:F:62:ARG:O	2:F:64:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:H	1:A:77:GLU:CD	2.14	0.55
1:B:232:HIS:CB	2:F:111:GLY:HA3	2.38	0.54
2:C:25:ARG:HD2	2:C:99:GLY:HA3	1.89	0.54
1:B:249:LYS:NZ	4:B:425:HOH:O	2.41	0.54
2:F:66:VAL:HG23	2:F:68:PRO:HD2	1.90	0.53
2:F:63:PRO:O	2:F:66:VAL:HG13	2.07	0.53
1:A:116:THR:HG21	1:A:344:GLN:O	2.08	0.53
1:B:178:ARG:NH2	4:B:423:HOH:O	2.40	0.53
1:B:325:GLU:OE1	4:B:413:HOH:O	2.19	0.53
1:A:1:MET:HB2	1:A:39:HIS:ND1	2.23	0.53
1:A:213:GLU:OE2	4:A:409:HOH:O	2.19	0.53
1:B:9:ASP:OD1	1:B:24:THR:HG21	2.09	0.52
1:B:77:GLU:OE1	1:B:77:GLU:N	2.37	0.52
2:C:64:ASP:HB2	4:C:401:HOH:O	2.08	0.52
2:F:27:LYS:HE2	4:F:364:HOH:O	2.09	0.52
2:F:25:ARG:CD	2:F:99:GLY:HA3	2.39	0.52
1:B:5:LEU:CD2	1:B:41:LEU:HD11	2.40	0.52
2:F:68:PRO:O	2:F:69:GLY:C	2.53	0.51
1:A:312:TYR:O	1:A:315:THR:HG22	2.10	0.51
2:F:19:SER:OG	2:F:22:GLU:HG3	2.10	0.51
2:C:71:ASN:OD1	2:C:121:THR:HB	2.10	0.51
2:C:134:LYS:O	2:C:138:THR:HB	2.11	0.51
1:B:77:GLU:H	1:B:77:GLU:CD	2.18	0.51
1:B:256:PRO:HG2	4:B:452:HOH:O	2.11	0.50
1:A:251:PRO:HD2	1:A:275:GLN:O	2.12	0.50
1:B:251:PRO:HD2	1:B:275:GLN:O	2.11	0.50
1:B:231:LEU:HA	1:B:235:THR:HG21	1.93	0.50
1:B:119:ASN:ND2	4:B:427:HOH:O	2.44	0.50
1:A:19:LYS:NZ	4:A:410:HOH:O	2.20	0.49
1:A:256:PRO:HG2	4:A:462:HOH:O	2.13	0.49
1:A:55:ASP:HA	1:A:58:ILE:HG22	1.94	0.49
1:B:292:ASP:OD2	4:B:414:HOH:O	2.19	0.48
1:A:77:GLU:OE2	1:A:77:GLU:N	2.40	0.48
2:F:110:VAL:HG13	2:F:111:GLY:H	1.78	0.48
1:B:53:VAL:N	4:B:411:HOH:O	2.17	0.48
1:B:277:ARG:NH2	4:B:428:HOH:O	2.45	0.48
1:A:5:LEU:CD2	1:A:41:LEU:HD11	2.44	0.48
1:B:116:THR:HG21	1:B:344:GLN:O	2.13	0.47
1:B:291:LYS:H	1:B:291:LYS:CD	2.10	0.47
2:C:68:PRO:O	2:C:69:GLY:C	2.57	0.47
2:C:117:LYS:NZ	4:C:310:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:THR:HG21	4:C:438:HOH:O	2.14	0.47
1:A:114:GLU:HG3	1:A:116:THR:HG22	1.98	0.46
2:F:112:VAL:O	2:F:113:ARG:CB	2.63	0.46
1:A:231:LEU:HA	1:A:235:THR:CG2	2.46	0.46
1:B:213:GLU:OE1	4:B:416:HOH:O	2.21	0.46
1:A:120:VAL:HG12	1:A:178:ARG:HD2	1.96	0.46
1:B:37:GLN:OE1	4:B:415:HOH:O	2.21	0.45
1:A:143:GLU:HG2	4:A:667:HOH:O	2.16	0.45
2:C:67:SER:O	2:C:68:PRO:O	2.35	0.45
2:C:25:ARG:HD2	2:C:99:GLY:CA	2.48	0.44
2:C:66:VAL:C	2:C:68:PRO:HD2	2.42	0.44
2:C:64:ASP:HA	2:C:66:VAL:HG22	1.99	0.44
2:C:100:ASP:OD1	4:C:303:HOH:O	2.21	0.44
4:B:661:HOH:O	2:C:27:LYS:HD3	2.18	0.44
1:A:232:HIS:H	1:A:235:THR:CG2	2.27	0.44
1:B:75:THR:O	1:B:79:ILE:HG13	2.16	0.44
1:B:111:SER:HB3	1:B:350:ASN:H	1.82	0.44
1:B:127:VAL:CG2	1:B:256:PRO:HG3	2.48	0.44
1:B:227:ILE:O	1:B:256:PRO:HD2	2.18	0.44
1:A:6:VAL:HA	1:A:44:THR:O	2.18	0.44
2:F:64:ASP:HB2	4:F:302:HOH:O	2.17	0.43
1:B:31:ALA:O	1:B:32:ASN:HB2	2.18	0.43
2:C:67:SER:N	2:C:68:PRO:HD2	2.33	0.43
1:B:201:LYS:HE3	1:B:205:GLU:OE2	2.19	0.43
1:B:292:ASP:HA	4:B:566:HOH:O	2.18	0.43
2:F:62:ARG:C	2:F:64:ASP:H	2.27	0.43
1:B:231:LEU:HA	1:B:235:THR:CG2	2.49	0.43
1:A:75:THR:O	1:A:79:ILE:HG13	2.19	0.43
2:F:27:LYS:HD3	4:A:649:HOH:O	2.18	0.43
1:A:231:LEU:HA	1:A:235:THR:HG21	2.00	0.43
1:A:265:GLU:HG3	4:A:469:HOH:O	2.18	0.43
1:A:120:VAL:CG1	1:A:178:ARG:HD2	2.50	0.42
1:B:76:LYS:HD2	1:B:102:TYR:CE1	2.55	0.42
2:F:114:GLU:CB	4:F:409:HOH:O	2.67	0.42
1:A:58:ILE:HG23	1:A:59:PRO:HD3	2.03	0.41
2:F:67:SER:O	2:F:68:PRO:O	2.39	0.41
1:B:6:VAL:HA	1:B:44:THR:O	2.19	0.40
1:B:265:GLU:HG3	4:B:487:HOH:O	2.22	0.40
1:A:227:ILE:O	1:A:256:PRO:HD2	2.21	0.40
1:B:197:GLN:HB3	4:B:422:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:750:HOH:O	4:F:449:HOH:O[3_555]	1.81	0.39
4:B:670:HOH:O	4:B:730:HOH:O[3_555]	2.11	0.09
4:B:440:HOH:O	4:A:608:HOH:O[5_445]	2.19	0.01

