



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2025 – 07:13 pm BST

PDB ID : 9IGQ / pdb\_00009igq  
Title : Crystal structure of PPK2 class III from Erysipelotrichaceae bacterium in complex with AppCH2p and polyphosphate  
Authors : Rasche, R.; Lawrence-Doerner, A.-M.; Cornelissen, N.V.; Kuemmel, D.  
Deposited on : 2025-02-20  
Resolution : 1.70 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 Phenix2.0rc1
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)	:	2.44

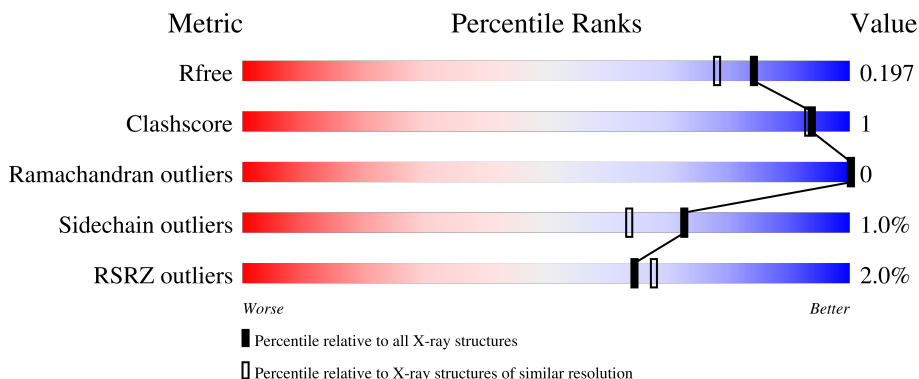
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	306	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div></div> </div> </div>
1	B	306	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div></div> </div> </div>
1	C	306	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>6%</div> </div> </div>
1	D	306	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20776 atoms, of which 9568 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 Polyphosphate--nucleotide phosphotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	H	N	O	S	0	2	0
			4876	1589	2388	418	476	5			
1	B	295	Total	C	H	N	O	S	0	3	0
			4895	1595	2399	418	478	5			
1	C	288	Total	C	H	N	O	S	0	7	0
			4812	1568	2356	412	471	5			
1	D	288	Total	C	H	N	O	S	0	1	0
			4756	1552	2326	408	465	5			

There are 36 discrepancies between the modelled and reference sequences:

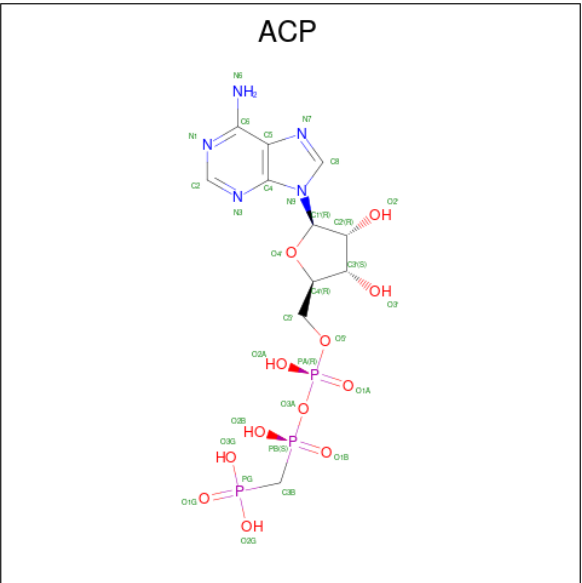
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
A	299	LEU	-	expression tag	UNP A0A3D5XRJ5
A	300	GLU	-	expression tag	UNP A0A3D5XRJ5
A	301	HIS	-	expression tag	UNP A0A3D5XRJ5
A	302	HIS	-	expression tag	UNP A0A3D5XRJ5
A	303	HIS	-	expression tag	UNP A0A3D5XRJ5
A	304	HIS	-	expression tag	UNP A0A3D5XRJ5
A	305	HIS	-	expression tag	UNP A0A3D5XRJ5
A	306	HIS	-	expression tag	UNP A0A3D5XRJ5
B	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
B	299	LEU	-	expression tag	UNP A0A3D5XRJ5
B	300	GLU	-	expression tag	UNP A0A3D5XRJ5
B	301	HIS	-	expression tag	UNP A0A3D5XRJ5
B	302	HIS	-	expression tag	UNP A0A3D5XRJ5
B	303	HIS	-	expression tag	UNP A0A3D5XRJ5
B	304	HIS	-	expression tag	UNP A0A3D5XRJ5
B	305	HIS	-	expression tag	UNP A0A3D5XRJ5
B	306	HIS	-	expression tag	UNP A0A3D5XRJ5
C	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
C	299	LEU	-	expression tag	UNP A0A3D5XRJ5
C	300	GLU	-	expression tag	UNP A0A3D5XRJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	301	HIS	-	expression tag	UNP A0A3D5XRJ5
C	302	HIS	-	expression tag	UNP A0A3D5XRJ5
C	303	HIS	-	expression tag	UNP A0A3D5XRJ5
C	304	HIS	-	expression tag	UNP A0A3D5XRJ5
C	305	HIS	-	expression tag	UNP A0A3D5XRJ5
C	306	HIS	-	expression tag	UNP A0A3D5XRJ5
D	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
D	299	LEU	-	expression tag	UNP A0A3D5XRJ5
D	300	GLU	-	expression tag	UNP A0A3D5XRJ5
D	301	HIS	-	expression tag	UNP A0A3D5XRJ5
D	302	HIS	-	expression tag	UNP A0A3D5XRJ5
D	303	HIS	-	expression tag	UNP A0A3D5XRJ5
D	304	HIS	-	expression tag	UNP A0A3D5XRJ5
D	305	HIS	-	expression tag	UNP A0A3D5XRJ5
D	306	HIS	-	expression tag	UNP A0A3D5XRJ5

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).



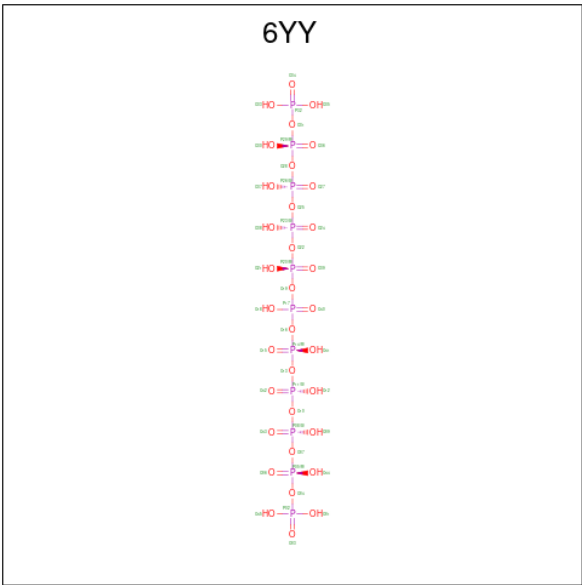
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	11	12	5	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	11	12	5	12	3		
2	C	1	Total	C	H	N	O	P	0	0
			43	11	12	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	D	1	Total	C	H	N	O	P	0	0
			43	11	12	5	12	3		

- Molecule 3 is bis[oxidanyl-[oxidanyl-[oxidanyl-[oxidanyl(phosphonooxy)phosphoryl]oxy-phosphoryl]oxy-phosphoryl]oxy-phosphoryl] hydrogen phosphate (CCD ID: 6YY) (formula: H<sub>13</sub>O<sub>34</sub>P<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



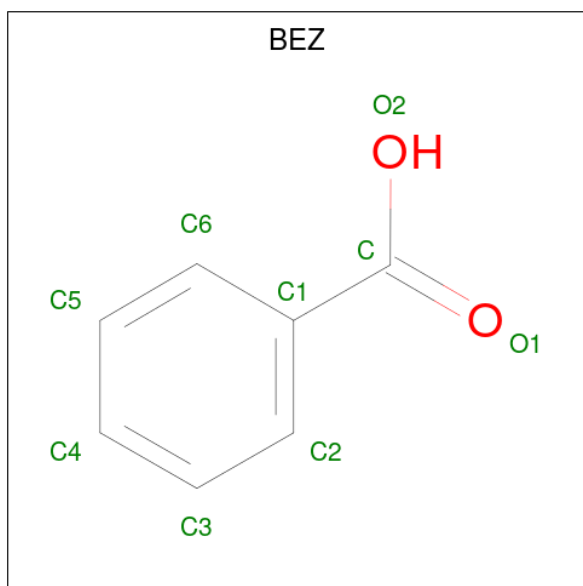
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			45	34	11		
3	B	1	Total	O	P	0	0
			45	34	11		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 5 is BENZOIC ACID (CCD ID: BEZ) (formula:  $C_7H_6O_2$ ).

