



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:22 AM EDT

PDB ID : 5KLQ  
Title : Crystal structure of HopZ1a in complex with IP6 and CoA  
Authors : Zhang, Z.-M.; Song, J.  
Deposited on : 2016-06-24  
Resolution : 3.40 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

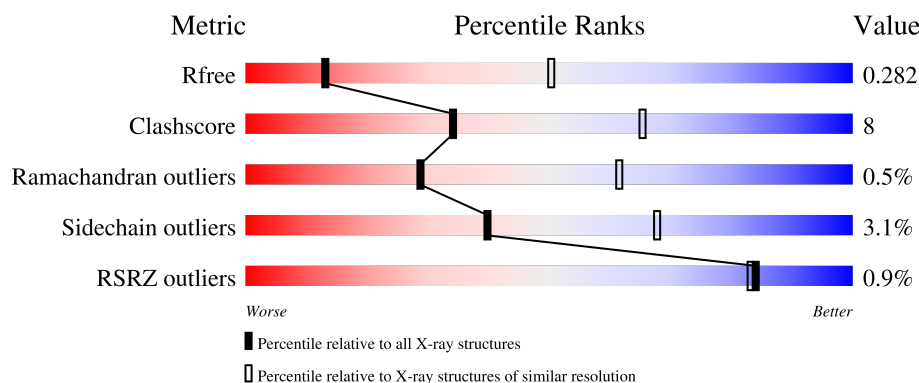
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	342	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	342	<div> <div></div> <div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div> </div>
1	C	342	<div> <div>%</div> <div> <div>73%</div> <div>20%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7575 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 Orf34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	320	Total	C	N	O	S	0	1	0
			2434	1521	444	461	8			
1	A	324	Total	C	N	O	S	0	1	0
			2466	1535	453	469	9			
1	B	320	Total	C	N	O	S	0	1	0
			2427	1513	449	457	8			

There are 27 discrepancies between the modelled and reference sequences:

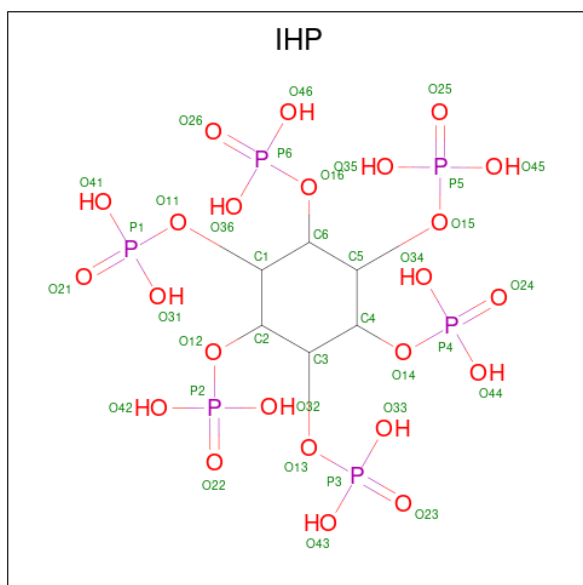
Chain	Residue	Modelled	Actual	Comment	Reference
C	28	SER	-	expression tag	UNP Q6VE93
C	82	ALA	LYS	engineered mutation	UNP Q6VE93
C	83	ALA	LYS	engineered mutation	UNP Q6VE93
C	119	TYR	LYS	engineered mutation	UNP Q6VE93
C	120	TYR	GLU	engineered mutation	UNP Q6VE93
C	298	TYR	LYS	engineered mutation	UNP Q6VE93
C	299	TYR	GLN	engineered mutation	UNP Q6VE93
C	366	ALA	GLU	engineered mutation	UNP Q6VE93
C	367	ALA	GLU	engineered mutation	UNP Q6VE93
A	28	SER	-	expression tag	UNP Q6VE93
A	82	ALA	LYS	engineered mutation	UNP Q6VE93
A	83	ALA	LYS	engineered mutation	UNP Q6VE93
A	119	TYR	LYS	engineered mutation	UNP Q6VE93
A	120	TYR	GLU	engineered mutation	UNP Q6VE93
A	298	TYR	LYS	engineered mutation	UNP Q6VE93
A	299	TYR	GLN	engineered mutation	UNP Q6VE93
A	366	ALA	GLU	engineered mutation	UNP Q6VE93
A	367	ALA	GLU	engineered mutation	UNP Q6VE93
B	28	SER	-	expression tag	UNP Q6VE93
B	82	ALA	LYS	engineered mutation	UNP Q6VE93
B	83	ALA	LYS	engineered mutation	UNP Q6VE93
B	119	TYR	LYS	engineered mutation	UNP Q6VE93
B	120	TYR	GLU	engineered mutation	UNP Q6VE93

