



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2025 – 11:11 pm BST

PDB ID : 8S1L / pdb\_00008s1l  
Title : Crystal structure of Renilla reniformis luciferase RLuc8-GFP BRET complex at pH 6.0  
Authors : Marek, M.; Smrckova, A.  
Deposited on : 2024-02-15  
Resolution : 2.40 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](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 Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

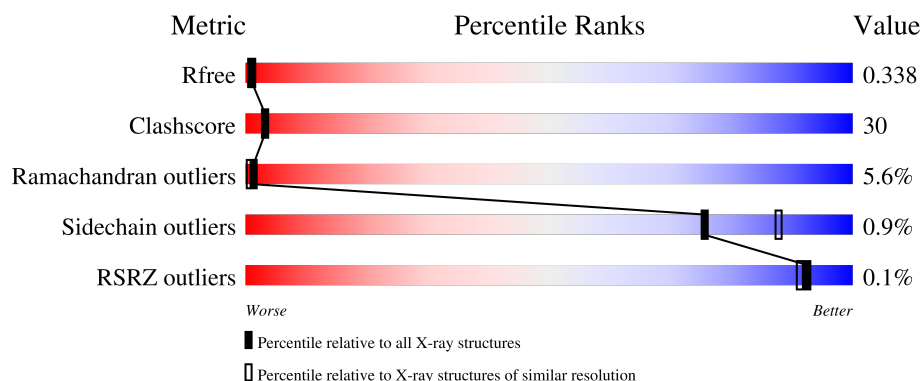
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	231	<div> <div style="width: 42%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div>
1	B	231	<div> <div style="width: 38%; background-color: green;"></div> <div style="width: 54%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div>
1	E	231	<div> <div style="width: 42%; background-color: green;"></div> <div style="width: 51%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div>
1	F	231	<div> <div style="width: 34%; background-color: green;"></div> <div style="width: 58%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div>
2	C	319	<div> <div style="width: 53%; background-color: green;"></div> <div style="width: 43%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	D	319	 49% 45% . .
2	G	319	 50% 44% . . .
2	H	319	 52% 43% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17772 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 Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1828	1171	301	346	10			
1	B	230	Total	C	N	O	S	0	0	0
			1820	1166	300	345	9			
1	E	231	Total	C	N	O	S	0	0	0
			1828	1171	301	346	10			
1	F	230	Total	C	N	O	S	0	0	0
			1820	1166	300	345	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CRO	SER	chromophore	UNP Q963I9
A	66	CRO	TYR	chromophore	UNP Q963I9
A	66	CRO	GLY	chromophore	UNP Q963I9
B	66	CRO	SER	chromophore	UNP Q963I9
B	66	CRO	TYR	chromophore	UNP Q963I9
B	66	CRO	GLY	chromophore	UNP Q963I9
E	66	CRO	SER	chromophore	UNP Q963I9
E	66	CRO	TYR	chromophore	UNP Q963I9
E	66	CRO	GLY	chromophore	UNP Q963I9
F	66	CRO	SER	chromophore	UNP Q963I9
F	66	CRO	TYR	chromophore	UNP Q963I9
F	66	CRO	GLY	chromophore	UNP Q963I9

- Molecule 2 is a protein called Coelenterazine h 2-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	316	Total	C	N	O	S	0	1	0
			2592	1677	433	473	9			
2	D	308	Total	C	N	O	S	0	1	0
			2532	1640	424	459	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	308	Total	C	N	O	S	0	1	0
			2532	1640	424	459	9			
2	H	318	Total	C	N	O	S	0	0	0
			2603	1686	435	473	9			

There are 64 discrepancies between the modelled and reference sequences:

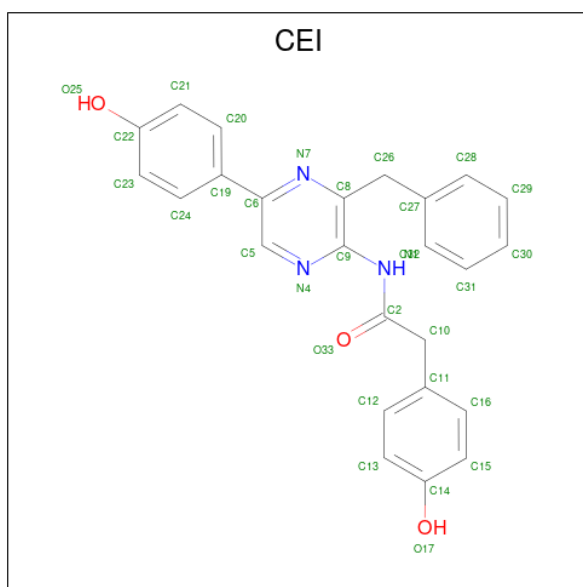
Chain	Residue	Modelled	Actual	Comment	Reference
C	55	THR	ALA	engineered mutation	UNP P27652
C	124	ALA	CYS	engineered mutation	UNP P27652
C	130	ALA	SER	engineered mutation	UNP P27652
C	136	ARG	LYS	engineered mutation	UNP P27652
C	143	MET	ALA	engineered mutation	UNP P27652
C	185	VAL	MET	engineered mutation	UNP P27652
C	253	LEU	MET	engineered mutation	UNP P27652
C	287	LEU	SER	engineered mutation	UNP P27652
C	312	SER	-	expression tag	UNP P27652
C	313	GLY	-	expression tag	UNP P27652
C	314	LEU	-	expression tag	UNP P27652
C	315	GLU	-	expression tag	UNP P27652
C	316	VAL	-	expression tag	UNP P27652
C	317	LEU	-	expression tag	UNP P27652
C	318	PHE	-	expression tag	UNP P27652
C	319	GLN	-	expression tag	UNP P27652
D	55	THR	ALA	engineered mutation	UNP P27652
D	124	ALA	CYS	engineered mutation	UNP P27652
D	130	ALA	SER	engineered mutation	UNP P27652
D	136	ARG	LYS	engineered mutation	UNP P27652
D	143	MET	ALA	engineered mutation	UNP P27652
D	185	VAL	MET	engineered mutation	UNP P27652
D	253	LEU	MET	engineered mutation	UNP P27652
D	287	LEU	SER	engineered mutation	UNP P27652
D	312	SER	-	expression tag	UNP P27652
D	313	GLY	-	expression tag	UNP P27652
D	314	LEU	-	expression tag	UNP P27652
D	315	GLU	-	expression tag	UNP P27652
D	316	VAL	-	expression tag	UNP P27652
D	317	LEU	-	expression tag	UNP P27652
D	318	PHE	-	expression tag	UNP P27652
D	319	GLN	-	expression tag	UNP P27652
G	55	THR	ALA	engineered mutation	UNP P27652
G	124	ALA	CYS	engineered mutation	UNP P27652