## 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	353/355 (99%)	339 (96%)	13 (4%)	1 (0%)	37	42
1	B	353/355 (99%)	338 (96%)	13 (4%)	2 (1%)	22	23
2	C	141/160 (88%)	134 (95%)	3 (2%)	4 (3%)	4	2
2	F	142/160 (89%)	131 (92%)	7 (5%)	4 (3%)	4	2
All	All	989/1030 (96%)	942 (95%)	36 (4%)	11 (1%)	12	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	32	ASN
2	F	68	PRO
2	F	113	ARG
2	C	68	PRO
2	C	110	VAL
2	F	70	GLY
2	C	70	GLY
2	F	63	PRO
1	A	256	PRO
1	B	256	PRO
2	C	63	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/292 (100%)	283 (97%)	9 (3%)	35	47
1	B	292/292 (100%)	280 (96%)	12 (4%)	26	34
2	C	110/124 (89%)	104 (94%)	6 (6%)	18	22
2	F	111/124 (90%)	105 (95%)	6 (5%)	18	23
All	All	805/832 (97%)	772 (96%)	33 (4%)	26	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	VAL
1	B	24	THR
1	B	115	VAL
1	B	116	THR
1	B	122	SER
1	B	235	THR
1	B	251	PRO
1	B	256	PRO
1	B	267	VAL
1	B	348	LEU
1	B	354	VAL
1	B	355	THR
2	F	18	LEU
2	F	19	SER
2	F	31	THR
2	F	47	ARG
2	F	67	SER
2	F	112	VAL
1	A	5	LEU
1	A	24	THR
1	A	116	THR
1	A	215	ILE
1	A	251	PRO
1	A	256	PRO