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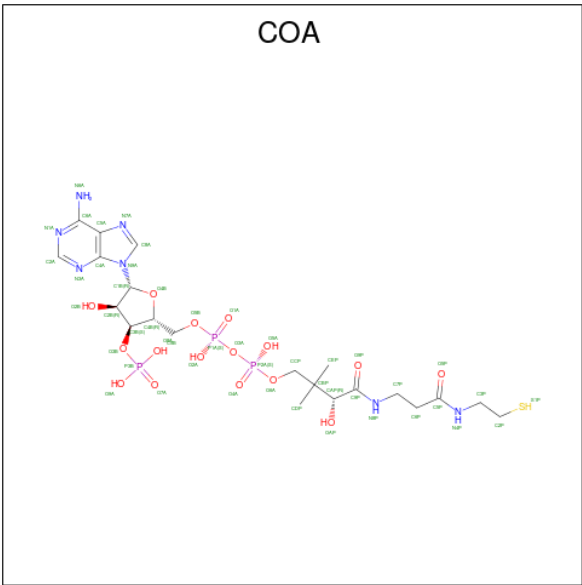
Chain	Residue	Modelled	Actual	Comment	Reference
B	298	TYR	LYS	engineered mutation	UNP Q6VE93
B	299	TYR	GLN	engineered mutation	UNP Q6VE93
B	366	ALA	GLU	engineered mutation	UNP Q6VE93
B	367	ALA	GLU	engineered mutation	UNP Q6VE93

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



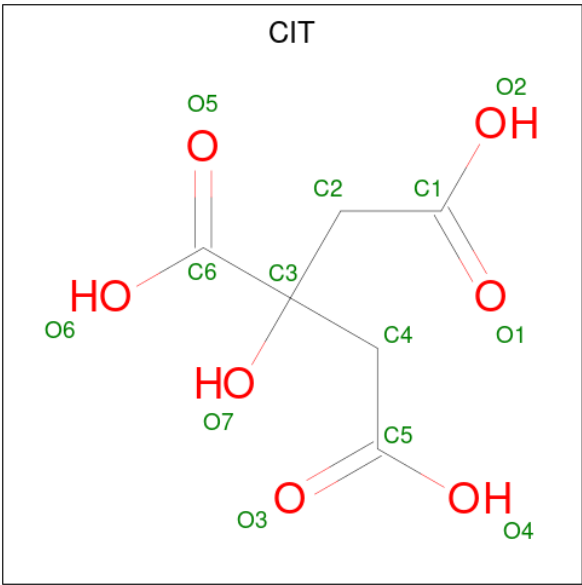
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			36	6	24	6		
2	A	1	Total	C	O	P	0	0
			36	6	24	6		
2	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P		0	0
			31	10	5	13	3			

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		



R335	E336	L337	L338	D339	T340	E341	T342	P343	S344	N345	T346	F355	Q358	E359	I360	K361	R362	Q368	ARG
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.13Å 82.30Å 86.27Å 64.20° 76.69° 89.35°	Depositor
Resolution (Å)	47.57 – 3.40 47.56 – 3.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.57-3.40) 97.3 (47.56-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.234 , 0.281 0.237 , 0.282	Depositor DCC
$R_{free}$ test set	1609 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 8.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for -h,k,k-l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: COA, CIT, IHP

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	0.27	0/2518	0.48	0/3416
1	B	0.27	0/2478	0.46	0/3362
1	C	0.27	0/2486	0.46	0/3375
All	All	0.27	0/7482	0.46	0/10153

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
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	GLU	Peptide
1	B	342	THR	Peptide

### 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2466	0	2352	42	0
1	B	2427	0	2323	36	0
1	C	2434	0	2331	50	0
2	A	36	0	6	1	0
2	B	36	0	6	2	0
2	C	36	0	6	7	0
3	A	48	0	32	5	0
3	B	31	0	11	0	0
3	C	48	0	32	3	0
4	B	13	0	5	0	0
All	All	7575	0	7104	123	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 8.