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Chain	Residue	Modelled	Actual	Comment	Reference
G	130	ALA	SER	engineered mutation	UNP P27652
G	136	ARG	LYS	engineered mutation	UNP P27652
G	143	MET	ALA	engineered mutation	UNP P27652
G	185	VAL	MET	engineered mutation	UNP P27652
G	253	LEU	MET	engineered mutation	UNP P27652
G	287	LEU	SER	engineered mutation	UNP P27652
G	312	SER	-	expression tag	UNP P27652
G	313	GLY	-	expression tag	UNP P27652
G	314	LEU	-	expression tag	UNP P27652
G	315	GLU	-	expression tag	UNP P27652
G	316	VAL	-	expression tag	UNP P27652
G	317	LEU	-	expression tag	UNP P27652
G	318	PHE	-	expression tag	UNP P27652
G	319	GLN	-	expression tag	UNP P27652
H	55	THR	ALA	engineered mutation	UNP P27652
H	124	ALA	CYS	engineered mutation	UNP P27652
H	130	ALA	SER	engineered mutation	UNP P27652
H	136	ARG	LYS	engineered mutation	UNP P27652
H	143	MET	ALA	engineered mutation	UNP P27652
H	185	VAL	MET	engineered mutation	UNP P27652
H	253	LEU	MET	engineered mutation	UNP P27652
H	287	LEU	SER	engineered mutation	UNP P27652
H	312	SER	-	expression tag	UNP P27652
H	313	GLY	-	expression tag	UNP P27652
H	314	LEU	-	expression tag	UNP P27652
H	315	GLU	-	expression tag	UNP P27652
H	316	VAL	-	expression tag	UNP P27652
H	317	LEU	-	expression tag	UNP P27652
H	318	PHE	-	expression tag	UNP P27652
H	319	GLN	-	expression tag	UNP P27652

- Molecule 3 is N-[3-BENZYL-5-(4-HYDROXYPHENYL)PYRAZIN-2-YL]-2-(4-HYDROXYPHENYL)ACETAMIDE (CCD ID: CEI) (formula: C<sub>25</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			31	25	3	3		
3	D	1	Total	C	N	O	0	0
			31	25	3	3		
3	G	1	Total	C	N	O	0	0
			31	25	3	3		
3	H	1	Total	C	N	O	0	0
			31	25	3	3		

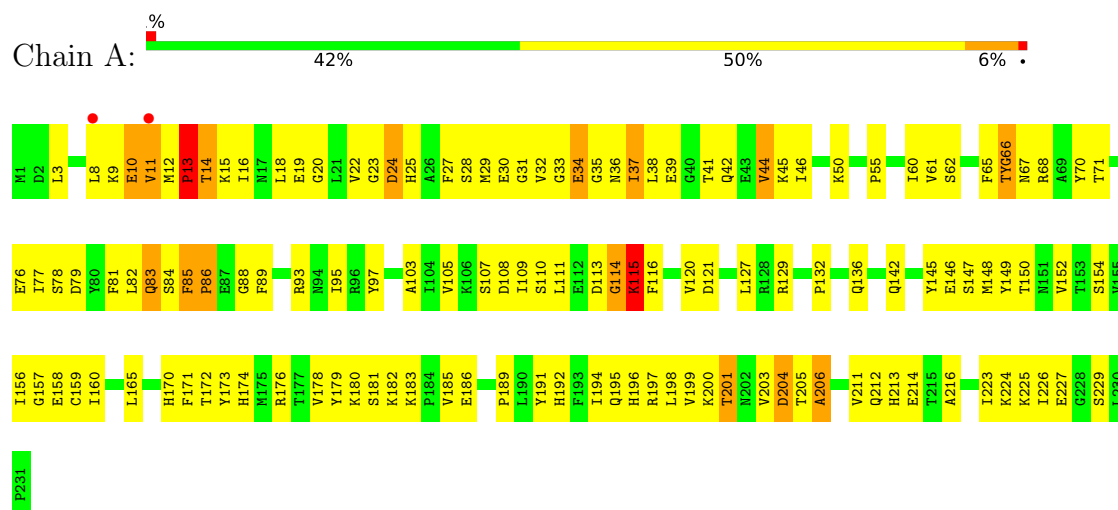
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	10	Total	O	0	0
			10	10		
4	C	23	Total	O	0	0
			23	23		
4	D	12	Total	O	0	0
			12	12		
4	E	3	Total	O	0	0
			3	3		
4	F	6	Total	O	0	0
			6	6		
4	G	11	Total	O	0	0
			11	11		
4	H	21	Total	O	0	0
			21	21		

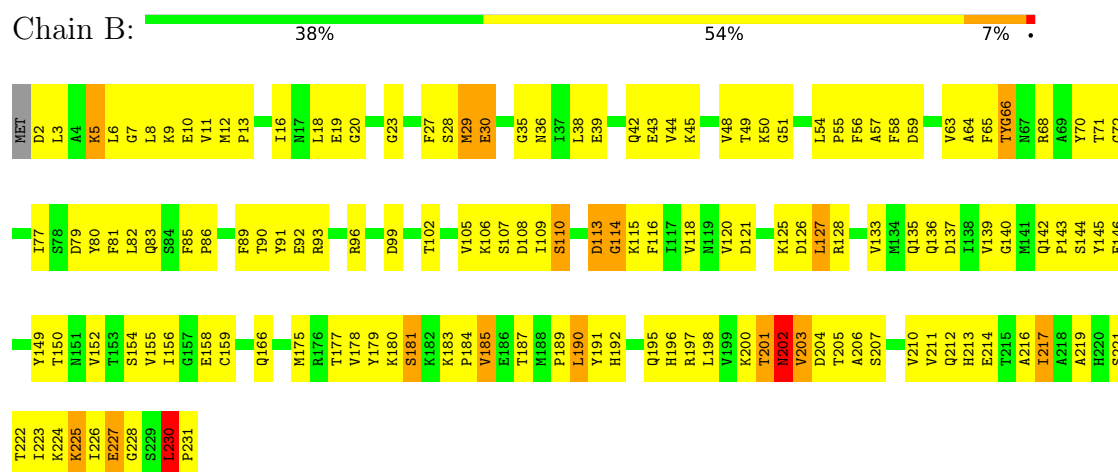
### 3 Residue-property plots

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: Green fluorescent protein



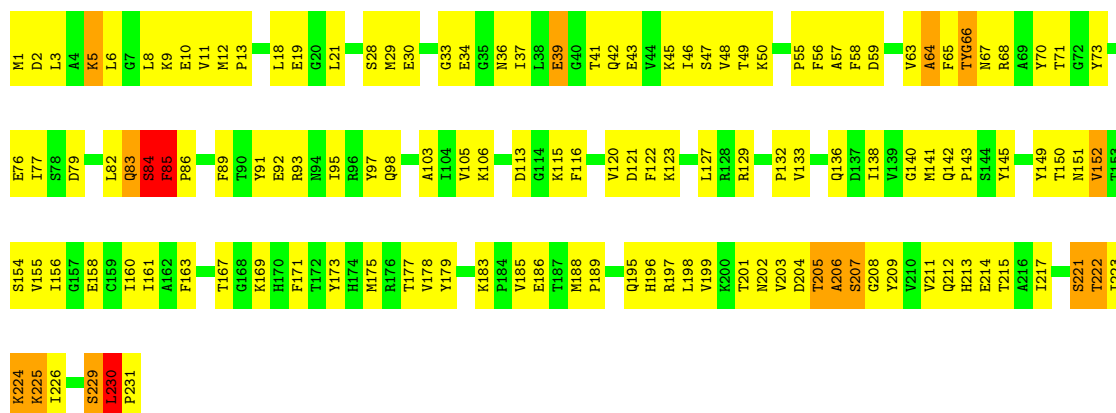
#### • Molecule 1: Green fluorescent protein