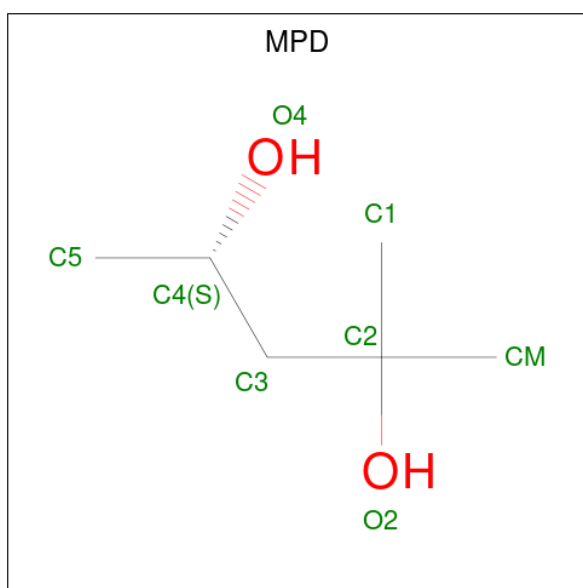


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	7	5	2		
5	C	1	Total	C	H	O	0	0
			14	7	5	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

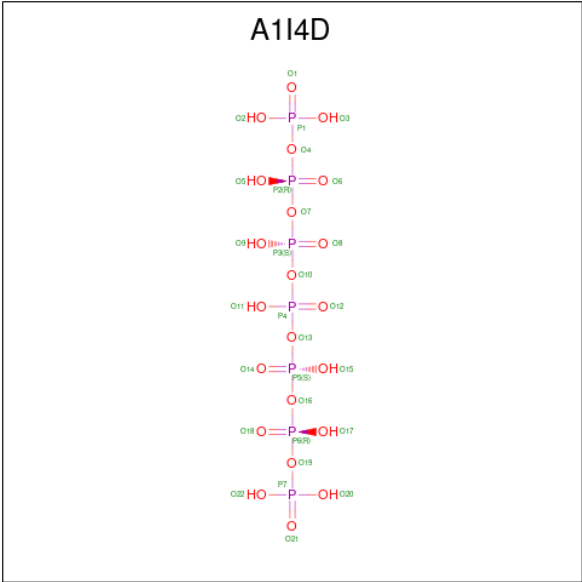
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Mg	0	0
			3	3		
6	B	3	Total	Mg	0	0
			3	3		
6	C	2	Total	Mg	0	0
			2	2		
6	D	2	Total	Mg	0	0
			2	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			20	6	12	2		
7	C	1	Total	C	H	O	0	0
			20	6	12	2		
7	D	1	Total	C	H	O	0	0
			20	6	12	2		

- Molecule 8 is bis[oxidanyl-[oxidanyl(phosphonooxy)phosphoryl]oxy-phosphoryl]hydrogen phosphate (CCD ID: A1I4D) (formula: H<sub>9</sub>O<sub>22</sub>P<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	P	0	0
			29	22	7		
8	D	1	Total	O	P	0	0
			29	22	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	231	Total	O	0	0
			231	231		
9	B	234	Total	O	0	0
			234	234		
9	C	270	Total	O	0	0
			270	270		
9	D	273	Total	O	0	0
			273	273		



### 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.

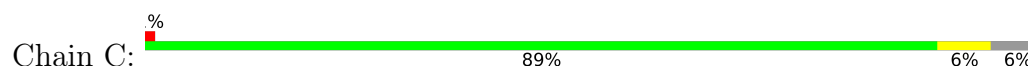
- Molecule 1: Polyphosphate--nucleotide phosphotransferase



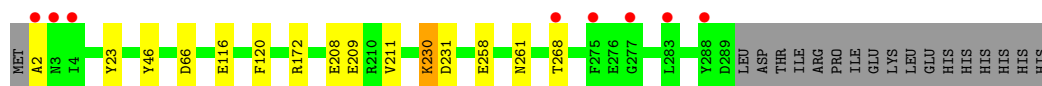
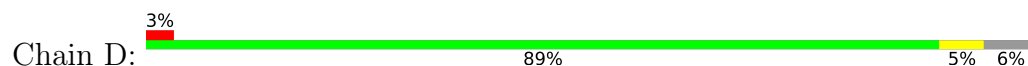
- Molecule 1: Polyphosphate--nucleotide phosphotransferase



- Molecule 1: Polyphosphate--nucleotide phosphotransferase



- Molecule 1: Polyphosphate--nucleotide phosphotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.89Å 110.73Å 152.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 1.70 48.90 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.90-1.70) 99.5 (48.90-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, $R_{free}$	0.167 , 0.197 0.167 , 0.197	Depositor DCC
$R_{free}$ test set	7187 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.63% 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: MG, A1I4D, GOL, BEZ, ACP, 6YY, MPD

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	0.88	1/2547 (0.0%)	1.19	6/3441 (0.2%)
1	B	0.90	2/2561 (0.1%)	1.23	8/3460 (0.2%)
1	C	0.94	1/2539 (0.0%)	1.25	9/3428 (0.3%)
1	D	0.95	2/2488 (0.1%)	1.25	6/3359 (0.2%)
All	All	0.92	6/10135 (0.1%)	1.23	29/13688 (0.2%)

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	1
1	B	0	1
1	D	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	GLU	CD-OE1	13.09	1.50	1.25
1	D	116	GLU	CD-OE1	11.27	1.46	1.25
1	D	261	ASN	C-O	-6.45	1.20	1.23
1	A	18	HIS	CE1-NE2	-5.83	1.26	1.32
1	B	172	ARG	NE-CZ	-5.42	1.27	1.33
1	B	101	HIS	ND1-CE1	5.09	1.37	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	GLU	CG-CD-OE2	-13.98	86.26	118.40
1	D	116	GLU	CG-CD-OE2	-12.76	89.05	118.40
1	C	116	GLU	CG-CD-OE1	10.70	143.01	118.40
1	D	116	GLU	CG-CD-OE1	10.15	141.74	118.40
1	D	116	GLU	CB-CG-CD	-8.74	97.75	112.60
1	C	116	GLU	CB-CG-CD	-8.44	98.26	112.60
1	B	267	VAL	N-CA-CB	-7.59	97.20	110.49
1	C	120	PHE	CA-CB-CG	7.07	120.87	113.80
1	A	209	GLU	CB-CG-CD	6.48	123.62	112.60
1	B	120	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	120	PHE	CA-CB-CG	6.23	120.03	113.80
1	D	120	PHE	CA-CB-CG	6.22	120.02	113.80
1	C	265	PRO	CB-CA-C	-5.93	103.64	111.23
1	C	168	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	116	GLU	CB-CG-CD	5.89	122.61	112.60
1	B	292	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	145	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	258	GLU	CB-CG-CD	-5.66	102.97	112.60
1	B	267	VAL	CB-CA-C	5.65	119.43	111.63
1	D	268	THR	CA-CB-OG1	-5.61	101.19	109.60
1	D	230	LYS	CB-CA-C	-5.58	102.11	110.88
1	A	230	LYS	CB-CA-C	5.56	120.01	110.79
1	B	251	GLU	CG-CD-OE2	-5.43	105.90	118.40
1	B	187	GLU	CB-CG-CD	5.38	121.75	112.60
1	C	206	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	116	GLU	CB-CG-CD	5.17	121.39	112.60
1	C	251	GLU	CG-CD-OE2	-5.13	106.59	118.40
1	A	189	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	275	PHE	CB-CA-C	-5.02	102.45	110.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	PRO	Peptide
1	B	172	ARG	Sidechain
1	D	172	ARG	Sidechain

## 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	2488	2388	2440	4	0
1	B	2496	2399	2453	7	0
1	C	2456	2356	2385	6	0
1	D	2430	2326	2378	6	0
2	A	31	12	14	0	0
2	B	31	12	14	0	0
2	C	31	12	14	1	0
2	D	31	12	14	0	0
3	A	45	0	0	0	0
3	B	45	0	0	0	0
4	A	6	5	8	0	0
5	A	9	5	5	0	0
5	C	9	5	5	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	B	8	12	14	0	0
7	C	8	12	14	1	0
7	D	8	12	14	4	1
8	C	29	0	0	0	0
8	D	29	0	0	0	0
9	A	231	0	0	1	1
9	B	234	0	0	1	0
9	C	270	0	0	5	0
9	D	273	0	0	3	0
All	All	11208	9568	9772	26	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 1.