All (123) 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:C:59:PRO:O	1:C:63:HIS:ND1	2.20	0.75
1:B:358:GLN:NE2	2:B:401:IHP:O45	2.20	0.73
1:A:294:LEU:N	3:A:402:COA:O8A	2.23	0.72
1:A:150[B]:HIS:NE2	3:A:402:COA:S1P	2.65	0.70
1:A:134:ARG:NH1	1:A:155:ASP:OD1	2.27	0.67
1:C:78:ARG:HH22	1:C:214:ASP:HB3	1.59	0.66
1:B:174:ILE:HG13	1:B:206:GLU:HB2	1.78	0.66
1:A:168:ILE:HB	1:A:204:ILE:HG12	1.79	0.65
1:A:292:ALA:HA	1:A:349:SER:HB3	1.79	0.63
1:B:175:VAL:HA	1:B:182:LEU:HB2	1.80	0.62
1:C:179:TYR:HD2	1:A:251:GLU:HG3	1.62	0.62
1:A:78:ARG:NH1	1:A:214:ASP:OD2	2.32	0.62
1:C:317:HIS:NE2	2:C:401:IHP:O36	2.32	0.61
1:B:141:CYS:HB2	1:B:148:LEU:HD11	1.81	0.61
1:A:44:ARG:HB2	1:A:81:GLY:HA2	1.84	0.60
1:A:344:SER:N	1:A:345:ASN:HA	2.16	0.60
1:B:72:GLY:HA2	1:B:360:ILE:HD13	1.84	0.59
1:A:311:ARG:NH1	1:A:314:SER:O	2.36	0.59
1:A:336:GLU:HB3	1:A:337:LEU:HA	1.84	0.58
1:A:343:PRO:C	1:A:345:ASN:HA	2.24	0.58
1:B:311:ARG:NH1	1:B:314:SER:O	2.37	0.57
1:C:317:HIS:HE2	2:C:401:IHP:P6	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:H	1:C:335:ARG:HH22	1.54	0.56
1:C:106:ARG:NH2	2:C:401:IHP:O24	2.34	0.56
1:B:130:PRO:HG2	1:B:133:PHE:HB3	1.87	0.56
1:C:99:MET:O	1:C:101:TYR:N	2.38	0.56
1:C:99:MET:O	1:C:100:VAL:C	2.43	0.56
1:A:77:ASP:HB3	1:A:82:ALA:HB3	1.88	0.55
1:C:219:TYR:OH	1:C:290:HIS:O	2.14	0.55
1:B:301:MET:HE1	1:B:324:VAL:H	1.72	0.55
1:A:103:GLU:OE2	1:A:362:ARG:NH1	2.36	0.54
1:A:148:LEU:O	1:A:150[A]:HIS:ND1	2.35	0.54
1:C:179:TYR:CD2	1:A:251:GLU:HG3	2.43	0.54
1:C:272:GLU:HG3	1:A:244:GLY:HA3	1.90	0.53
1:B:118:HIS:NE2	1:B:191:ASP:OD2	2.39	0.53
1:B:335:ARG:HG3	1:B:336:GLU:H	1.73	0.53
1:C:294:LEU:N	3:C:402:COA:O9A	2.42	0.53
1:B:208:GLN:O	1:B:211:LYS:NZ	2.40	0.53
1:C:253:ARG:NH2	1:C:262:GLU:OE2	2.41	0.52
1:A:78:ARG:HH22	1:A:214:ASP:HB3	1.73	0.52
1:B:249:GLU:HG3	1:B:276:ALA:O	2.10	0.52
1:B:341:GLU:O	1:B:343:PRO:HD2	2.11	0.51
1:A:46:GLN:N	1:A:46:GLN:OE1	2.44	0.51
1:B:106:ARG:NH2	2:B:401:IHP:O43	2.43	0.51
1:C:265:SER:HB2	1:C:267:TYR:CZ	2.45	0.51
1:C:343:PRO:O	1:C:344:SER:OG	2.25	0.51
1:A:174:ILE:HG13	1:A:206:GLU:HB2	1.93	0.51
1:A:343:PRO:O	1:A:344:SER:OG	2.27	0.50
1:C:334:ARG:NH2	3:C:402:COA:H2B	2.27	0.50
1:B:334:ARG:N	1:B:346:THR:O	2.45	0.50
1:C:226:LYS:HD2	1:C:286:ASP:HB3	1.94	0.50
1:C:233:GLN:O	1:C:237:ILE:HG13	2.11	0.50
1:C:99:MET:HE3	1:C:359:GLU:HB2	1.93	0.50
1:A:134:ARG:HB3	1:A:153:MET:HE1	1.94	0.50
1:A:334:ARG:N	1:A:346:THR:O	2.45	0.50
1:B:280:ALA:O	1:B:307:ARG:NH1	2.40	0.49
1:A:150[B]:HIS:CD2	3:A:402:COA:HS1	2.27	0.49
1:C:208:GLN:HE21	1:C:278:PHE:HE1	1.60	0.49
1:C:99:MET:CE	1:C:359:GLU:CB	2.91	0.48
1:B:192:LEU:O	1:B:195:SER:OG	2.26	0.48
1:C:311:ARG:NH1	1:C:314:SER:O	2.45	0.48
1:C:290:HIS:NE2	2:C:401:IHP:O32	2.43	0.48
1:C:134:ARG:NH1	1:C:155:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLY:O	1:C:111:ASN:ND2	2.45	0.48
1:A:170:GLU:OE2	1:A:181:GLN:NE2	2.47	0.47