#### • Molecule 1: Green fluorescent protein

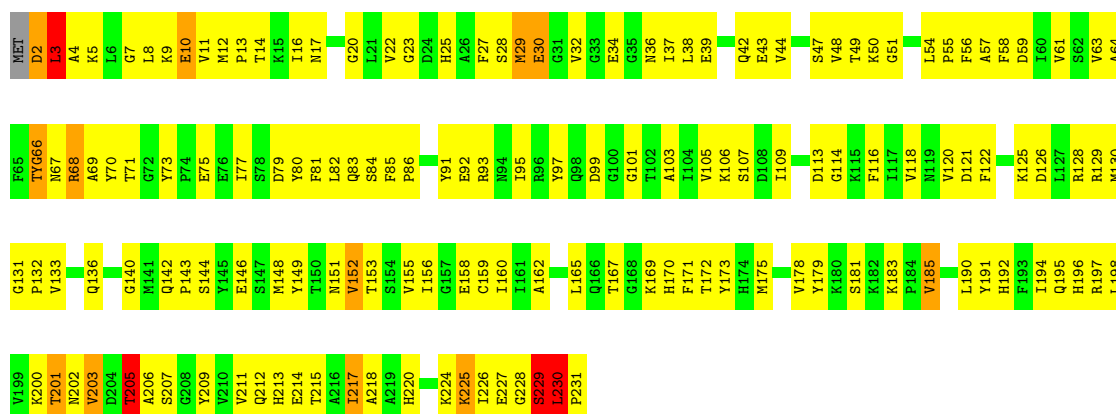






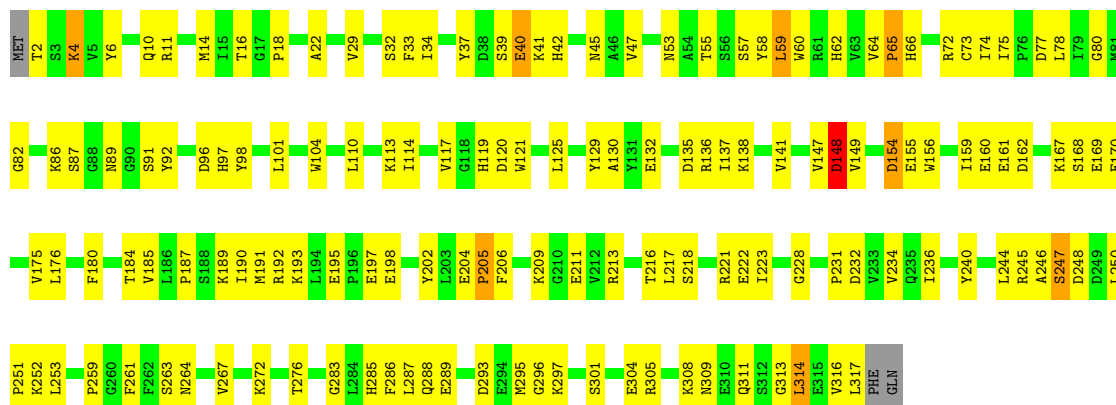
- Molecule 1: Green fluorescent protein

Chain F: 34% 58% 5% •



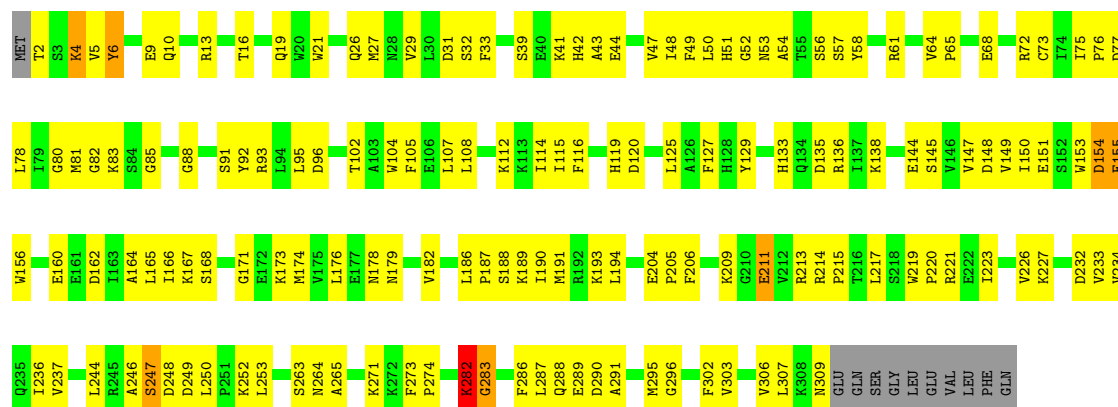
- Molecule 2: Coelenterazine h 2-monooxygenase