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Mol	Chain	Res	Type
1	A	267	VAL
1	A	348	LEU
1	A	355	THR
2	C	19	SER
2	C	31	THR
2	C	46	SER
2	C	67	SER
2	C	121	THR
2	C	138	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS
1	A	70	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 oligosaccharides 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
3	CYC	F	201	2	42,46,46	1.48	3 (7%)	50,67,67	1.16	3 (6%)
3	CYC	C	201	2	42,46,46	1.43	2 (4%)	50,67,67	1.23	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
3	CYC	F	201	2	-	6/25/74/74	0/4/4/4
3	CYC	C	201	2	-	8/25/74/74	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	CYC	CHA-C1A	7.11	1.41	1.35
3	C	201	CYC	CHA-C1A	7.09	1.41	1.35
3	F	201	CYC	CHB-C4A	2.81	1.47	1.40
3	C	201	CYC	CHB-C4A	2.67	1.46	1.40
3	F	201	CYC	C1B-C2B	2.02	1.48	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	CYC	C4D-CHA-C1A	3.61	133.13	128.81
3	F	201	CYC	C4D-CHA-C1A	3.45	132.93	128.81
3	F	201	CYC	CHA-C1A-NA	-3.12	124.50	128.83
3	C	201	CYC	CHA-C1A-NA	-2.81	124.92	128.83
3	C	201	CYC	C2C-C3C-C4C	2.60	105.23	101.34
3	F	201	CYC	C2C-C3C-C4C	2.41	104.95	101.34
3	C	201	CYC	OC-C1C-C2C	2.16	127.89	126.17

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	201	CYC	NA-C4A-CHB-C1B
3	F	201	CYC	C3A-C4A-CHB-C1B
3	F	201	CYC	ND-C1D-CHD-C4C
3	F	201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
3	C	201	CYC	NA-C4A-CHB-C1B
3	C	201	CYC	C3A-C4A-CHB-C1B
3	C	201	CYC	ND-C1D-CHD-C4C
3	C	201	CYC	C2D-C1D-CHD-C4C
3	C	201	CYC	C1A-C2A-CAA-CBA
3	C	201	CYC	C3A-C2A-CAA-CBA
3	C	201	CYC	CAA-CBA-CGA-O1A
3	C	201	CYC	CAA-CBA-CGA-O2A
3	F	201	CYC	C3A-C2A-CAA-CBA
3	F	201	CYC	C1A-C2A-CAA-CBA