All (26) 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:40:ILE:HG23	1:A:80:ALA:HB2	1.62	0.82
1:D:230:LYS:H	7:D:403:MPD:H11	1.45	0.80
7:D:403:MPD:H12	9:D:551:HOH:O	1.96	0.66
1:B:40:ILE:HG23	1:B:80:ALA:HB2	1.77	0.65
1:D:231:ASP:OD2	7:D:403:MPD:H51	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:TYR:OH	1:D:258:GLU:HG2	2.01	0.61
7:C:403:MPD:H51	9:C:620:HOH:O	2.01	0.59
1:C:290:LEU:C	9:C:503:HOH:O	2.46	0.58
1:B:267:VAL:HG22	1:B:271:THR:HG21	1.88	0.55
1:D:208:GLU:O	1:D:211:VAL:HG22	2.08	0.54
1:A:40:ILE:HG23	1:A:80:ALA:CB	2.37	0.52
1:D:2:ALA:N	9:D:503:HOH:O	2.44	0.49
1:C:66:ASP:OD2	1:C:209:GLU:OE1	2.31	0.48
1:C:268:THR:HG23	1:C:271:THR:H	1.79	0.47
1:B:120:PHE:HB3	1:B:122:ARG:O	2.15	0.46
1:B:267:VAL:CG2	1:B:271:THR:HG21	2.46	0.46
1:D:66:ASP:OD2	1:D:209:GLU:OE1	2.34	0.46
7:D:403:MPD:H13	9:D:709:HOH:O	2.17	0.44
1:B:40:ILE:HG23	1:B:80:ALA:CB	2.43	0.44
1:C:217:GLN:NE2	9:C:505:HOH:O	2.45	0.43
2:C:401:ACP:H3B2	9:C:725:HOH:O	2.19	0.42
1:A:174:ILE:HA	9:A:532:HOH:O	2.20	0.41
1:C:109[A]:ASN:ND2	9:C:512:HOH:O	2.54	0.41
1:B:278:TYR:OH	1:C:204:ASP:OD1	2.34	0.41
1:A:120:PHE:HB3	1:A:122:ARG:O	2.21	0.40
1:B:18:HIS:HE1	9:B:654:HOH:O	2.03	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:D:403:MPD:C5	9:A:713:HOH:O[4_455]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/306 (96%)	289 (98%)	5 (2%)	0	100	100
1	B	296/306 (97%)	291 (98%)	5 (2%)	0	100	100
1	C	293/306 (96%)	287 (98%)	6 (2%)	0	100	100
1	D	287/306 (94%)	282 (98%)	5 (2%)	0	100	100
All	All	1170/1224 (96%)	1149 (98%)	21 (2%)	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	273/282 (97%)	269 (98%)	4 (2%)	60	47
1	B	274/282 (97%)	270 (98%)	4 (2%)	60	47
1	C	271/282 (96%)	269 (99%)	2 (1%)	81	75
1	D	265/282 (94%)	264 (100%)	1 (0%)	89	85
All	All	1083/1128 (96%)	1072 (99%)	11 (1%)	73	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	23	TYR
1	A	164	LYS
1	A	296	ILE
1	B	23	TYR
1	B	209	GLU
1	B	263	LYS
1	B	267	VAL
1	C	16	ASN
1	C	23	TYR
1	D	23	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	12	ASN
1	A	18	HIS
1	A	63	GLN
1	B	18	HIS
1	C	18	HIS
1	C	141	ASN
1	C	161	ASN
1	C	168	ASN
1	C	217	GLN
1	D	17	ASN
1	D	18	HIS
1	D	169	ASN
1	D	218	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 10 are monoatomic - leaving 14 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	ACP	A	401	6	27,33,33	0.96	1 (3%)	32,52,52	1.17	2 (6%)
7	MPD	C	403	-	7,7,7	0.36	0	9,10,10	0.82	0
8	A1I4D	C	402	6	16,28,28	1.37	1 (6%)	23,48,48	1.60	5 (21%)
7	MPD	B	403	-	7,7,7	0.45	0	9,10,10	0.73	0
2	ACP	D	401	6	27,33,33	0.99	1 (3%)	32,52,52	1.30	5 (15%)
4	GOL	A	403	-	5,5,5	0.13	0	5,5,5	0.28	0
7	MPD	D	403	-	7,7,7	0.45	0	9,10,10	1.08	1 (11%)
8	A1I4D	D	402	6	16,28,28	0.95	0	23,48,48	1.42	3 (13%)
3	6YY	B	402	6	24,44,44	1.14	0	31,76,76	1.59	3 (9%)
3	6YY	A	402	6	24,44,44	0.96	0	31,76,76	1.91	7 (22%)
5	BEZ	A	404	-	9,9,9	1.27	1 (11%)	11,11,11	1.43	2 (18%)
5	BEZ	C	404	-	9,9,9	1.53	2 (22%)	11,11,11	1.00	0
2	ACP	C	401	6	27,33,33	1.12	2 (7%)	32,52,52	1.32	6 (18%)
2	ACP	B	401	6	27,33,33	0.86	1 (3%)	32,52,52	1.18	2 (6%)

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	ACP	A	401	6	-	9/15/38/38	0/3/3/3
7	MPD	C	403	-	-	2/5/5/5	-
8	A1I4D	C	402	6	-	3/36/36/36	-
7	MPD	B	403	-	-	0/5/5/5	-
2	ACP	D	401	6	-	4/15/38/38	0/3/3/3
4	GOL	A	403	-	-	0/4/4/4	-
7	MPD	D	403	-	-	1/5/5/5	-
8	A1I4D	D	402	6	-	5/36/36/36	-
3	6YY	B	402	6	-	9/60/60/60	-
3	6YY	A	402	6	-	12/60/60/60	-
5	BEZ	A	404	-	-	0/4/4/4	0/1/1/1
5	BEZ	C	404	-	-	0/4/4/4	0/1/1/1
2	ACP	C	401	6	-	4/15/38/38	0/3/3/3
2	ACP	B	401	6	-	6/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ACP	PB-O3A	4.15	1.63	1.58
5	A	404	BEZ	C1-C	-3.42	1.42	1.49
5	C	404	BEZ	C1-C	-3.38	1.42	1.49
5	C	404	BEZ	O2-C	-2.94	1.21	1.30
2	A	401	ACP	PB-O3A	2.79	1.61	1.58
8	C	402	A1I4D	P1-O3	2.47	1.64	1.54
2	B	401	ACP	PB-O2B	-2.30	1.51	1.56
2	D	401	ACP	PB-O3A	2.06	1.60	1.58
2	C	401	ACP	PB-O2B	-2.02	1.51	1.56

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	6YY	P11-O10-P08	4.73	149.05	132.83
3	B	402	6YY	P14-O13-P11	4.59	148.57	132.83
3	A	402	6YY	P14-O13-P11	4.32	147.66	132.83
8	C	402	A1I4D	O3-P1-O4	3.44	116.17	104.64
3	B	402	6YY	P08-O07-P05	3.39	144.44	132.83
2	C	401	ACP	O1G-PG-C3B	-3.31	104.11	111.24
2	A	401	ACP	PB-O3A-PA	3.25	142.88	132.56
3	A	402	6YY	P26-O25-P23	-3.18	121.91	132.83
2	B	401	ACP	O1G-PG-C3B	-3.08	104.60	111.24
3	A	402	6YY	O45-P02-O01	3.06	119.33	107.64
2	A	401	ACP	O1G-PG-C3B	-2.92	104.94	111.24
2	D	401	ACP	O1G-PG-C3B	-2.89	105.01	111.24
3	B	402	6YY	P26-O25-P23	-2.83	123.12	132.83
8	D	402	A1I4D	O5-P2-O6	2.76	125.89	112.24
5	A	404	BEZ	O1-C-C1	-2.74	114.15	121.45
2	C	401	ACP	O1B-PB-C3B	2.69	116.19	109.07
2	D	401	ACP	O2B-PB-O1B	2.67	118.97	110.07
3	A	402	6YY	O35-P32-O33	2.65	117.78	107.64
3	A	402	6YY	O45-P02-O03	-2.64	100.36	110.68
8	D	402	A1I4D	O2-P1-O4	2.62	113.43	104.64
2	D	401	ACP	O1B-PB-C3B	-2.60	102.21	109.07
8	D	402	A1I4D	P5-O13-P4	-2.47	124.35	132.83
8	C	402	A1I4D	O3-P1-O2	2.33	116.56	107.64
2	D	401	ACP	PB-O3A-PA	2.33	139.96	132.56
2	D	401	ACP	C4-C5-N7	2.32	111.81	109.40
2	C	401	ACP	O3G-PG-O2G	2.26	114.67	108.08
2	B	401	ACP	O2B-PB-O1B	2.25	117.58	110.07
8	C	402	A1I4D	P5-O13-P4	-2.23	125.18	132.83
7	D	403	MPD	O2-C2-C3	-2.18	101.61	109.80
3	A	402	6YY	O21-P20-O39	2.18	123.00	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	A1I4D	O3-P1-O1	-2.14	102.30	110.68
2	C	401	ACP	O4'-C1'-C2'	-2.11	103.84	106.93
5	A	404	BEZ	C6-C1-C2	2.05	121.51	118.59
8	C	402	A1I4D	O17-P6-O18	2.05	122.36	112.24
2	C	401	ACP	O2A-PA-O1A	2.03	122.29	112.24
2	C	401	ACP	O2B-PB-O1B	2.02	116.83	110.07