Chain C: 53% 43% • •

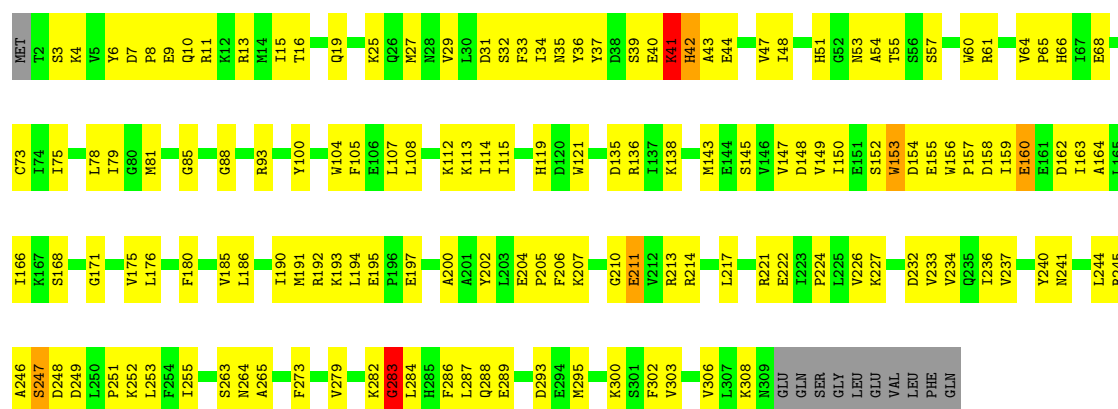


- Molecule 2: Coelenterazine h 2-monooxygenase

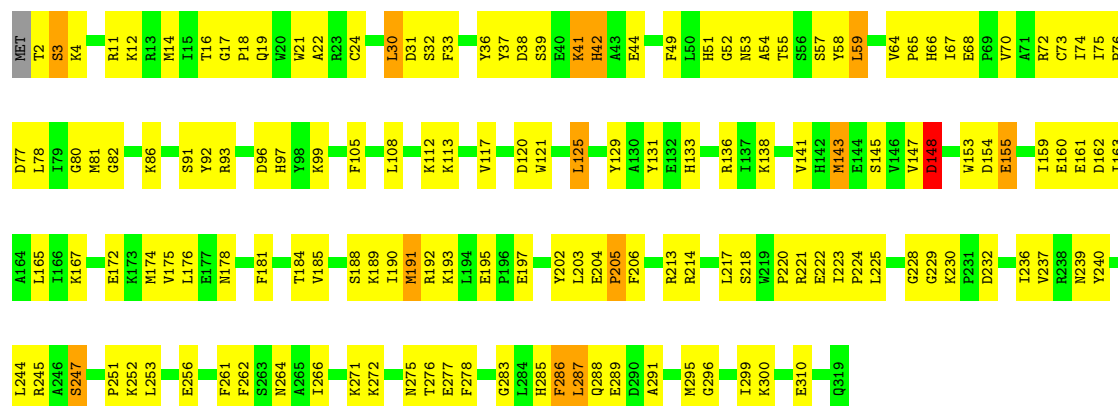
Chain D: 49% 45% • •



• Molecule 2: Coelenterazine h 2-monooxygenase



• Molecule 2: Coelenterazine h 2-monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.93Å 95.93Å 357.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.54 – 2.40 47.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.54-2.40) 99.0 (47.54-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, $R_{free}$	0.268 , 0.340 0.270 , 0.338	Depositor DCC
$R_{free}$ test set	7116 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.478 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: CRO, CEI

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	0.61	1/1845 (0.1%)	1.00	8/2489 (0.3%)
1	B	0.51	1/1837 (0.1%)	0.89	4/2479 (0.2%)
1	E	0.50	0/1845	0.88	1/2489 (0.0%)
1	F	0.51	0/1837	0.88	2/2479 (0.1%)
2	C	0.53	0/2664	0.81	1/3607 (0.0%)
2	D	0.47	0/2604	0.79	3/3526 (0.1%)
2	G	0.47	0/2604	0.78	2/3526 (0.1%)
2	H	0.54	1/2676 (0.0%)	0.79	2/3623 (0.1%)
All	All	0.52	3/17912 (0.0%)	0.84	23/24218 (0.1%)

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
1	A	0	2
1	B	0	3
1	E	0	4
1	F	0	2
2	D	0	3
2	G	0	1
2	H	0	1
All	All	0	16

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	PRO	N-CD	-10.64	1.32	1.47
2	H	155	GLU	CA-C	9.69	1.65	1.52
1	B	219	ALA	CA-CB	-5.34	1.50	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	283	GLY	N-CA-C	10.98	124.44	110.38
1	A	85	PHE	C-N-CD	-8.79	101.26	120.60
1	B	201	THR	CA-C-N	-7.89	109.55	122.65
1	B	201	THR	C-N-CA	-7.89	109.55	122.65
1	A	85	PHE	CA-C-N	6.56	142.74	127.00

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	VAL	Peptide
1	A	86	PRO	Peptide
1	B	196	HIS	Peptide
1	B	202	ASN	Peptide
1	B	225	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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	1828	0	1814	175	0
1	B	1820	0	1802	138	0
1	E	1828	0	1813	148	0
1	F	1820	0	1803	147	0
2	C	2592	0	2552	125	0
2	D	2532	0	2493	133	0
2	G	2532	0	2493	128	0
2	H	2603	0	2564	114	0
3	C	31	0	21	4	0
3	D	31	0	21	1	0
3	G	31	0	21	1	0
3	H	31	0	21	5	0
4	A	7	0	0	0	0
4	B	10	0	0	0	0
4	C	23	0	0	2	0
4	D	12	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	0	0
4	F	6	0	0	1	0
4	G	11	0	0	1	0
4	H	21	0	0	2	0
All	All	17772	0	17418	1068	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 30.

The worst 5 of 1068 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:E:85:PHE:CZ	1:E:89:PHE:CD2	2.23	1.25
1:A:13:PRO:HD2	1:A:115:LYS:CE	1.69	1.21
1:A:13:PRO:HD2	1:A:115:LYS:HE2	1.18	1.18
1:F:50:LYS:HD2	1:F:51:GLY:N	1.58	1.18
1:E:11:VAL:HG12	1:E:36:ASN:HA	1.17	1.15

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	226/231 (98%)	179 (79%)	29 (13%)	18 (8%)	1	0
1	B	225/231 (97%)	171 (76%)	38 (17%)	16 (7%)	1	0
1	E	226/231 (98%)	188 (83%)	22 (10%)	16 (7%)	1	0
1	F	225/231 (97%)	172 (76%)	35 (16%)	18 (8%)	1	0
2	C	315/319 (99%)	255 (81%)	45 (14%)	15 (5%)	2	1
2	D	307/319 (96%)	256 (83%)	42 (14%)	9 (3%)	3	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	307/319 (96%)	254 (83%)	42 (14%)	11 (4%)	3	2
2	H	316/319 (99%)	255 (81%)	43 (14%)	18 (6%)	1	0
All	All	2147/2200 (98%)	1730 (81%)	296 (14%)	121 (6%)	1	1

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	37	ILE
1	A	86	PRO
1	A	114	GLY
1	A	186	GLU

### 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	198/198 (100%)	197 (100%)	1 (0%)	86	94
1	B	197/198 (100%)	192 (98%)	5 (2%)	42	63
1	E	198/198 (100%)	195 (98%)	3 (2%)	60	77
1	F	197/198 (100%)	194 (98%)	3 (2%)	60	77
2	C	280/282 (99%)	280 (100%)	0	100	100
2	D	273/282 (97%)	269 (98%)	4 (2%)	60	77
2	G	273/282 (97%)	270 (99%)	3 (1%)	70	84
2	H	281/282 (100%)	281 (100%)	0	100	100
All	All	1897/1920 (99%)	1878 (99%)	19 (1%)	75	86

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	229	SER
2	G	211[A]	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	211[B]	GLU
2	G	41	LYS
2	D	271	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	119	HIS
1	F	196	HIS
2	H	178	ASN
1	F	67	ASN
2	G	19	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CRO	B	66	1	22,22,24	2.24	7 (31%)	27,30,34	2.84	9 (33%)
1	CRO	E	66	1	22,22,24	2.94	7 (31%)	27,30,34	2.80	9 (33%)
1	CRO	A	66	1	22,22,24	2.69	6 (27%)	27,30,34	2.84	8 (29%)
1	CRO	F	66	1	22,22,24	2.35	5 (22%)	27,30,34	2.96	7 (25%)

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
1	CRO	B	66	1	-	5/9/29/32	0/2/2/2
1	CRO	E	66	1	-	6/9/29/32	0/2/2/2
1	CRO	A	66	1	-	3/9/29/32	0/2/2/2
1	CRO	F	66	1	-	4/9/29/32	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	66	CRO	CA2-C2	-10.74	1.38	1.48
1	A	66	CRO	CA2-C2	-9.37	1.39	1.48
1	F	66	CRO	CA2-C2	-8.54	1.40	1.48
1	B	66	CRO	CA2-C2	-7.73	1.41	1.48
1	A	66	CRO	C1-N2	4.63	1.39	1.32

