



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:22 PM EST

PDB ID : 5RC2  
Title : PanDDA analysis group deposition – Endothiapepsin changed state model for fragment F2X-Entry Library E11b  
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Deposited on : 2020-03-24  
Resolution : 0.97 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

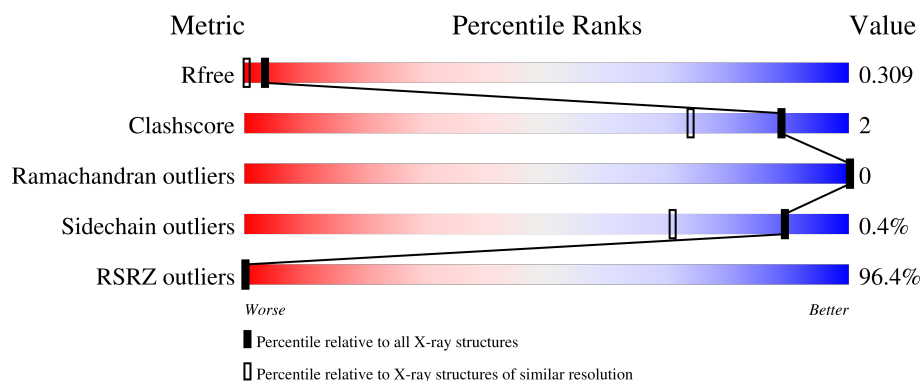
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 0.97 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	1026 (1.02-0.94)
Clashscore	180529	1154 (1.02-0.94)
Ramachandran outliers	177936	1094 (1.02-0.94)
Sidechain outliers	177891	1095 (1.02-0.94)
RSRZ outliers	164620	1025 (1.02-0.94)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	419	<div> <div>76%</div> <div>76%</div> <div>21%</div> </div>

## 2 Entry composition [i](#)

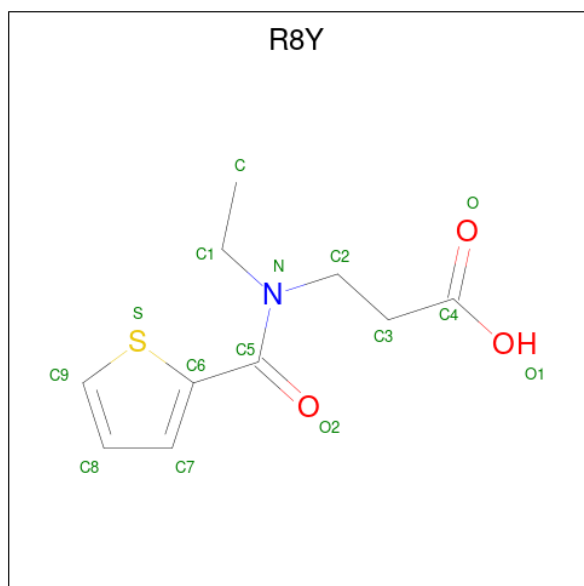
There are 7 unique types of molecules in this entry. The entry contains 3741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endothiapepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	3412	2157	515	732	8	22	52	0

- Molecule 2 is N-ethyl-N-(thiophene-2-carbonyl)-beta-alanine (three-letter code: R8Y) (formula: C<sub>10</sub>H<sub>13</sub>NO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	30	20	2	6	2	0	1