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ACP	PB-C3B-PG-O1G
2	A	401	ACP	PB-C3B-PG-O2G
2	A	401	ACP	C5'-O5'-PA-O3A
2	B	401	ACP	PG-C3B-PB-O1B
2	B	401	ACP	C5'-O5'-PA-O2A
2	C	401	ACP	PB-C3B-PG-O1G
2	C	401	ACP	PB-C3B-PG-O2G
2	C	401	ACP	PB-C3B-PG-O3G
3	A	402	6YY	P05-O04-P02-O01
3	A	402	6YY	P29-O31-P32-O33
3	B	402	6YY	P29-O31-P32-O33
8	D	402	A1I4D	P6-O19-P7-O22
2	A	401	ACP	O4'-C4'-C5'-O5'
2	A	401	ACP	PB-O3A-PA-O1A
2	A	401	ACP	C3'-C4'-C5'-O5'
3	B	402	6YY	P29-O31-P32-O34
8	C	402	A1I4D	P6-O19-P7-O21
8	D	402	A1I4D	P6-O19-P7-O21
3	A	402	6YY	P14-O13-P11-O42
2	A	401	ACP	PB-O3A-PA-O5'
2	D	401	ACP	O4'-C4'-C5'-O5'
3	B	402	6YY	P05-O04-P02-O01
3	B	402	6YY	P05-O04-P02-O45
8	C	402	A1I4D	P6-O19-P7-O22
2	B	401	ACP	C5'-O5'-PA-O3A
2	D	401	ACP	C5'-O5'-PA-O3A
3	B	402	6YY	P14-O16-P17-O40
7	C	403	MPD	C2-C3-C4-C5
7	D	403	MPD	C2-C3-C4-C5
2	A	401	ACP	C5'-O5'-PA-O1A
7	C	403	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	A	401	ACP	PB-C3B-PG-O3G
2	B	401	ACP	PG-C3B-PB-O3A
3	A	402	6YY	P05-O07-P08-O09
3	B	402	6YY	P11-O13-P14-O41
3	A	402	6YY	P29-O31-P32-O34
2	B	401	ACP	O4'-C4'-C5'-O5'
3	A	402	6YY	P14-O13-P11-O12
3	B	402	6YY	P08-O07-P05-O06
8	D	402	A1I4D	P1-O4-P2-O6
8	D	402	A1I4D	P5-O16-P6-O17
3	A	402	6YY	P05-O04-P02-O03
3	A	402	6YY	P05-O04-P02-O45
2	D	401	ACP	PB-O3A-PA-O1A
2	D	401	ACP	PB-O3A-PA-O2A
3	A	402	6YY	P05-O07-P08-O43
3	A	402	6YY	P11-O10-P08-O43
3	A	402	6YY	P14-O16-P17-O18
3	A	402	6YY	P26-O28-P29-O36
3	B	402	6YY	P11-O13-P14-O15
3	B	402	6YY	P14-O16-P17-O18
8	C	402	A1I4D	P5-O16-P6-O18
8	D	402	A1I4D	P5-O16-P6-O18
2	B	401	ACP	C5'-O5'-PA-O1A
2	C	401	ACP	O4'-C4'-C5'-O5'

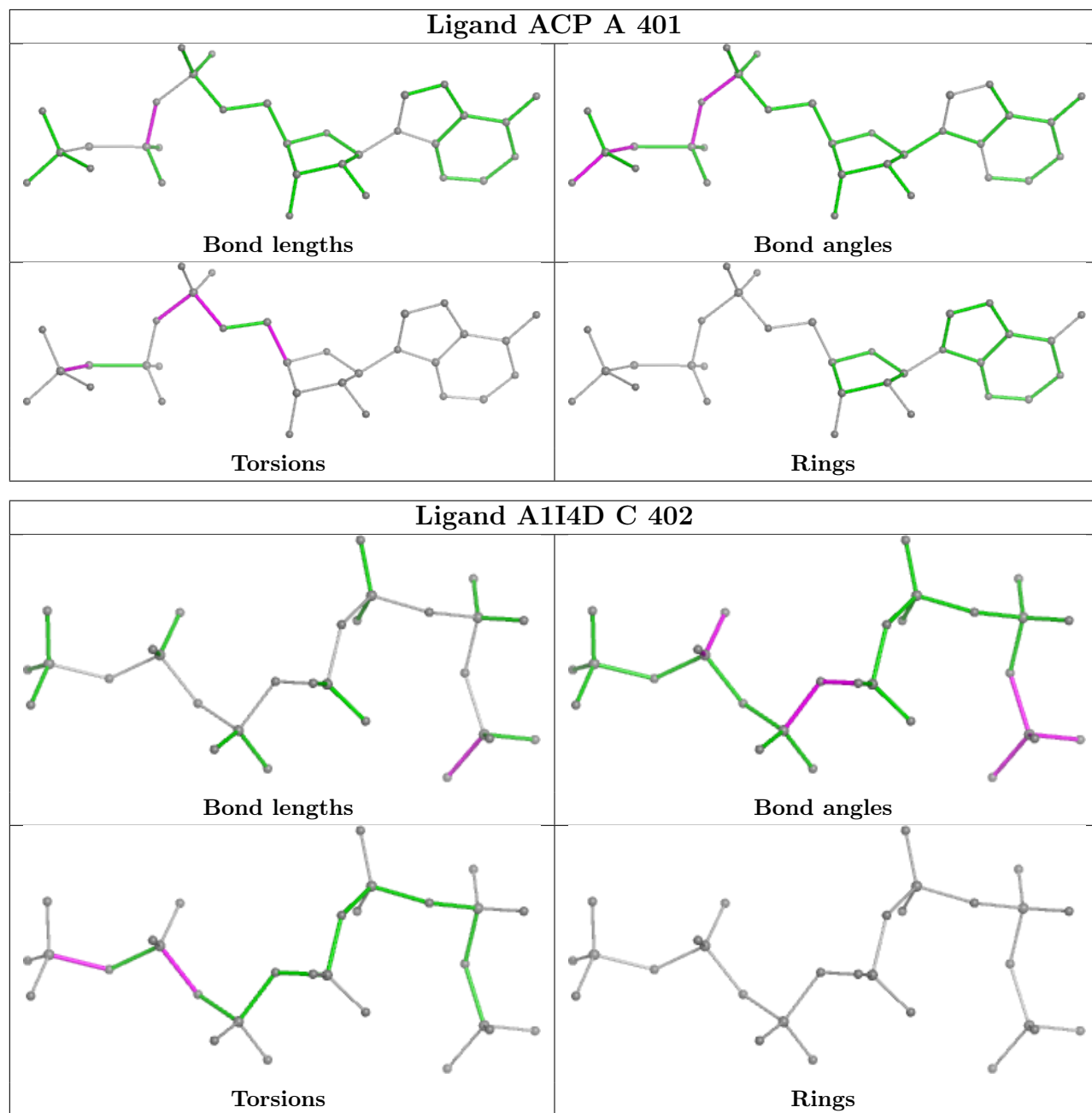
There are no ring outliers.