1:C:99:MET:HE2	1:C:359:GLU:HB3	1.96	0.47
1:C:337:LEU:HD21	1:B:70:ALA:HB2	1.96	0.47
1:A:51:GLN:HA	1:A:54:ILE:HD12	1.96	0.47
1:A:57:LEU:HB3	1:A:76:LEU:HD21	1.97	0.47
1:A:348:PHE:CD2	3:A:402:COA:H2A	2.50	0.47
1:C:99:MET:HE2	1:C:359:GLU:CB	2.45	0.47
1:C:326:ARG:NH2	2:C:401:IHP:O22	2.47	0.46
1:B:203:ALA:HB2	1:B:241:LEU:HD21	1.96	0.46
1:C:362:ARG:NH2	2:C:401:IHP:O25	2.47	0.46
1:B:303:ARG:NH1	1:B:305:ASP:OD1	2.48	0.46
1:C:348:PHE:HB3	3:C:402:COA:H8A	1.98	0.46
1:B:71:TYR:OH	1:B:92:ASP:OD1	2.24	0.46
1:A:334:ARG:HD3	3:A:402:COA:C2A	2.46	0.46
1:A:265:SER:HB2	1:A:267:TYR:CZ	2.51	0.46
1:B:54:ILE:HG23	1:B:76:LEU:HD22	1.97	0.45
1:B:296:GLN:O	1:B:300:LEU:HG	2.16	0.45
1:B:233:GLN:O	1:B:236:ASP:HB2	2.16	0.45
1:A:311:ARG:HH12	1:A:317:HIS:HB2	1.81	0.45
1:B:155:ASP:OD2	1:B:238:HIS:NE2	2.43	0.45
1:A:175:VAL:HA	1:A:182:LEU:HB2	1.98	0.45
1:C:78:ARG:HD3	1:C:88:PHE:CE1	2.51	0.45
1:C:174:ILE:HG13	1:C:206:GLU:HB2	1.98	0.44
1:C:283:LEU:O	1:C:307:ARG:NH2	2.46	0.44
1:A:45:THR:H	1:A:332:VAL:CG1	2.31	0.44
1:A:54:ILE:HG23	1:A:76:LEU:HD22	1.99	0.44
1:B:334:ARG:HD3	1:B:346:THR:O	2.18	0.44
1:B:107:ASN:OD1	1:B:107:ASN:N	2.50	0.44
1:C:303:ARG:NH1	1:C:305:ASP:OD1	2.51	0.44
1:C:57:LEU:HD11	1:C:360:ILE:HG22	2.00	0.43
1:A:53:LYS:NZ	2:A:401:IHP:O46	2.33	0.43
1:B:180:GLN:O	1:B:183:GLN:HG2	2.18	0.43
1:C:303:ARG:HA	1:C:304:PRO:HD3	1.79	0.43
1:B:337:LEU:O	1:B:338:LEU:HB2	2.19	0.43
1:A:336:GLU:N	1:A:336:GLU:OE1	2.52	0.43
1:C:336:GLU:HG3	1:B:66:GLY:HA2	2.00	0.43
1:B:338:LEU:HB3	1:B:339:ASP:H	1.50	0.43
1:C:112:LEU:HD11	1:C:136:ILE:HG13	1.99	0.42
1:C:178:ARG:O	1:C:180:GLN:NE2	2.40	0.42
1:C:54:ILE:HG23	1:C:76:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:MET:O	1:C:102:ILE:N	2.52	0.42
1:C:226:LYS:HD3	1:C:226:LYS:HA	1.86	0.42
1:C:355:PHE:O	1:C:359:GLU:HG2	2.20	0.42
1:C:189:LEU:O	1:C:199:LEU:HD21	2.19	0.42
1:A:289:LYS:HE2	1:A:289:LYS:HB3	1.79	0.42
1:A:72:GLY:HA2	1:A:360:ILE:HD13	2.02	0.42
1:C:71:TYR:CE1	1:C:91:LEU:HB3	2.54	0.41
1:B:355:PHE:O	1:B:359:GLU:HG2	2.21	0.41
1:A:258:LEU:O	1:A:262:GLU:HG3	2.20	0.41
1:A:303:ARG:NH1	1:A:305:ASP:OD1	2.54	0.41
1:C:326:ARG:NH1	2:C:401:IHP:O41	2.53	0.41
1:A:141:CYS:HA	1:A:142:PRO:HD3	1.91	0.41
1:B:255:ARG:NH1	1:B:281:ASP:OD2	2.53	0.41
1:C:355:PHE:O	1:C:358:GLN:HB3	2.21	0.41
1:B:303:ARG:HA	1:B:304:PRO:HD3	1.88	0.41
1:B:183:GLN:HA	1:B:186:ASN:HB2	2.04	0.40
1:B:103:GLU:OE2	1:B:362:ARG:NH1	2.45	0.40
1:C:210:GLN:HG3	1:C:219:TYR:CE2	2.57	0.40
1:A:45:THR:H	1:A:332:VAL:HG11	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/342 (94%)	305 (95%)	16 (5%)	0	100	100
1	B	317/342 (93%)	299 (94%)	13 (4%)	5 (2%)	9	34
1	C	317/342 (93%)	300 (95%)	16 (5%)	1 (0%)	41	72
All	All	955/1026 (93%)	904 (95%)	45 (5%)	6 (1%)	29	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	LEU
1	B	342	THR
1	B	343	PRO
1	B	150[A]	HIS
1	B	150[B]	HIS
1	C	100	VAL