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRO	CA2-C2-N3	10.04	108.12	103.37
1	F	66	CRO	O2-C2-CA2	-9.49	125.63	130.96
1	F	66	CRO	CA2-C2-N3	8.94	107.60	103.37
1	E	66	CRO	CA2-C2-N3	7.98	107.14	103.37
1	A	66	CRO	O2-C2-CA2	-7.09	126.98	130.96

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	66	CRO	N1-CA1-CB1-OG1
1	B	66	CRO	C1-CA1-CB1-OG1
1	E	66	CRO	N1-CA1-CB1-OG1
1	E	66	CRO	C1-CA1-CB1-OG1
1	E	66	CRO	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CRO	5	0
1	E	66	CRO	1	0
1	A	66	CRO	4	0
1	F	66	CRO	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	CEI	G	401	-	31,34,34	1.37	4 (12%)	38,46,46	1.47	4 (10%)
3	CEI	H	401	-	31,34,34	1.37	4 (12%)	38,46,46	1.38	8 (21%)
3	CEI	D	401	-	31,34,34	1.34	5 (16%)	38,46,46	1.36	4 (10%)
3	CEI	C	401	-	31,34,34	1.50	4 (12%)	38,46,46	1.24	4 (10%)

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	CEI	G	401	-	-	3/12/16/16	0/4/4/4
3	CEI	H	401	-	-	2/12/16/16	0/4/4/4
3	CEI	D	401	-	-	3/12/16/16	0/4/4/4
3	CEI	C	401	-	-	0/12/16/16	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	CEI	C2-N1	4.05	1.44	1.35
3	H	401	CEI	C2-N1	4.02	1.44	1.35
3	G	401	CEI	C2-N1	3.90	1.44	1.35
3	C	401	CEI	C26-C8	3.43	1.54	1.51
3	D	401	CEI	C2-N1	3.35	1.43	1.35

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	CEI	C26-C8-N7	4.79	125.88	116.36
3	G	401	CEI	C8-C9-N1	-4.54	112.17	118.40
3	G	401	CEI	C26-C8-N7	4.28	124.86	116.36
3	H	401	CEI	C26-C8-N7	3.27	122.85	116.36
3	C	401	CEI	C27-C26-C8	-3.22	104.14	112.40

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

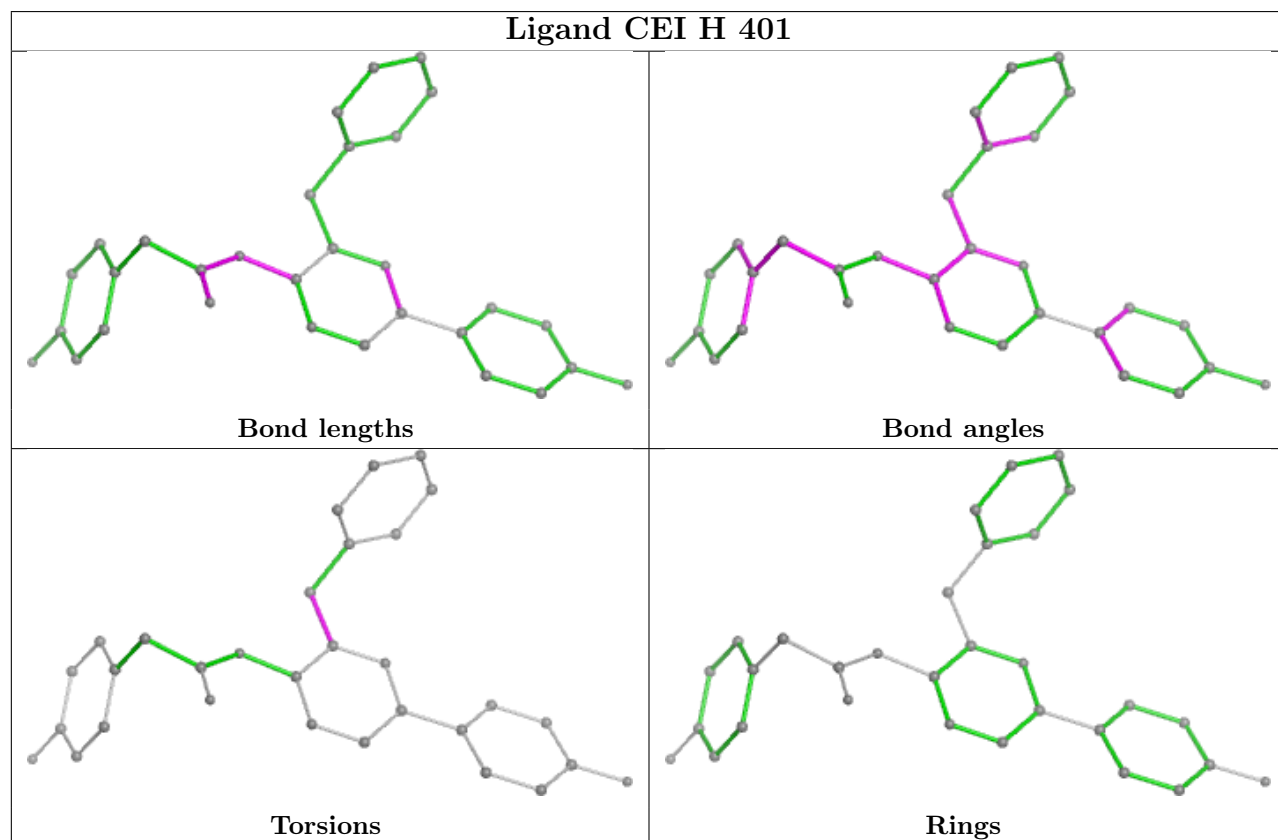
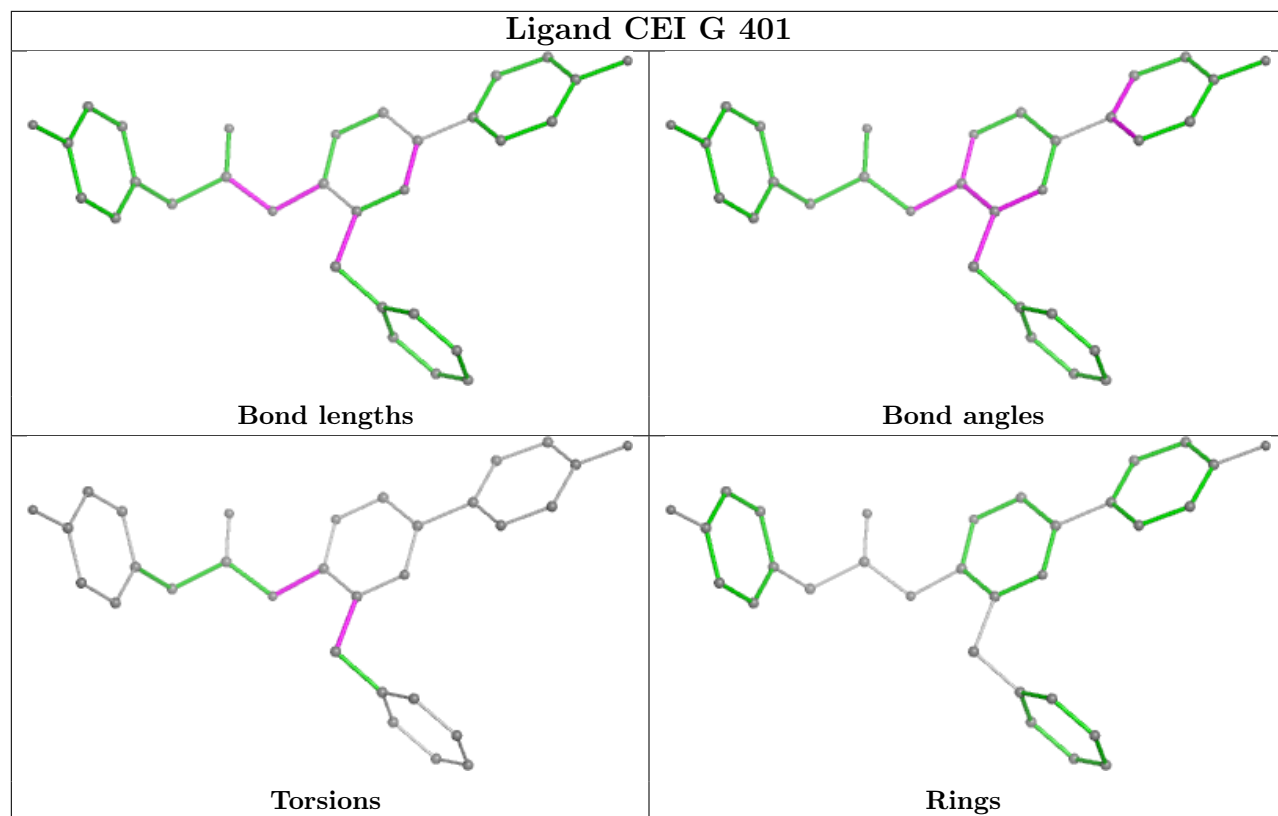
Mol	Chain	Res	Type	Atoms
3	G	401	CEI	C27-C26-C8-C9
3	G	401	CEI	C27-C26-C8-N7
3	H	401	CEI	C27-C26-C8-N7
3	D	401	CEI	C8-C9-N1-C2
3	G	401	CEI	C8-C9-N1-C2