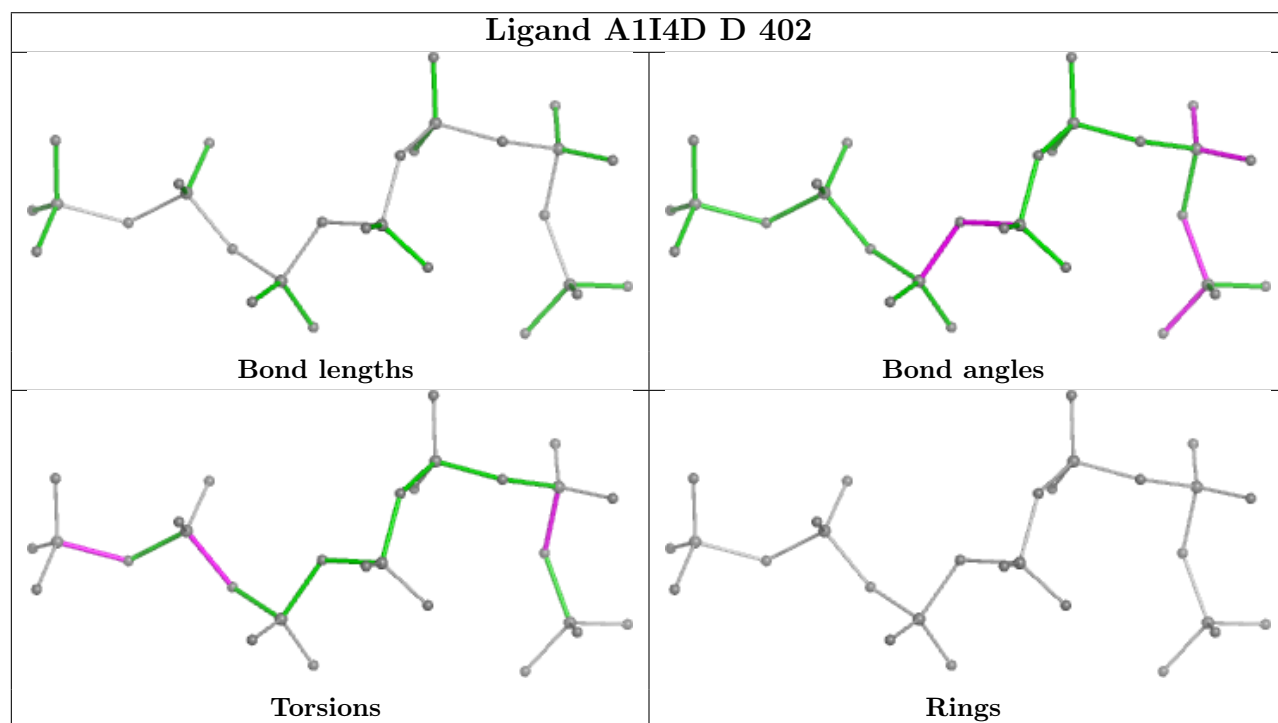
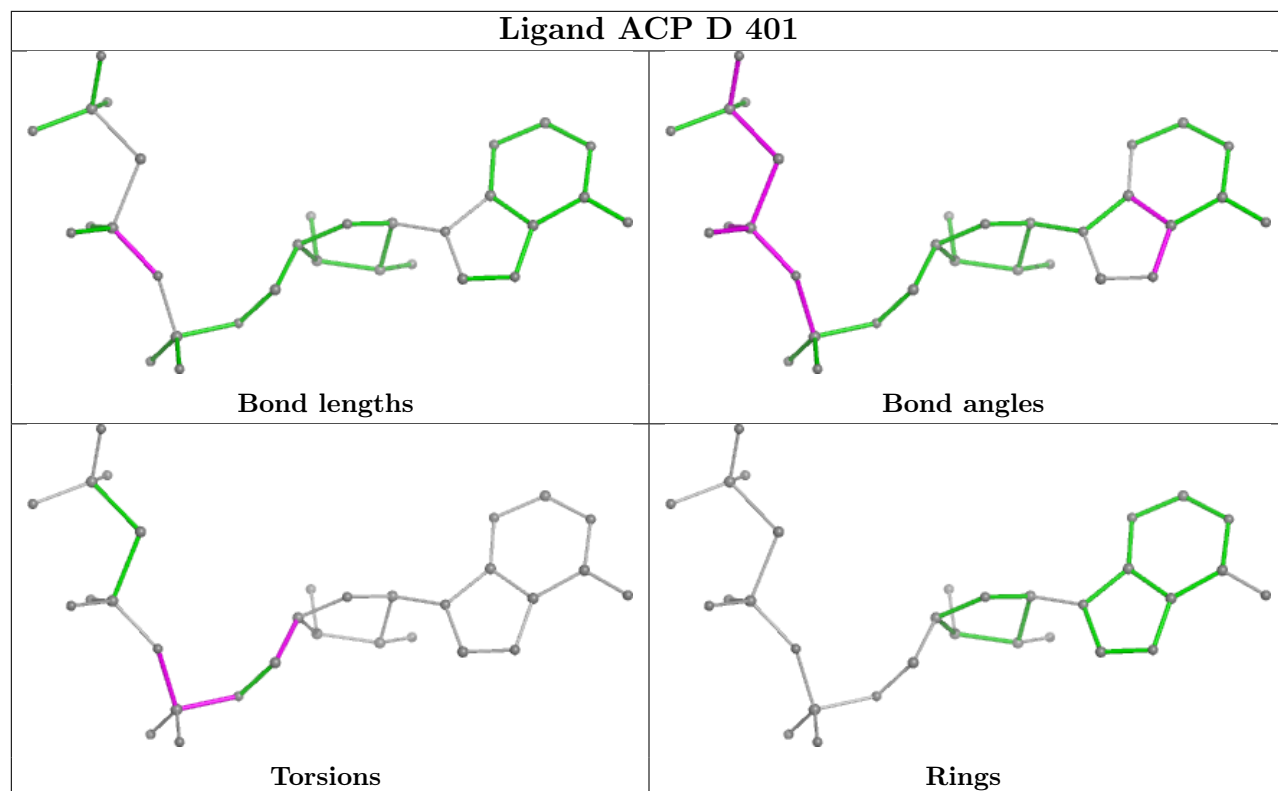
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	403	MPD	1	0
7	D	403	MPD	4	1
2	C	401	ACP	1	0

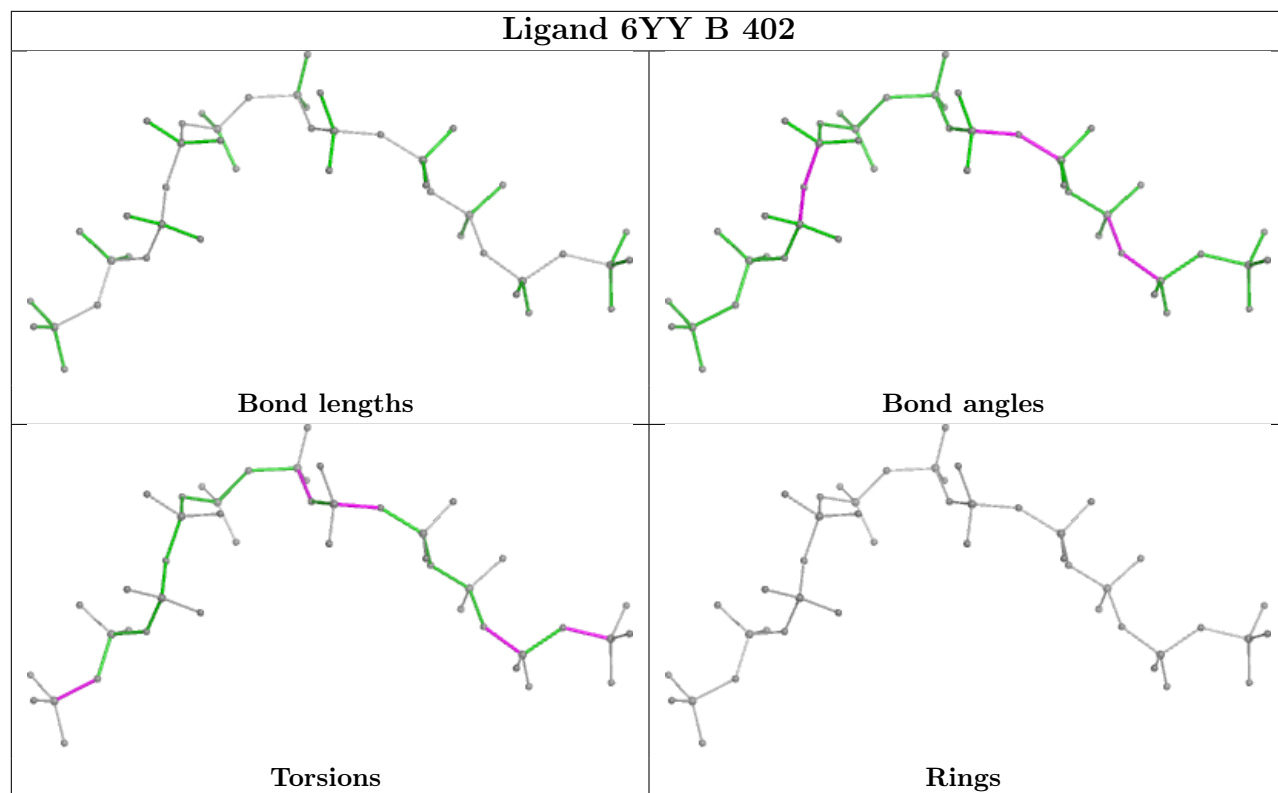
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