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

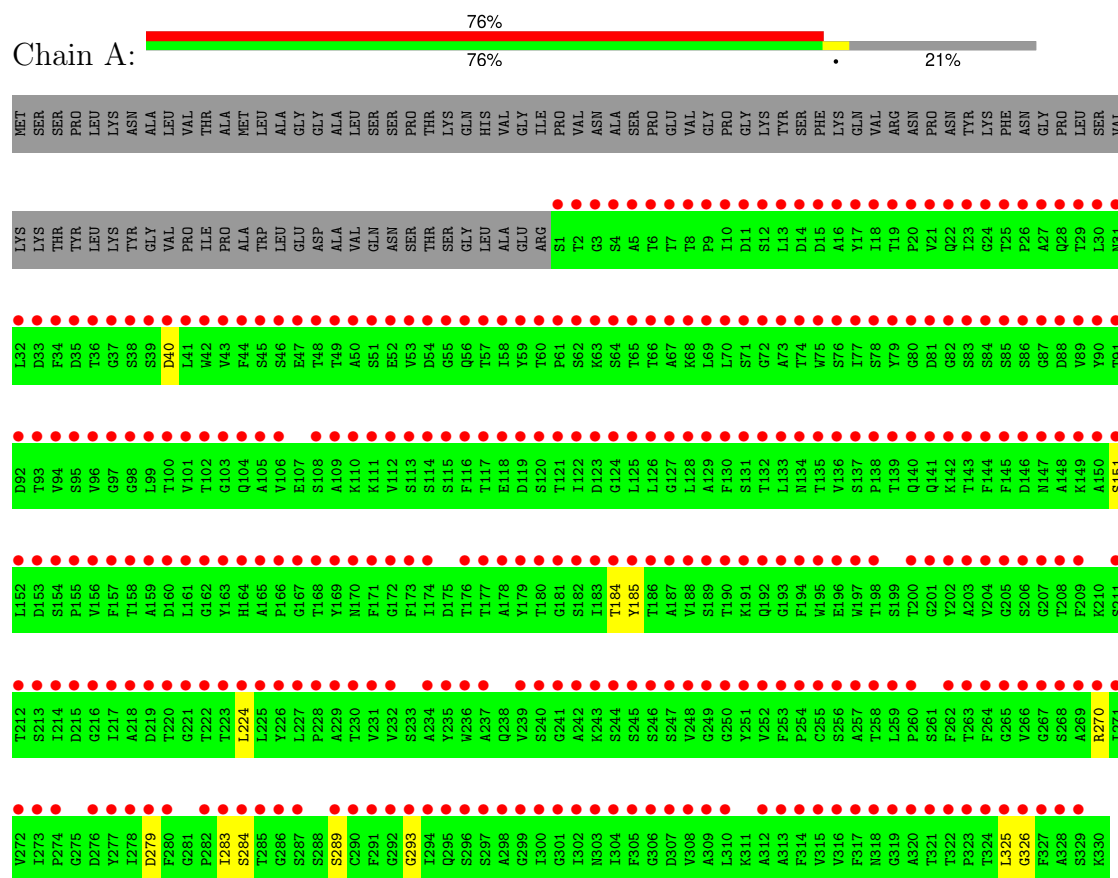
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	229	Total	O	0	14
			263	263		

### 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. 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: Endothiapepsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.23Å 73.01Å 52.51Å 90.00° 108.95° 90.00°	Depositor
Resolution (Å)	42.82 – 0.97 42.82 – 0.97	Depositor EDS
% Data completeness (in resolution range)	97.6 (42.82-0.97) 97.8 (42.82-0.97)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 0.97Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, $R_{free}$	0.154 , 0.154 0.314 , 0.309	Depositor DCC
$R_{free}$ test set	9536 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.6	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3741	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, R8Y, NA, DMS, PG4

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	0.83	1/3492 (0.0%)	0.92	3/4776 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	SER	CA-CB	-5.50	1.44	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	279[A]	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	279[B]	ASP	CB-CG-OD1	-5.12	113.69	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3412	0	3168	7	0
2	A	30	0	0	4	0
3	A	4	0	6	0	0
4	A	18	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	13	0	18	0	0
6	A	1	0	0	0	0
7	A	263	0	0	3	1
All	All	3741	0	3216	12	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (12) 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)
2:A:401[D]:R8Y:O2	7:A:502[D]:HOH:O	2.07	0.71
4:A:404[B]:GOL:O3	7:A:501:HOH:O	2.10	0.69
2:A:401[C]:R8Y:O2	7:A:502[C]:HOH:O	2.13	0.65
1:A:185[C]:TYR:HA	1:A:325[C]:LEU:O	2.12	0.49
1:A:283[B]:ILE:HG23	1:A:289[B]:SER:O	2.16	0.46
2:A:401[D]:R8Y:C2	2:A:401[D]:R8Y:S	3.06	0.44
2:A:401[C]:R8Y:C2	2:A:401[C]:R8Y:S	3.06	0.43
1:A:184[D]:THR:O	1:A:326[D]:GLY:HA2	2.19	0.43
1:A:184[C]:THR:O	1:A:326[C]:GLY:HA2	2.19	0.42
1:A:224:LEU:HD22	1:A:293:GLY:HA2	2.02	0.41
1:A:283[C]:ILE:HG13	1:A:284[C]:SER:N	2.36	0.41
1:A:283[D]:ILE:HG13	1:A:284[D]:SER:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:510:HOH:O	7:A:566:HOH:O[1_655]	2.18	0.02