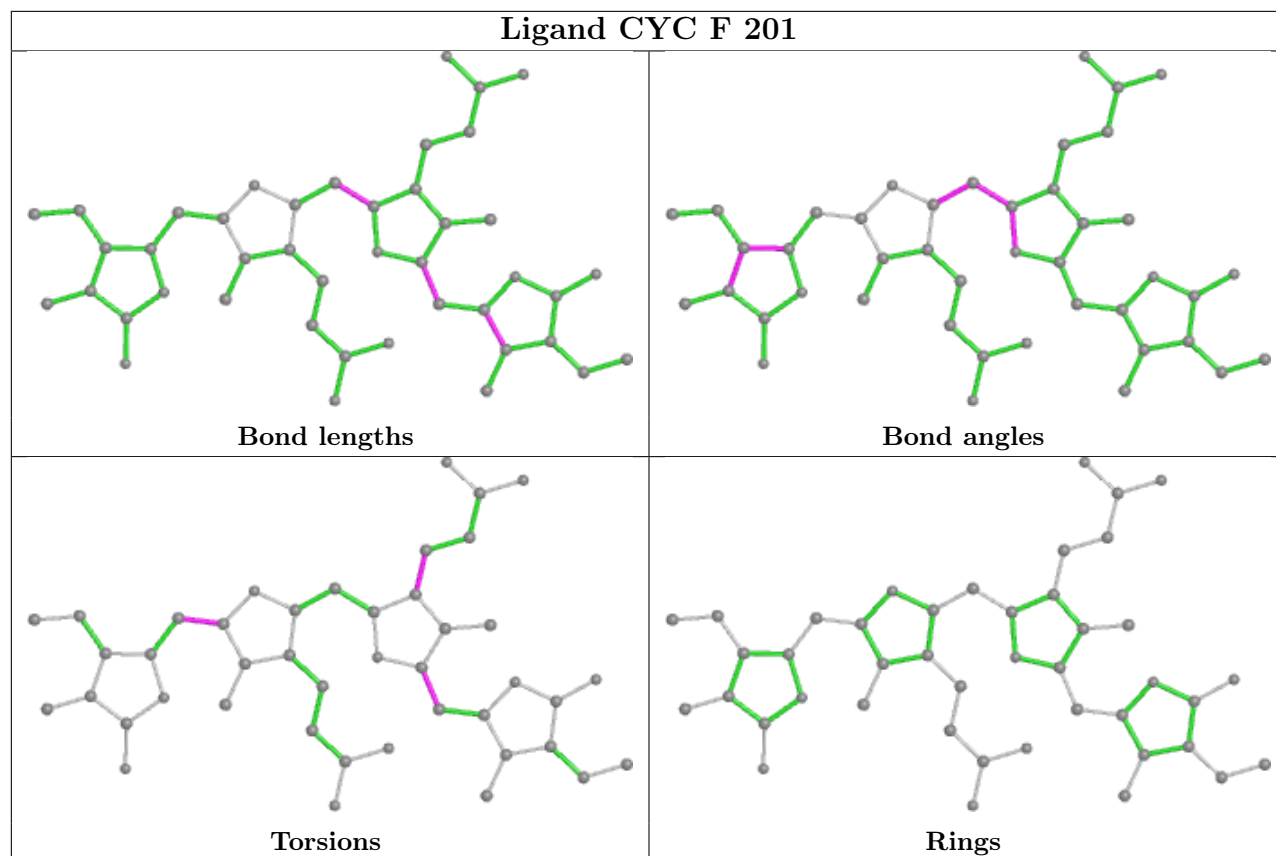
There are no ring outliers.

No monomer is involved in short contacts.