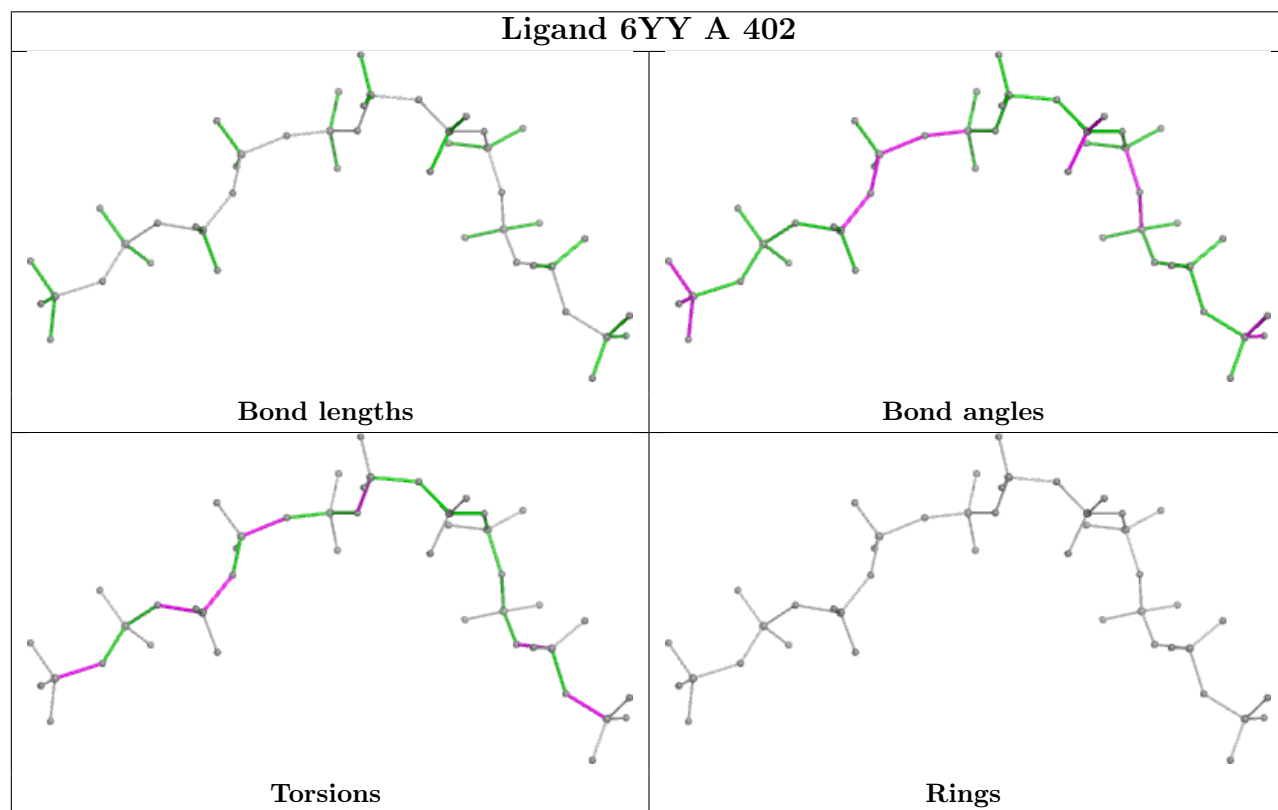


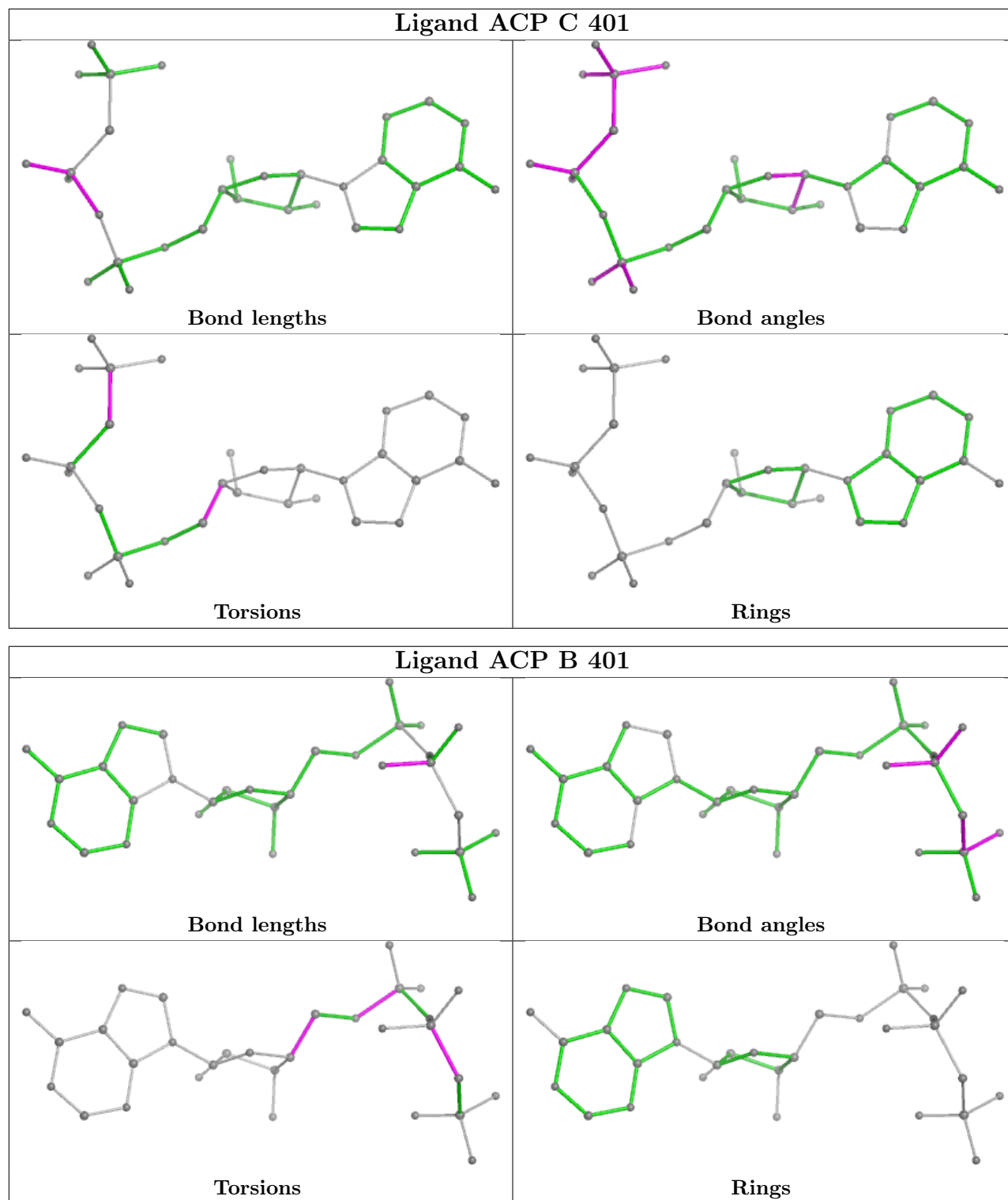


## Ligand 6YY B 402



## Ligand 6YY A 402





## 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

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	294/306 (96%)	-0.23	6 (2%) 64 68	11, 29, 57, 102	2 (0%)
1	B	295/306 (96%)	-0.33	5 (1%) 69 71	12, 27, 50, 96	3 (1%)
1	C	288/306 (94%)	-0.49	4 (1%) 73 76	9, 24, 54, 89	4 (1%)
1	D	288/306 (94%)	-0.48	8 (2%) 55 58	11, 23, 70, 99	1 (0%)
All	All	1165/1224 (95%)	-0.38	23 (1%) 64 68	9, 26, 57, 102	10 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	ILE	7.4
1	A	296	ILE	7.3
1	D	2	ALA	5.4
1	A	4	ILE	4.8
1	B	2	ALA	4.2
1	D	288	TYR	4.1
1	A	202	PHE	4.1
1	C	4	ILE	3.6
1	B	295	PRO	3.5
1	B	4	ILE	3.4
1	B	3	ASN	3.1
1	C	290	LEU	2.9
1	D	275	PHE	2.9
1	D	283	LEU	2.4
1	A	3	ASN	2.4
1	C	268	THR	2.3
1	A	196	PRO	2.3
1	C	3	ASN	2.1
1	D	277	GLY	2.1
1	A	295	PRO	2.1
1	D	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	3	ASN	2.1
1	D	268	THR	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 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.