## 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	482/419 (115%)	479 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	370/336 (110%)	369 (100%)	1 (0%)	91	72

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	R8Y	A	401[C]	-	14,15,15	2.43	1 (7%)	14,19,19	1.40	1 (7%)
3	DMS	A	402	-	3,3,3	0.23	0	3,3,3	0.53	0
4	GOL	A	404[A]	-	5,5,5	0.15	0	5,5,5	0.30	0
2	R8Y	A	401[D]	-	14,15,15	2.36	1 (7%)	14,19,19	1.37	1 (7%)
5	PG4	A	405	6	12,12,12	0.13	0	11,11,11	0.24	0
4	GOL	A	404[B]	-	5,5,5	0.12	0	5,5,5	0.45	0
4	GOL	A	403	-	5,5,5	0.12	0	5,5,5	0.42	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
2	R8Y	A	401[C]	-	-	2/11/15/15	0/1/1/1
4	GOL	A	404[A]	-	-	0/4/4/4	-
2	R8Y	A	401[D]	-	-	2/11/15/15	0/1/1/1
5	PG4	A	405	6	-	0/10/10/10	-
4	GOL	A	404[B]	-	-	2/4/4/4	-
4	GOL	A	403	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[C]	R8Y	C6-S	-8.57	1.62	1.72
2	A	401[D]	R8Y	C6-S	-8.36	1.62	1.72

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[D]	R8Y	C2-C3-C4	-2.71	106.94	112.84
2	A	401[C]	R8Y	C2-C3-C4	-2.69	106.97	112.84

There are no chirality outliers.

All (6) torsion outliers are listed below:

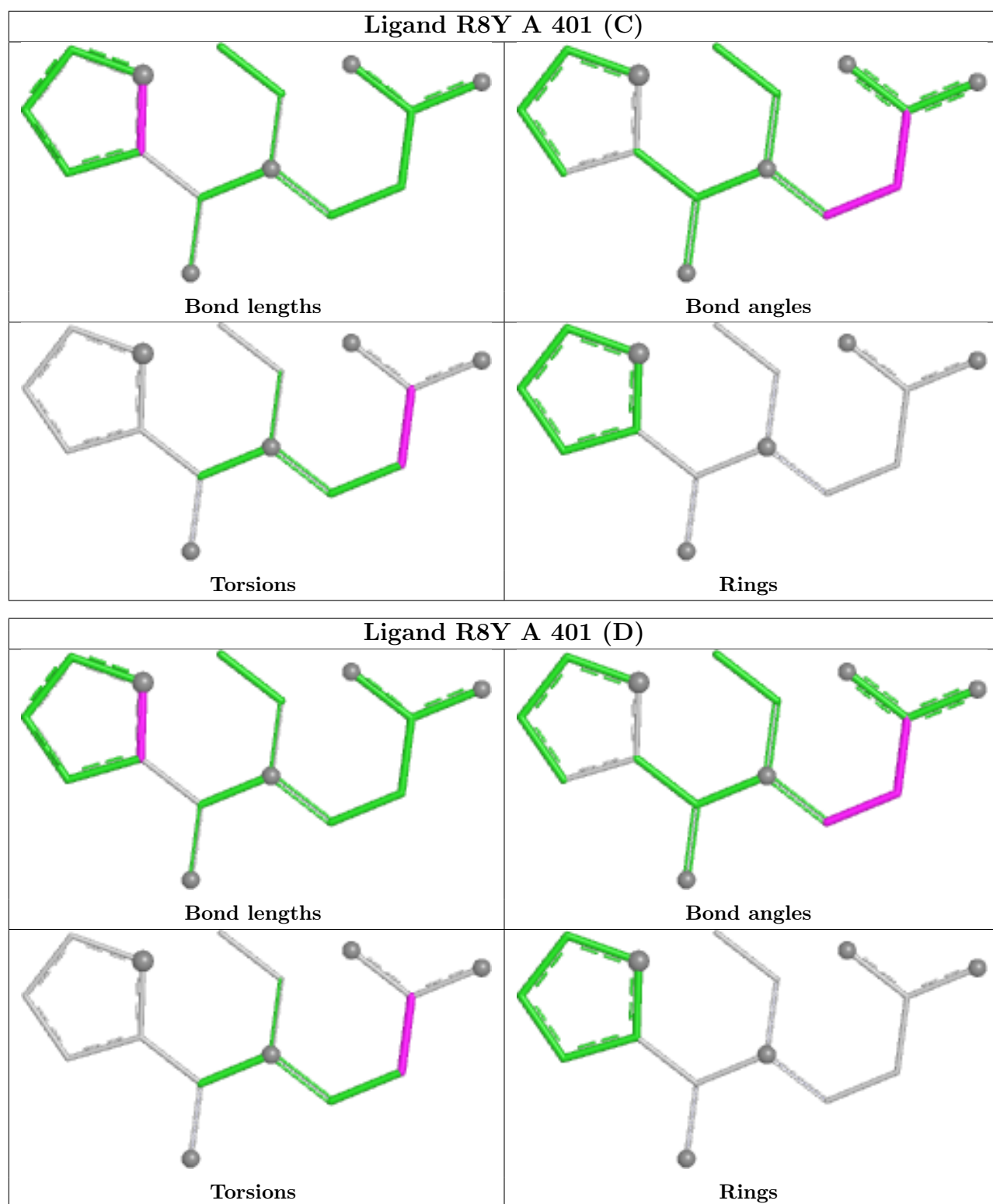
Mol	Chain	Res	Type	Atoms
4	A	404[B]	GOL	O1-C1-C2-C3
4	A	404[B]	GOL	O1-C1-C2-O2
2	A	401[C]	R8Y	C2-C3-C4-O
2	A	401[D]	R8Y	C2-C3-C4-O
2	A	401[C]	R8Y	C2-C3-C4-O1
2	A	401[D]	R8Y	C2-C3-C4-O1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401[C]	R8Y	2	0
2	A	401[D]	R8Y	2	0
4	A	404[B]	GOL	1	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

**Warning:** The R factor obtained from EDS is 0.3229, which does not match the depositor's R factor of 0.15366. Please interpret the results in this section carefully.

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	330/419 (78%)	4.13	318 (96%) 0 0	2, 13, 22, 31	52 (15%)