### 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	249/279 (89%)	241 (97%)	8 (3%)	39	67
1	B	244/279 (88%)	238 (98%)	6 (2%)	47	72
1	C	246/279 (88%)	237 (96%)	9 (4%)	34	62
All	All	739/837 (88%)	716 (97%)	23 (3%)	40	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	99	MET
1	C	114	HIS
1	C	195	SER
1	C	212	THR
1	C	270	MET
1	C	331	ARG
1	C	334	ARG
1	C	337	LEU
1	C	342	THR
1	A	102	ILE
1	A	153	MET
1	A	212	THR
1	A	331	ARG
1	A	332	VAL
1	A	341	GLU
1	A	342	THR
1	A	346	THR

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Mol	Chain	Res	Type
1	B	107	ASN
1	B	153	MET
1	B	242	GLN
1	B	267	TYR
1	B	334	ARG
1	B	345	ASN

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

Mol	Chain	Res	Type
1	A	271	HIS
1	B	183	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	IHP	A	401	-	36,36,36	3.28	13 (36%)	54,60,60	1.50	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	COA	A	402	-	41,50,50	2.56	8 (19%)	52,75,75	1.76	10 (19%)
4	CIT	B	403	-	12,12,12	0.98	0	17,17,17	1.61	2 (11%)
3	COA	C	402	-	41,50,50	2.53	6 (14%)	52,75,75	1.80	10 (19%)
3	COA	B	402	-	28,33,50	3.15	4 (14%)	35,52,75	1.91	9 (25%)
2	IHP	C	401	-	36,36,36	3.37	15 (41%)	54,60,60	1.70	10 (18%)
2	IHP	B	401	-	36,36,36	3.62	11 (30%)	54,60,60	2.21	14 (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
2	IHP	A	401	-	-	6/30/54/54	0/1/1/1
3	COA	A	402	-	-	19/44/64/64	0/3/3/3
4	CIT	B	403	-	-	4/16/16/16	-
3	COA	C	402	-	-	17/44/64/64	0/3/3/3
3	COA	B	402	-	-	7/17/37/64	0/3/3/3
2	IHP	C	401	-	-	7/30/54/54	0/1/1/1
2	IHP	B	401	-	-	14/30/54/54	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	COA	P3B-O3B	14.59	1.86	1.59
3	A	402	COA	P3B-O3B	13.43	1.84	1.59
3	C	402	COA	P3B-O3B	13.41	1.84	1.59
2	B	401	IHP	P1-O11	10.38	1.78	1.59
2	C	401	IHP	P1-O11	8.34	1.75	1.59
2	C	401	IHP	P5-O15	7.99	1.74	1.59
2	B	401	IHP	P5-O15	7.63	1.73	1.59
2	B	401	IHP	P3-O13	7.59	1.73	1.59
2	A	401	IHP	P3-O13	7.52	1.73	1.59
2	B	401	IHP	C2-C1	7.25	1.67	1.52
2	A	401	IHP	P5-O15	7.02	1.72	1.59
2	B	401	IHP	P4-O14	6.81	1.72	1.59
2	A	401	IHP	C5-C4	6.74	1.66	1.52
2	C	401	IHP	P2-O12	6.54	1.71	1.59
2	C	401	IHP	C3-C2	6.50	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	IHP	P4-O14	6.28	1.71	1.59