There are no ring outliers.

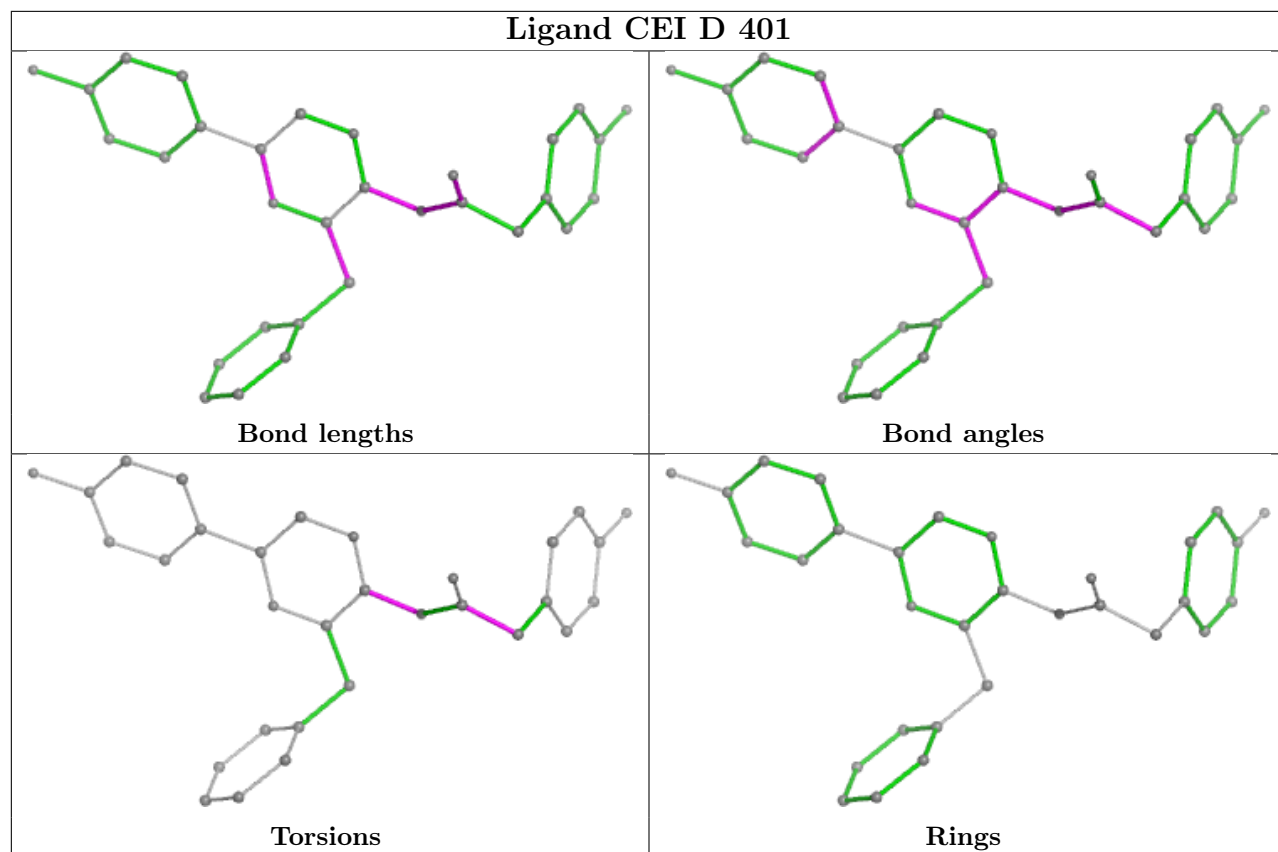
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	CEI	1	0
3	H	401	CEI	5	0
3	D	401	CEI	1	0
3	C	401	CEI	4	0