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300[A]	ILE	10.9
1	A	136	VAL	8.9
1	A	150	ALA	8.6
1	A	75	TRP	8.5
1	A	53	VAL	7.6
1	A	49	THR	7.4
1	A	125	LEU	7.3
1	A	89	VAL	7.2
1	A	246[A]	SER	7.1
1	A	247[A]	SER	7.1
1	A	70	LEU	7.0
1	A	77	ILE	7.0
1	A	73	ALA	6.9
1	A	116	PHE	6.9
1	A	321	THR	6.9
1	A	79	TYR	6.8
1	A	80	GLY	6.7
1	A	248[A]	VAL	6.7
1	A	298[A]	ALA	6.6
1	A	43	VAL	6.6
1	A	58	ILE	6.6
1	A	42	TRP	6.3
1	A	69	LEU	6.2
1	A	55	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	25	THR	6.2
1	A	41	LEU	6.1
1	A	84	SER	6.1
1	A	90	TYR	6.1
1	A	285	THR	6.1
1	A	109	ALA	6.0
1	A	114	SER	6.0
1	A	105	ALA	6.0
1	A	50	ALA	6.0
1	A	102	THR	5.9
1	A	249[A]	GLY	5.9
1	A	115	SER	5.9
1	A	106	VAL	5.9
1	A	51	SER	5.9
1	A	86	SER	5.8
1	A	144	PHE	5.8
1	A	59	TYR	5.8
1	A	299[A]	GLY	5.8
1	A	60	THR	5.8
1	A	122	ILE	5.8
1	A	13	LEU	5.8
1	A	146	ASP	5.8
1	A	139	THR	5.7
1	A	74	THR	5.7
1	A	112	VAL	5.7
1	A	164	HIS	5.6
1	A	322	THR	5.6
1	A	324[A]	THR	5.6
1	A	101	VAL	5.6
1	A	195	TRP	5.5
1	A	68[A]	LYS	5.5
1	A	72	GLY	5.5
1	A	190	THR	5.5
1	A	67	ALA	5.5
1	A	157	PHE	5.4
1	A	65	THR	5.4
1	A	48	THR	5.3
1	A	44	PHE	5.3
1	A	82	GLY	5.3
1	A	66	THR	5.3
1	A	32	LEU	5.3
1	A	163	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	78	SER	5.3
1	A	208	THR	5.2
1	A	10	ILE	5.2
1	A	30	LEU	5.2
1	A	2	THR	5.1
1	A	145	PHE	5.1
1	A	17	TYR	5.1
1	A	94	VAL	5.0
1	A	193	GLY	5.0
1	A	99	LEU	5.0
1	A	61	PRO	5.0
1	A	169	TYR	5.0
1	A	24	GLY	5.0
1	A	315	VAL	5.0
1	A	188	VAL	4.9
1	A	113	SER	4.9
1	A	117	THR	4.9
1	A	87	GLY	4.9
1	A	221	GLY	4.9
1	A	21	VAL	4.9
1	A	290[A]	CYS	4.9
1	A	91	THR	4.8
1	A	62	SER	4.8
1	A	23	ILE	4.8
1	A	130	PHE	4.8
1	A	71[A]	SER	4.8
1	A	57	THR	4.7
1	A	121	THR	4.7
1	A	189	SER	4.7
1	A	26	PRO	4.7
1	A	138	PRO	4.7
1	A	212	THR	4.7
1	A	148	ALA	4.7
1	A	178	ALA	4.7
1	A	54	ASP	4.7
1	A	132	THR	4.7
1	A	85	SER	4.6
1	A	236	TRP	4.6
1	A	16	ALA	4.6
1	A	19	THR	4.6
1	A	320	ALA	4.6
1	A	174[A]	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	302	ILE	4.6
1	A	291[A]	PHE	4.6
1	A	317	PHE	4.6
1	A	177	THR	4.6
1	A	152	LEU	4.5
1	A	76	SER	4.5
1	A	187[A]	ALA	4.5
1	A	209	PHE	4.5
1	A	253[A]	PHE	4.5
1	A	155	PRO	4.5
1	A	206[A]	SER	4.5
1	A	149[A]	LYS	4.4
1	A	34	PHE	4.4
1	A	156	VAL	4.4
1	A	134	ASN	4.4
1	A	135	THR	4.4
1	A	103	GLY	4.4
1	A	133	LEU	4.4
1	A	45	SER	4.3
1	A	108	SER	4.3
1	A	127	GLY	4.3
1	A	314	PHE	4.3
1	A	204	VAL	4.3
1	A	27	ALA	4.3
1	A	129	ALA	4.3
1	A	251[A]	TYR	4.3
1	A	126	LEU	4.3
1	A	217	ILE	4.3
1	A	218	ALA	4.2
1	A	176	THR	4.2
1	A	258	THR	4.2
1	A	197	TRP	4.2
1	A	192	GLN	4.2
1	A	46	SER	4.2
1	A	179	TYR	4.1
1	A	310	LEU	4.1
1	A	214	ILE	4.1
1	A	5	ALA	4.1
1	A	252[A]	VAL	4.1
1	A	180	THR	4.1
1	A	151	SER	4.1
1	A	159	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	165	ALA	4.1
1	A	173	PHE	4.1
1	A	83	SER	4.1
1	A	168	THR	4.1
1	A	186[A]	THR	4.1
1	A	12	SER	4.0
1	A	329	SER	4.0
1	A	224	LEU	4.0
1	A	119	ASP	4.0