2	B	401	IHP	P6-O16	6.23	1.71	1.59
2	C	401	IHP	P3-O13	6.22	1.71	1.59
2	A	401	IHP	P1-O11	6.07	1.70	1.59
2	A	401	IHP	P6-O16	5.94	1.70	1.59
3	B	402	COA	P2A-O6A	5.56	1.76	1.54
2	A	401	IHP	C4-C3	5.46	1.63	1.52
2	A	401	IHP	P2-O12	5.36	1.69	1.59
2	C	401	IHP	C2-C1	5.33	1.63	1.52
2	B	401	IHP	C3-C2	5.28	1.63	1.52
2	C	401	IHP	P4-O14	5.14	1.69	1.59
2	B	401	IHP	P2-O12	4.66	1.68	1.59
3	A	402	COA	P2A-O6A	4.65	1.78	1.59
2	A	401	IHP	C6-C5	4.50	1.61	1.52
3	C	402	COA	P2A-O6A	4.40	1.77	1.59
2	C	401	IHP	P6-O16	4.22	1.67	1.59
2	C	401	IHP	C4-C3	4.04	1.60	1.52
2	B	401	IHP	C5-C4	3.97	1.60	1.52
2	C	401	IHP	C5-C4	3.81	1.60	1.52
2	C	401	IHP	C6-C1	3.71	1.59	1.52
2	B	401	IHP	C6-C5	3.53	1.59	1.52
2	A	401	IHP	C3-C2	3.27	1.59	1.52
3	A	402	COA	C5P-N4P	3.22	1.40	1.33
3	C	402	COA	C5P-N4P	3.05	1.40	1.33
3	C	402	COA	C9P-N8P	3.02	1.40	1.33
3	A	402	COA	C9P-N8P	2.97	1.40	1.33
3	C	402	COA	O3B-C3B	-2.75	1.34	1.44
3	A	402	COA	O3B-C3B	-2.67	1.34	1.44
3	B	402	COA	O3B-C3B	-2.66	1.34	1.44
3	A	402	COA	C2A-N1A	2.60	1.38	1.33
2	A	401	IHP	O11-C1	-2.40	1.35	1.44
2	C	401	IHP	O13-C3	-2.39	1.35	1.44
3	A	402	COA	C4A-N3A	2.38	1.38	1.35
2	C	401	IHP	C6-C5	2.38	1.57	1.52
2	B	401	IHP	O13-C3	-2.26	1.35	1.44
2	C	401	IHP	O15-C5	-2.20	1.36	1.44
3	C	402	COA	C2A-N1A	2.15	1.37	1.33
2	C	401	IHP	O16-C6	-2.15	1.36	1.44
2	A	401	IHP	O15-C5	-2.07	1.36	1.44
2	A	401	IHP	O13-C3	-2.05	1.36	1.44
3	A	402	COA	O2B-C2B	-2.01	1.38	1.43
3	B	402	COA	C2A-N1A	2.01	1.37	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	COA	P2A-O3A-P1A	-7.57	106.84	132.83
3	B	402	COA	P1A-O3A-P2A	-6.85	109.31	132.83
3	A	402	COA	P2A-O3A-P1A	-6.73	109.74	132.83
2	B	401	IHP	C6-C5-C4	-6.05	97.17	110.41
2	B	401	IHP	O11-C1-C2	5.92	122.64	108.69
2	B	401	IHP	O13-C3-C2	4.98	120.43	108.69
2	B	401	IHP	C6-C1-C2	-4.94	99.59	110.41
2	C	401	IHP	C3-C2-C1	4.79	120.90	110.41
2	B	401	IHP	O16-C6-C5	4.76	119.91	108.69
4	B	403	CIT	O6-C6-C3	4.54	120.94	113.05
2	A	401	IHP	C5-C4-C3	4.22	119.66	110.41
2	C	401	IHP	O15-C5-C4	4.01	118.14	108.69
2	B	401	IHP	O14-C4-C5	3.90	117.89	108.69
3	A	402	COA	O3B-P3B-O7A	-3.76	94.86	109.39