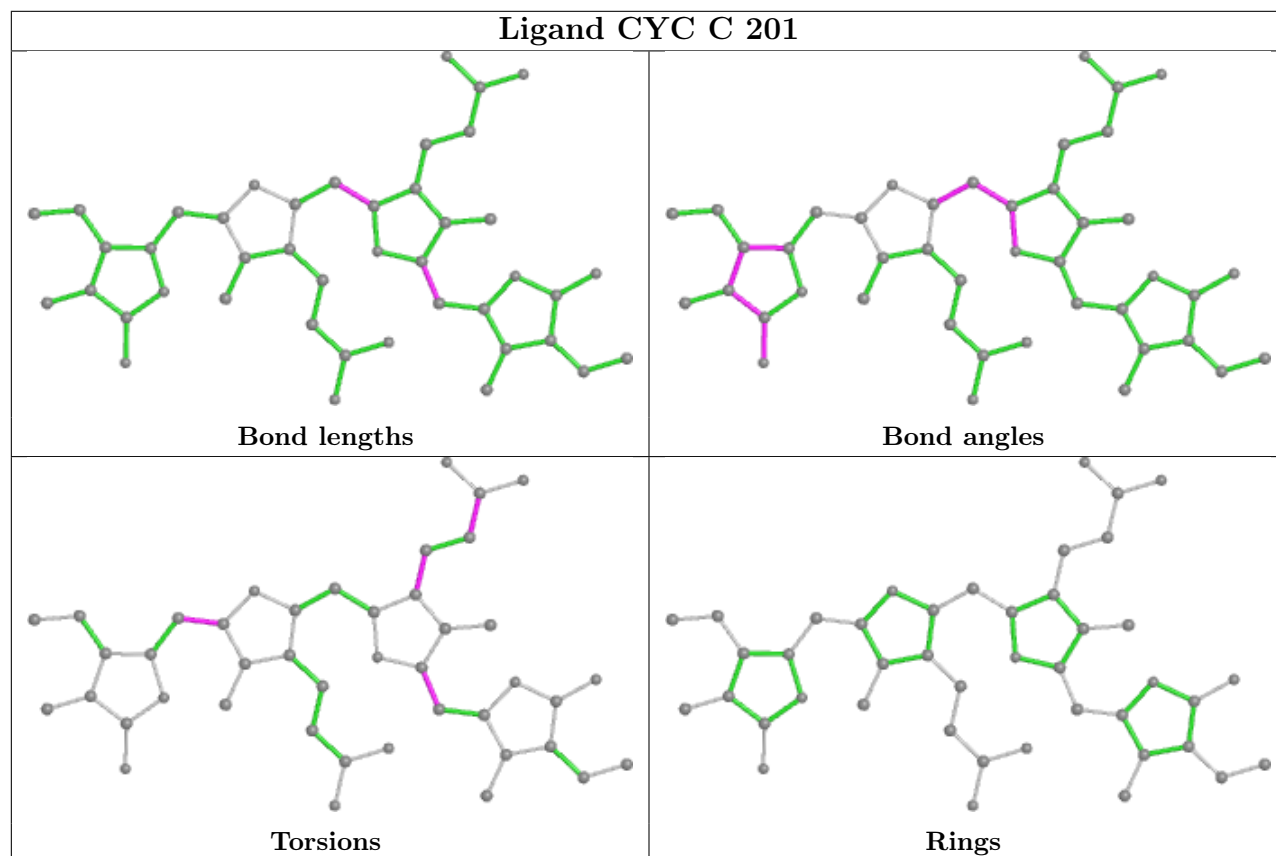
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand CYC F 201