1	A	305	PHE	4.0
1	A	93	THR	4.0
1	A	222	THR	4.0
1	A	88	ASP	4.0
1	A	266[A]	VAL	4.0
1	A	167	GLY	4.0
1	A	18	ILE	4.0
1	A	283[A]	ILE	4.0
1	A	171	PHE	3.9
1	A	4	SER	3.9
1	A	97	GLY	3.9
1	A	128	LEU	3.9
1	A	96	VAL	3.9
1	A	81	ASP	3.9
1	A	278	ILE	3.9
1	A	100	THR	3.9
1	A	194	PHE	3.9
1	A	226	TYR	3.9
1	A	120	SER	3.9
1	A	137	SER	3.9
1	A	245[A]	SER	3.9
1	A	257	ALA	3.8
1	A	185[A]	TYR	3.8
1	A	202	TYR	3.8
1	A	98	GLY	3.8
1	A	207	GLY	3.8
1	A	110	LYS	3.8
1	A	294	ILE	3.8
1	A	284[A]	SER	3.8
1	A	216	GLY	3.8
1	A	225	LEU	3.8
1	A	231	VAL	3.8
1	A	227	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1	SER	3.8
1	A	39	SER	3.8
1	A	131	SER	3.7
1	A	220	THR	3.7
1	A	118	GLU	3.7
1	A	9[A]	PRO	3.7
1	A	123	ASP	3.7
1	A	47	GLU	3.6
1	A	319	GLY	3.6
1	A	38	SER	3.6
1	A	95	SER	3.6
1	A	8	THR	3.6
1	A	29	THR	3.6
1	A	124	GLY	3.6
1	A	286	GLY	3.6
1	A	7	THR	3.6
1	A	223	THR	3.5
1	A	312	ALA	3.5
1	A	215[A]	ASP	3.5
1	A	268[A]	SER	3.5
1	A	304	ILE	3.5
1	A	104	GLN	3.5
1	A	269[A]	ALA	3.5
1	A	63	LYS	3.4
1	A	142	LYS	3.4
1	A	276[A]	ASP	3.4
1	A	282[A]	PRO	3.4
1	A	198	THR	3.4
1	A	327[A]	PHE	3.4
1	A	162	GLY	3.4
1	A	15	ASP	3.4
1	A	40	ASP	3.4
1	A	323	PRO	3.4
1	A	64	SER	3.4
1	A	35	ASP	3.3
1	A	161	LEU	3.3
1	A	52	GLU	3.3
1	A	228	PRO	3.3
1	A	232	VAL	3.3
1	A	203	ALA	3.3
1	A	183[A]	ILE	3.3
1	A	36	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	ASP	3.3
1	A	239	VAL	3.3
1	A	20	PRO	3.2
1	A	254[A]	PRO	3.2
1	A	306	GLY	3.2
1	A	3	GLY	3.2
1	A	255[A]	CYS	3.2
1	A	308	VAL	3.2
1	A	316	VAL	3.2
1	A	280	PHE	3.2
1	A	6	THR	3.2
1	A	277	TYR	3.2
1	A	37	GLY	3.2
1	A	244[A]	SER	3.2
1	A	301	GLY	3.1
1	A	141	GLN	3.1
1	A	154[A]	SER	3.1
1	A	318	ASN	3.1
1	A	313	ALA	3.1
1	A	325[A]	LEU	3.1
1	A	271	ILE	3.1
1	A	56	GLN	3.1
1	A	240[A]	SER	3.1
1	A	181	GLY	3.0
1	A	241	GLY	3.0
1	A	264	PHE	3.0
1	A	263	THR	3.0
1	A	237	ALA	3.0
1	A	272	VAL	2.9
1	A	328[A]	ALA	2.9
1	A	229	ALA	2.9
1	A	309	ALA	2.9
1	A	147	ASN	2.9
1	A	184[A]	THR	2.9
1	A	250[A]	GLY	2.9
1	A	170	ASN	2.9
1	A	200	THR	2.9
1	A	267[A]	GLY	2.9
1	A	326[A]	GLY	2.8
1	A	230	THR	2.8
1	A	273	ILE	2.8
1	A	11	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	92	ASP	2.8
1	A	153	ASP	2.8
1	A	172	GLY	2.8
1	A	158	THR	2.8
1	A	262	PHE	2.8
1	A	201	GLY	2.8
1	A	213	SER	2.7
1	A	234	ALA	2.7
1	A	33	ASP	2.7
1	A	279[A]	ASP	2.7
1	A	182[A]	SER	2.7
1	A	235	TYR	2.7
1	A	256	SER	2.7
1	A	196	GLU	2.6
1	A	242	ALA	2.6
1	A	143	THR	2.6
1	A	31	ASN	2.6
1	A	211	SER	2.5
1	A	297	SER	2.5
1	A	259	LEU	2.5
1	A	265	GLY	2.5
1	A	140	GLN	2.5
1	A	260	PRO	2.5
1	A	243[A]	LYS	2.5
1	A	274	PRO	2.5
1	A	191	LYS	2.4
1	A	205	GLY	2.4
1	A	303	ASN	2.4
1	A	293	GLY	2.4
1	A	287[A]	SER	2.3
1	A	166	PRO	2.3
1	A	292	GLY	2.3
1	A	289[A]	SER	2.3
1	A	307	ASP	2.2
1	A	111	LYS	2.2
1	A	296	SER	2.2
1	A	28	GLN	2.2
1	A	22	GLN	2.1
1	A	160	ASP	2.1
1	A	270	ARG	2.0
1	A	14	ASP	2.0
1	A	295	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