2	B	401	IHP	C4-C3-C2	-3.54	102.66	110.41
3	C	402	COA	O3B-P3B-O7A	-3.44	96.10	109.39
2	B	401	IHP	O12-C2-C1	3.42	116.74	108.69
2	C	401	IHP	O15-C5-C6	3.41	116.72	108.69
2	C	401	IHP	O13-C3-C2	3.36	116.61	108.69
2	C	401	IHP	O11-C1-C2	3.35	116.58	108.69
2	B	401	IHP	C3-C2-C1	3.32	117.69	110.41
2	A	401	IHP	O15-C5-C4	3.26	116.37	108.69
2	B	401	IHP	O15-C5-C4	3.18	116.17	108.69
2	A	401	IHP	O13-C3-C2	3.11	116.03	108.69
2	A	401	IHP	O11-C1-C2	3.06	115.89	108.69
2	C	401	IHP	C5-C4-C3	3.02	117.02	110.41
3	C	402	COA	P1A-O5B-C5B	-2.97	104.25	121.68
3	B	402	COA	O5A-P2A-O3A	2.97	114.59	104.64
3	A	402	COA	C7P-C6P-C5P	-2.96	107.43	112.36
2	C	401	IHP	O11-C1-C6	2.93	115.60	108.69
3	C	402	COA	O9A-P3B-O8A	2.92	118.79	107.64
3	B	402	COA	P1A-O5B-C5B	-2.91	104.64	121.68
3	B	402	COA	O5A-P2A-O4A	2.82	121.74	110.68
3	A	402	COA	O9A-P3B-O8A	2.80	118.34	107.64
3	A	402	COA	P1A-O5B-C5B	-2.74	105.63	121.68
3	C	402	COA	P2A-O6A-CCP	-2.62	106.42	121.56
2	A	401	IHP	O13-C3-C4	2.61	114.84	108.69
2	A	401	IHP	O15-C5-C6	2.61	114.83	108.69
2	A	401	IHP	C6-C1-C2	-2.58	104.77	110.41
2	A	401	IHP	O11-C1-C6	2.54	114.66	108.69
2	C	401	IHP	C5-C6-C1	2.50	115.88	110.41
2	C	401	IHP	C6-C5-C4	-2.44	105.07	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	P2A-O6A-CCP	-2.43	107.53	121.56
3	C	402	COA	O6A-P2A-O4A	-2.41	99.66	109.07
3	A	402	COA	CEP-CBP-CAP	2.34	112.87	108.82
3	B	402	COA	O8A-P3B-O3B	-2.33	95.55	105.99
3	C	402	COA	O5P-C5P-N4P	-2.30	118.67	123.01
2	B	401	IHP	O12-C2-C3	2.30	114.12	108.69
3	C	402	COA	C2A-N1A-C6A	-2.28	114.86	118.75
3	B	402	COA	O6A-P2A-O4A	-2.22	101.97	110.68
3	A	402	COA	C2A-N1A-C6A	-2.21	114.98	118.75
3	C	402	COA	O5A-P2A-O4A	2.20	123.13	112.24
3	A	402	COA	O6A-P2A-O4A	-2.20	100.49	109.07
3	B	402	COA	C2A-N1A-C6A	-2.18	115.03	118.75
2	C	401	IHP	O13-C3-C4	2.17	113.80	108.69
3	B	402	COA	C2B-C3B-C4B	-2.13	99.45	103.22
3	B	402	COA	O9A-P3B-O7A	2.08	118.84	110.68
4	B	403	CIT	O2-C1-C2	2.08	121.04	114.35
2	B	401	IHP	O15-C5-C6	2.07	113.57	108.69
3	A	402	COA	C3P-N4P-C5P	-2.06	119.02	122.84
3	C	402	COA	C4A-C5A-N7A	2.06	111.54	109.40
2	B	401	IHP	O11-C1-C6	2.03	113.48	108.69
2	B	401	IHP	O13-C3-C4	2.02	113.44	108.69