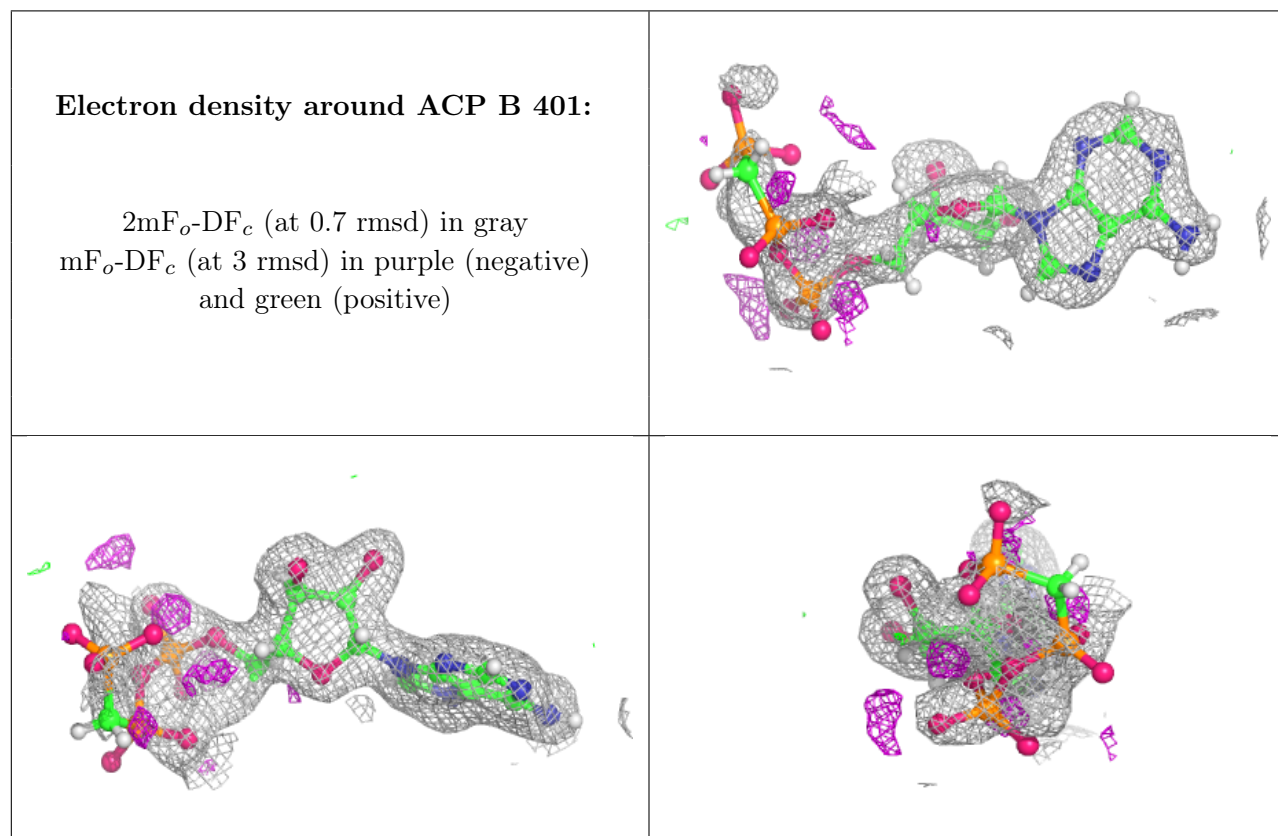
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MPD	B	403	8/8	0.67	0.21	40,54,59,85	0
6	MG	A	407	1/1	0.73	0.16	65,65,65,65	0
4	GOL	A	403	6/6	0.86	0.20	61,65,70,76	0
7	MPD	C	403	8/8	0.87	0.15	52,64,67,75	0
6	MG	D	405	1/1	0.88	0.14	46,46,46,46	0
2	ACP	B	401	31/31	0.89	0.11	30,40,129,141	0
2	ACP	A	401	31/31	0.89	0.11	29,42,139,161	0
7	MPD	D	403	8/8	0.89	0.10	24,33,37,51	0
6	MG	A	406	1/1	0.91	0.15	50,50,50,50	0
2	ACP	D	401	31/31	0.91	0.10	21,31,126,141	0
6	MG	B	405	1/1	0.91	0.10	62,62,62,62	0
6	MG	C	406	1/1	0.91	0.10	50,50,50,50	0
2	ACP	C	401	31/31	0.92	0.10	23,30,101,128	0
6	MG	B	406	1/1	0.94	0.15	41,41,41,41	0
5	BEZ	A	404	9/9	0.94	0.09	27,30,41,41	0
6	MG	C	405	1/1	0.97	0.11	37,37,37,37	0
3	6YY	A	402	45/45	0.97	0.07	21,35,91,99	0
5	BEZ	C	404	9/9	0.97	0.05	20,22,35,35	0
3	6YY	B	402	45/45	0.98	0.08	19,29,103,115	0
6	MG	D	404	1/1	0.98	0.07	37,37,37,37	0
6	MG	B	404	1/1	0.99	0.02	21,21,21,21	0

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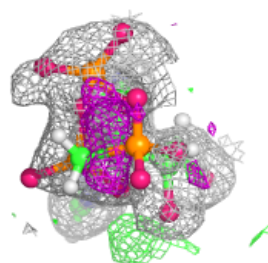
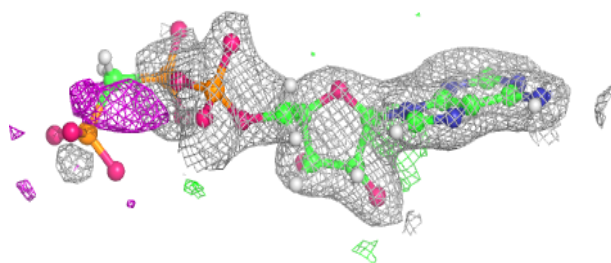
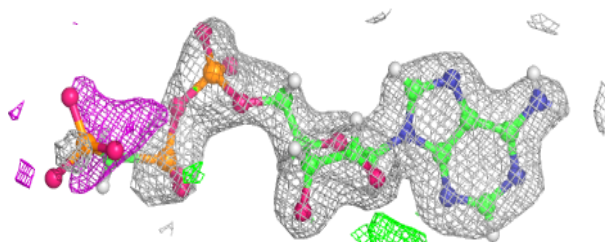
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	A	405	1/1	0.99	0.03	22,22,22,22	0
8	A1I4D	C	402	29/29	0.99	0.05	17,21,48,52	0
8	A1I4D	D	402	29/29	0.99	0.04	16,20,34,49	0

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.

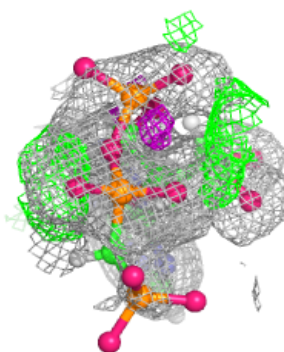
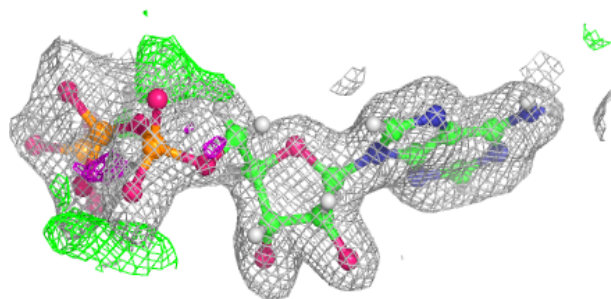
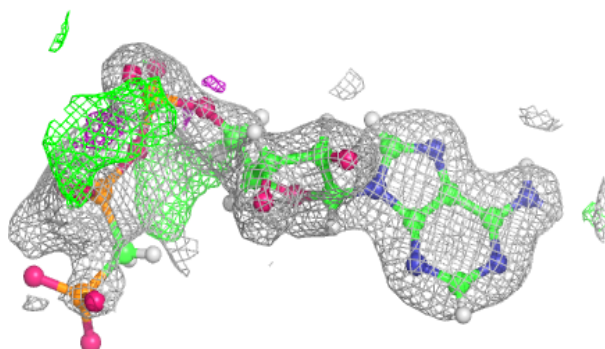