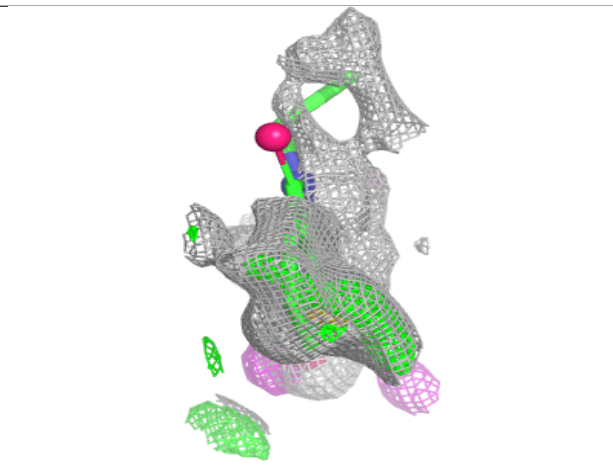
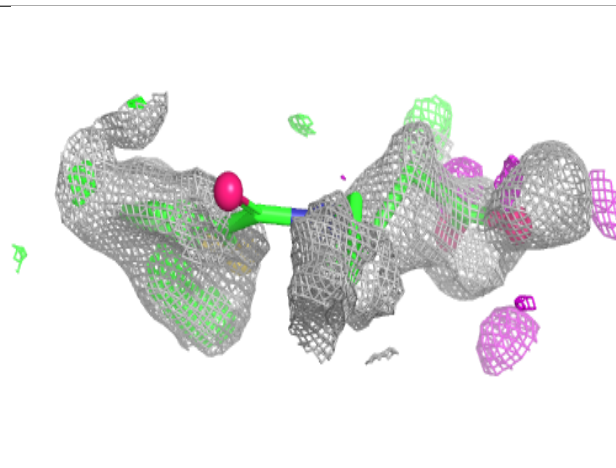
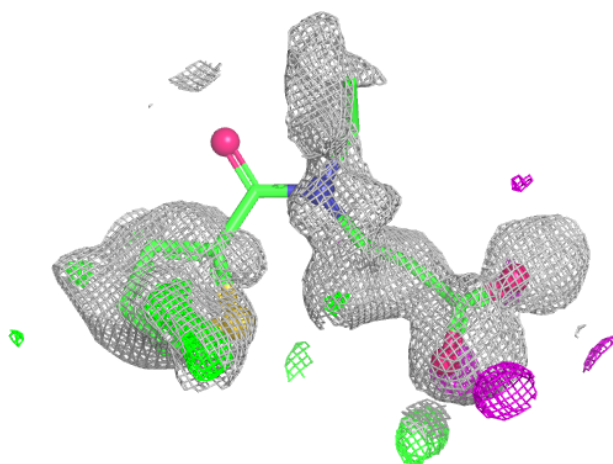
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	PG4	A	405	13/13	0.68	0.30	39,46,51,53	0
6	NA	A	406	1/1	0.69	0.31	59,59,59,59	0
4	GOL	A	404[A]	6/6	0.73	0.24	18,27,28,30	6
4	GOL	A	404[B]	6/6	0.73	0.24	21,33,38,38	6
2	R8Y	A	401[C]	15/15	0.73	0.33	15,19,21,22	15
2	R8Y	A	401[D]	15/15	0.73	0.33	15,19,21,22	15
4	GOL	A	403	6/6	0.76	0.23	15,20,26,28	6
3	DMS	A	402	4/4	0.83	0.20	19,29,37,42	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 R8Y A 401 (C):**