## Ligand CYC C 201



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	355/355 (100%)	-1.61	0 100 100	23, 36, 62, 95	0
1	B	355/355 (100%)	-1.59	0 100 100	23, 36, 62, 94	0
2	C	143/160 (89%)	-1.58	0 100 100	29, 37, 48, 68	0
2	F	144/160 (90%)	-1.58	0 100 100	28, 37, 51, 69	0
All	All	997/1030 (96%)	-1.59	0 100 100	23, 37, 60, 95	0

There are no RSRZ outliers to report.

### 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.

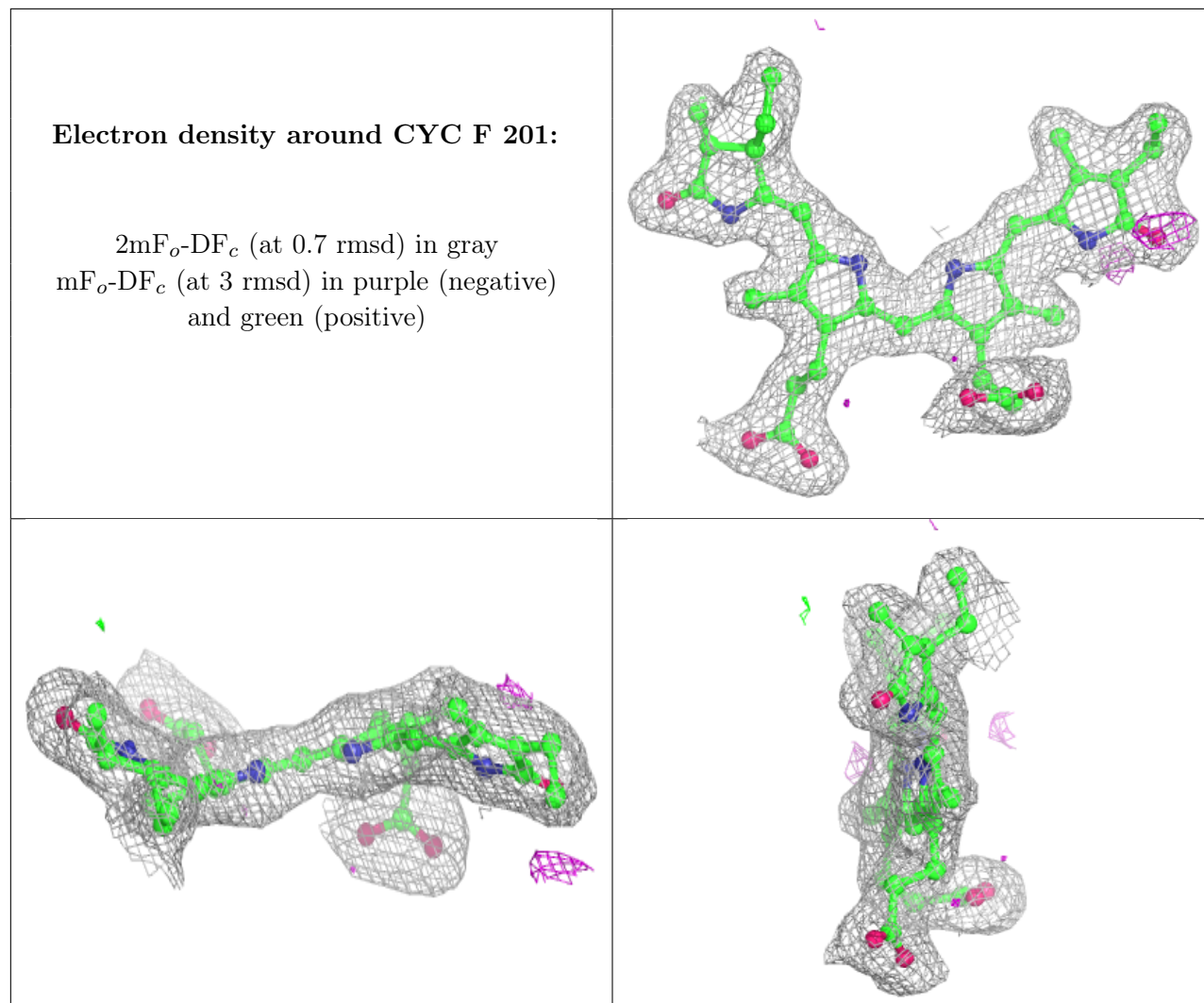
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CYC	F	201	43/43	0.99	0.03	27,32,38,40	0
3	CYC	C	201	43/43	0.99	0.03	27,31,38,41	0

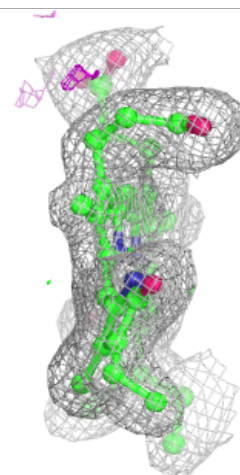
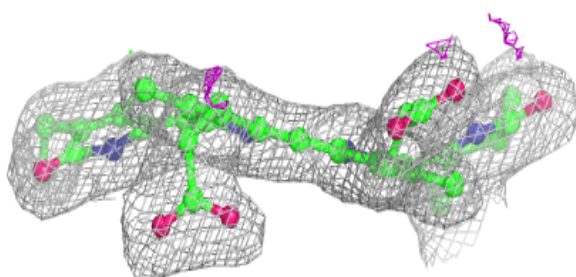
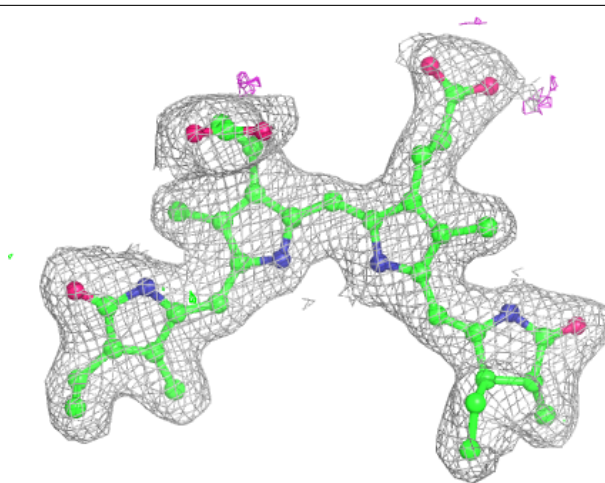
The following is a graphical depiction of the model fit to experimental electron density of all

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 CYC C 201:**

$2mF_o-DF_c$  (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.