**Electron density around ACP A 401:**

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

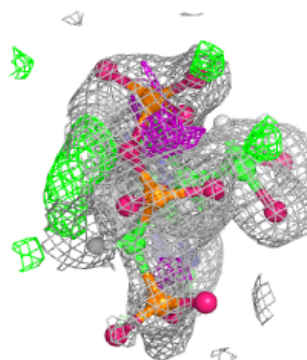
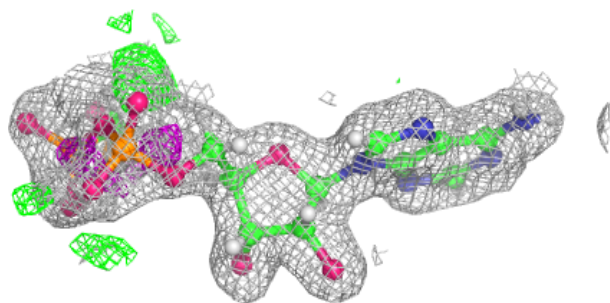
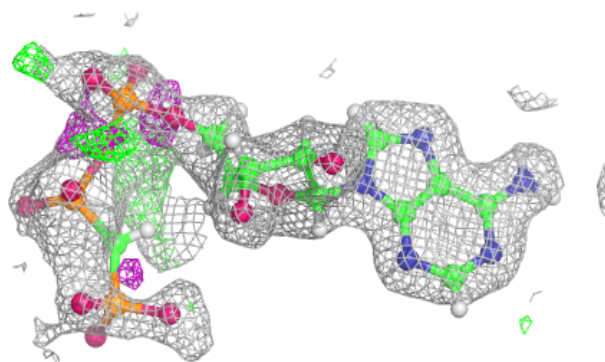
**Electron density around ACP D 401:**

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

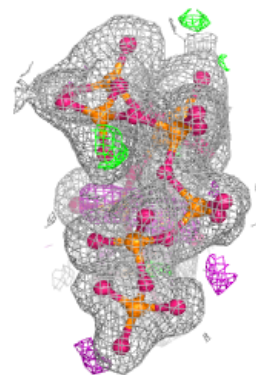
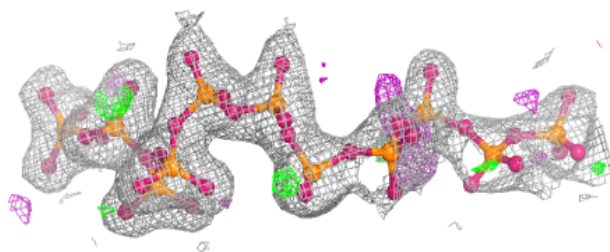
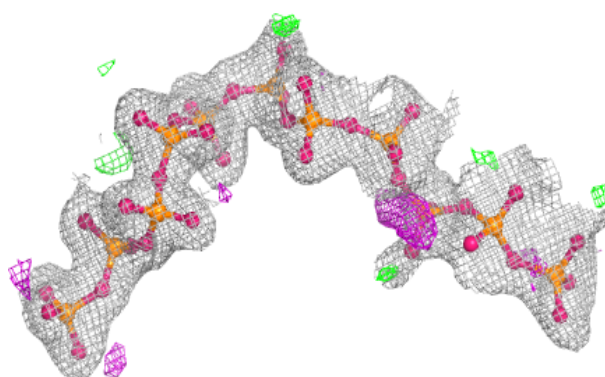


**Electron density around ACP C 401:**

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

**Electron density around 6YY A 402:**

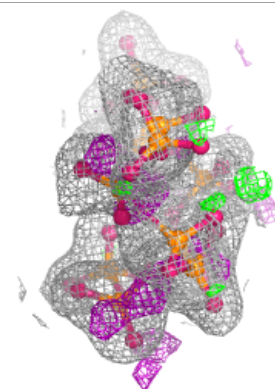
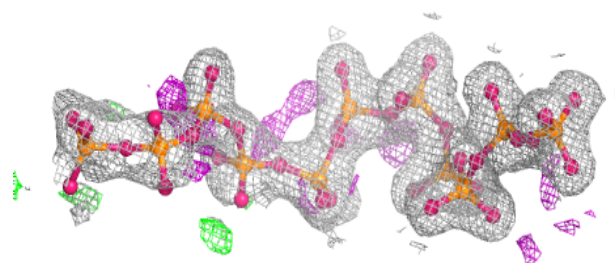
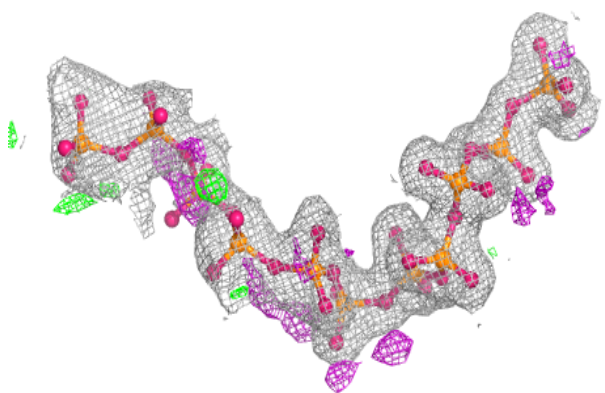
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



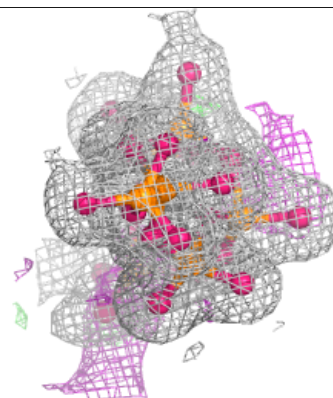
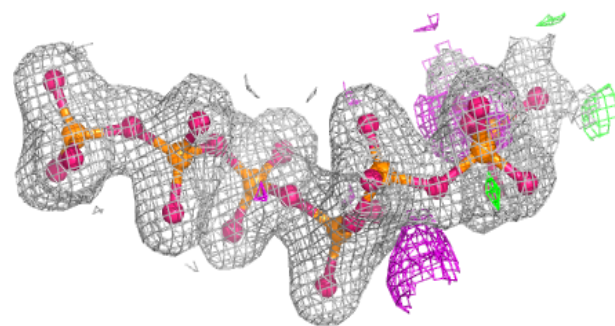
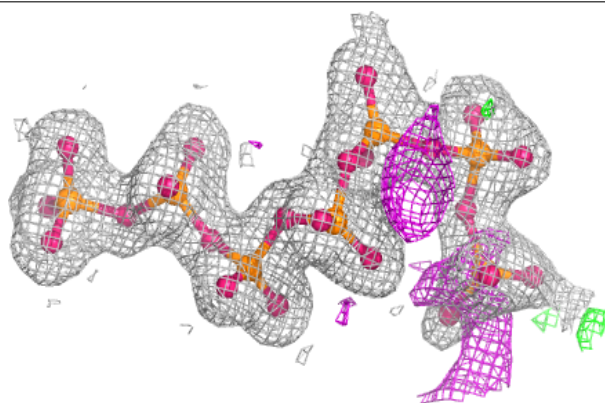


**Electron density around 6YY B 402:**

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

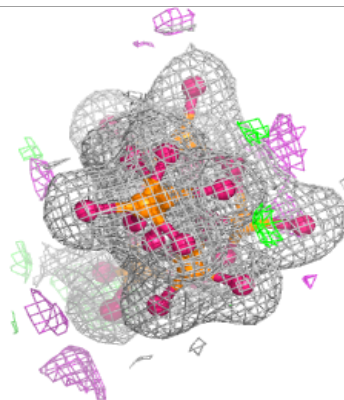
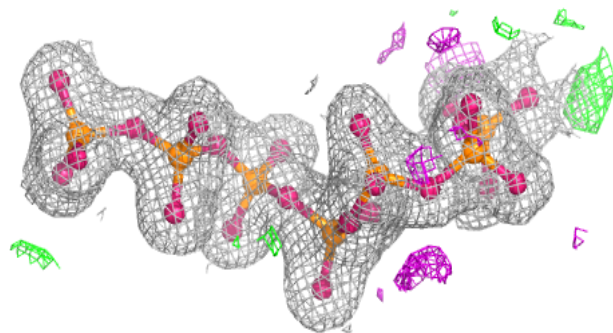
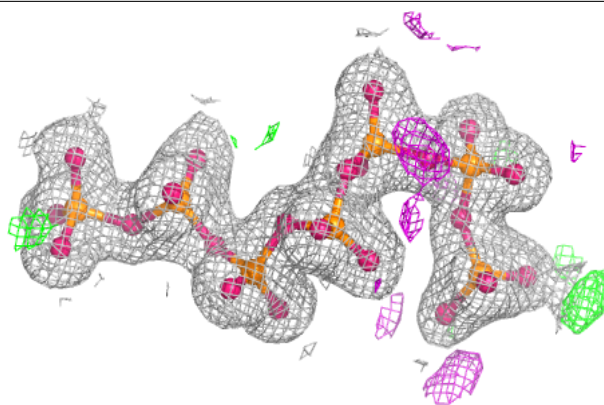
**Electron density around A1I4D C 402:**

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



**Electron density around A1I4D D 402:**

$2mF_o-DF_c$  (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.