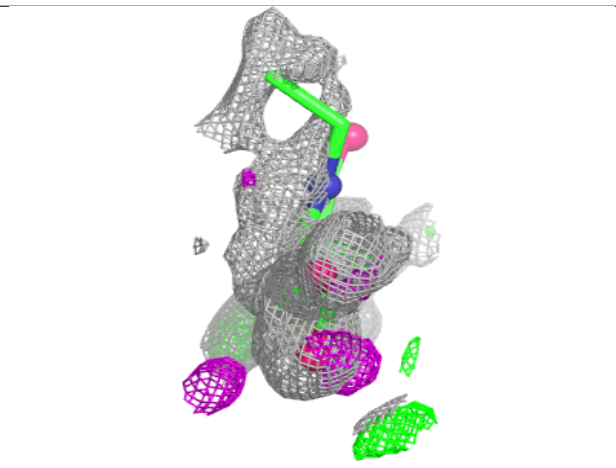
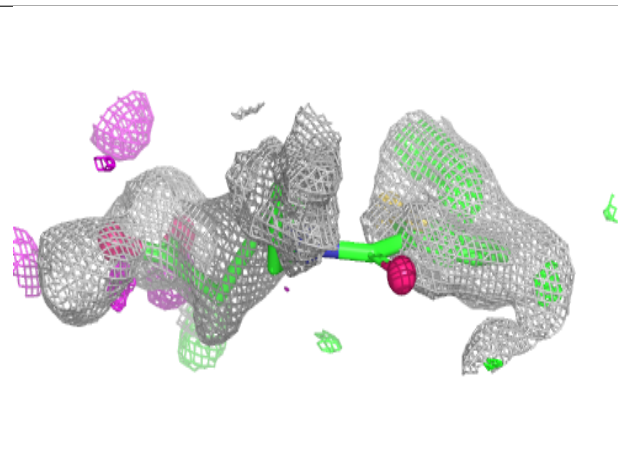
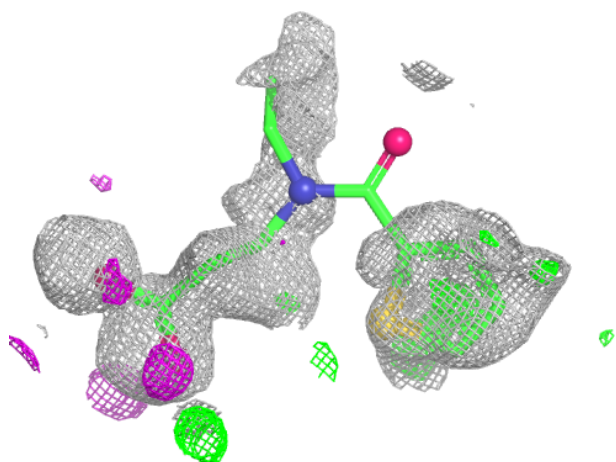
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around R8Y A 401 (D):**

$2mF_o-DF_c$  (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.