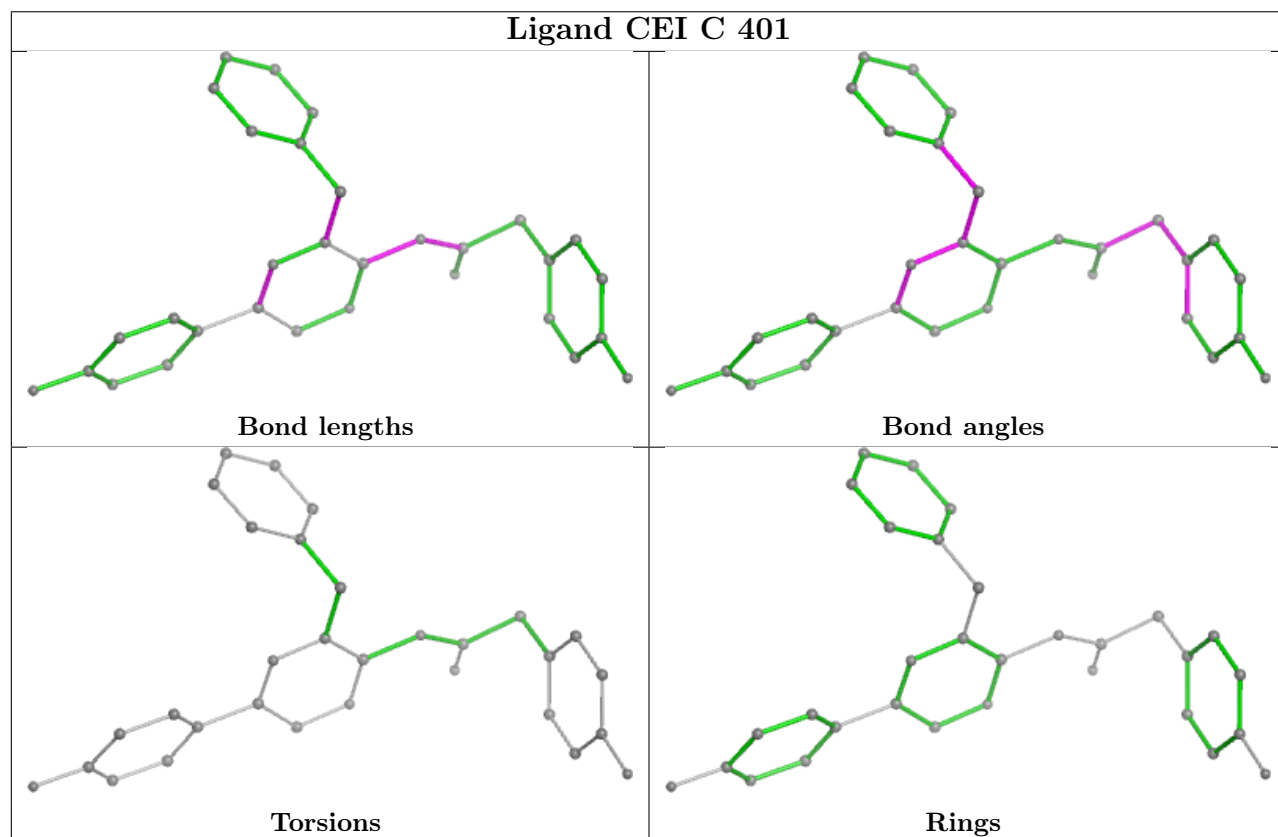
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



## Ligand CEI D 401



## Ligand CEI C 401



## 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	230/231 (99%)	-0.82	2 (0%) 81 78	48, 86, 127, 144	0
1	B	229/231 (99%)	-0.84	0 100 100	49, 87, 107, 134	0
1	E	230/231 (99%)	-0.83	0 100 100	52, 90, 126, 142	0
1	F	229/231 (99%)	-0.83	0 100 100	56, 87, 112, 131	0
2	C	316/319 (99%)	-0.98	0 100 100	33, 67, 92, 113	1 (0%)
2	D	308/319 (96%)	-0.92	0 100 100	35, 71, 93, 115	1 (0%)
2	G	308/319 (96%)	-0.81	0 100 100	37, 76, 101, 116	1 (0%)
2	H	318/319 (99%)	-1.03	0 100 100	45, 65, 87, 102	0
All	All	2168/2200 (98%)	-0.89	2 (0%) 92 91	33, 76, 112, 144	3 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	VAL	2.6
1	A	8	LEU	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CRO	A	66	21/23	0.99	0.07	59,73,93,102	0
1	CRO	B	66	21/23	0.99	0.04	65,90,107,115	0
1	CRO	E	66	21/23	0.99	0.05	55,83,98,104	0
1	CRO	F	66	21/23	0.99	0.06	72,87,109,118	0

### 6.3 Carbohydrates [i](#)

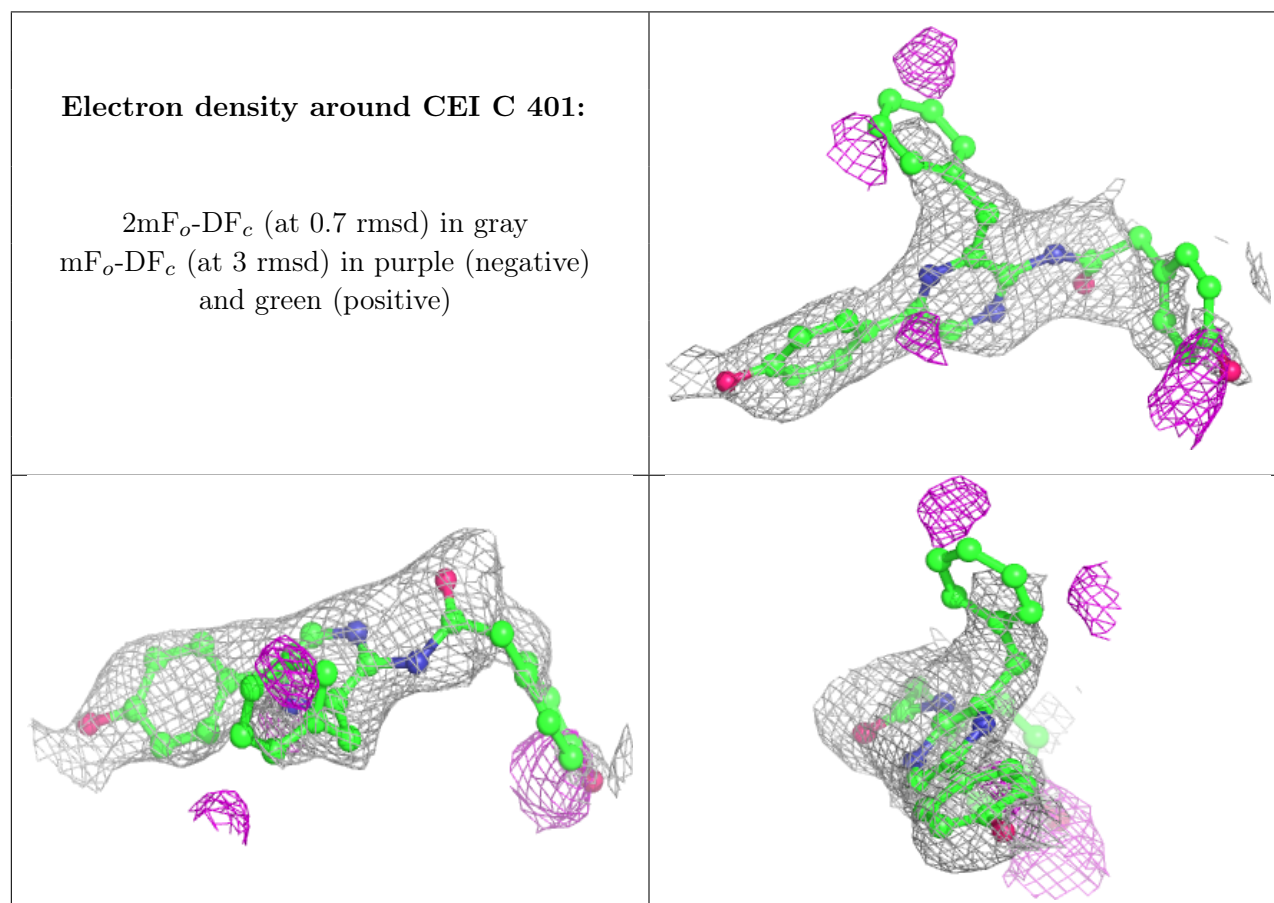
There are no oligosaccharides in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
3	CEI	C	401	31/31	0.98	0.07	67,79,95,101	0
3	CEI	D	401	31/31	0.99	0.07	58,82,118,121	0
3	CEI	G	401	31/31	0.99	0.07	66,88,120,123	0
3	CEI	H	401	31/31	0.99	0.07	51,80,103,108	0

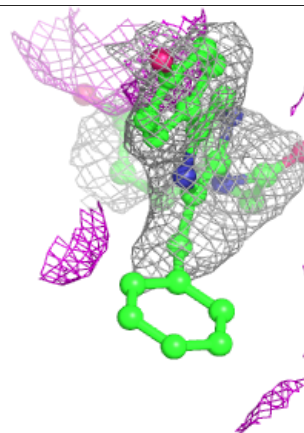
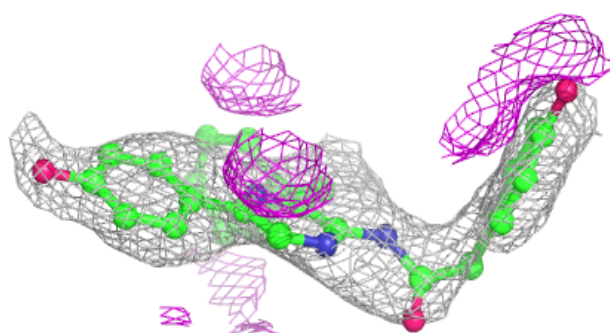
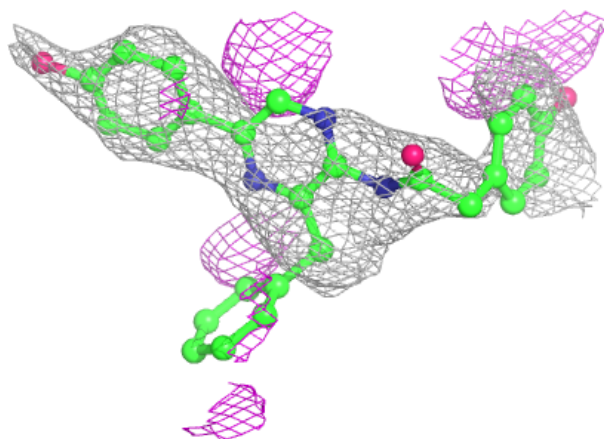
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



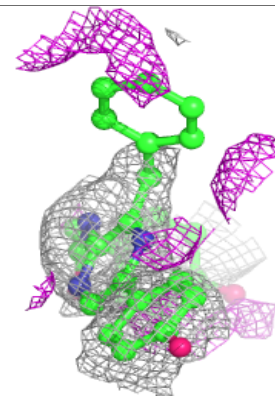
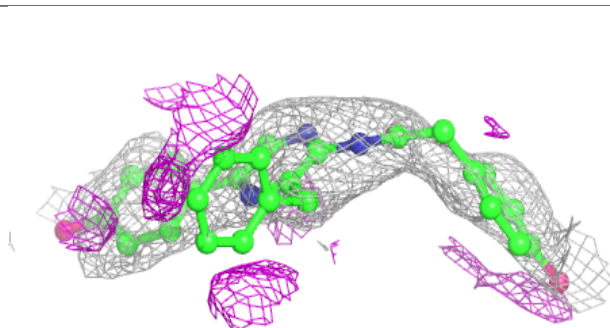
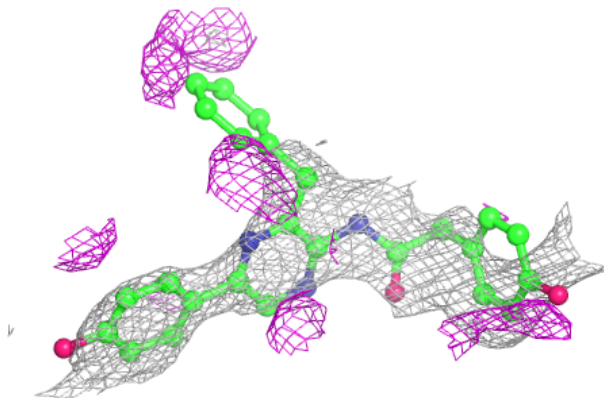


**Electron density around CEI D 401:**

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

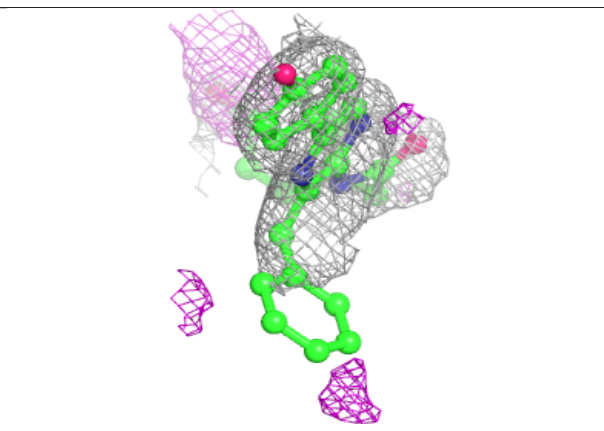
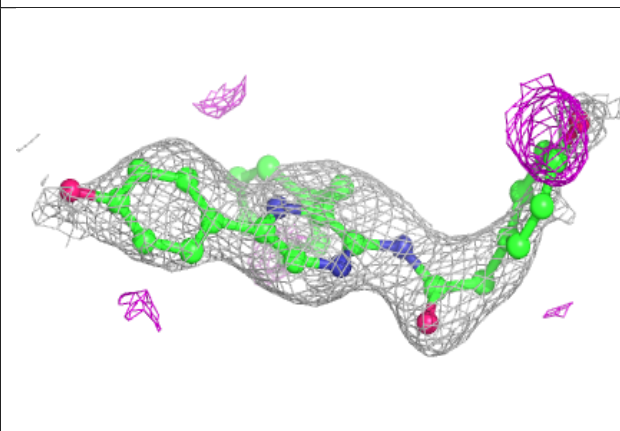
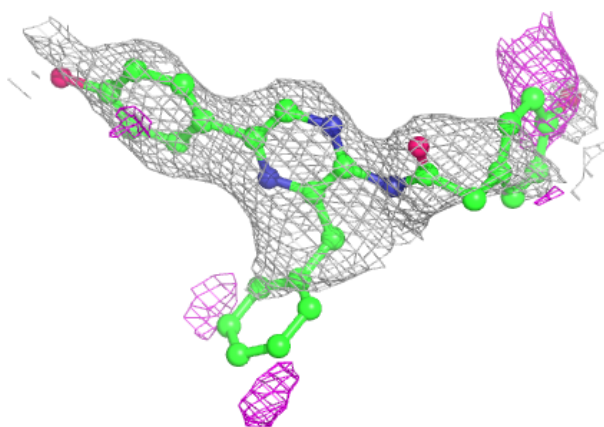
**Electron density around CEI G 401:**

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



**Electron density around CEI H 401:**

$2mF_o-DF_c$  (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.