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	IHP	C4-O14-P4-O24
2	B	401	IHP	C2-C1-O11-P1
2	B	401	IHP	C6-C1-O11-P1
2	B	401	IHP	C3-C4-O14-P4
2	B	401	IHP	C1-C6-O16-P6
2	B	401	IHP	C1-O11-P1-O21
2	B	401	IHP	C3-O13-P3-O43
3	C	402	COA	C3B-C4B-C5B-O5B
3	C	402	COA	O4B-C4B-C5B-O5B
3	C	402	COA	C5B-O5B-P1A-O1A
3	C	402	COA	C5B-O5B-P1A-O2A
3	C	402	COA	C5B-O5B-P1A-O3A
3	C	402	COA	CCP-O6A-P2A-O3A
3	C	402	COA	CAP-CBP-CCP-O6A
3	C	402	COA	C5P-C6P-C7P-N8P
3	C	402	COA	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
3	A	402	COA	C3B-C4B-C5B-O5B
3	A	402	COA	O4B-C4B-C5B-O5B
3	A	402	COA	C5B-O5B-P1A-O2A
3	A	402	COA	C5B-O5B-P1A-O3A
3	A	402	COA	CCP-O6A-P2A-O3A
3	A	402	COA	CDP-CBP-CCP-O6A
3	A	402	COA	CAP-CBP-CCP-O6A
3	A	402	COA	O9P-C9P-CAP-OAP
3	A	402	COA	CAP-C9P-N8P-C7P
3	B	402	COA	C5B-O5B-P1A-O1A
3	B	402	COA	C5B-O5B-P1A-O3A
3	C	402	COA	C6P-C5P-N4P-C3P
3	A	402	COA	O9P-C9P-N8P-C7P
3	B	402	COA	C3B-C4B-C5B-O5B
3	C	402	COA	O5P-C5P-N4P-C3P
3	C	402	COA	CDP-CBP-CCP-O6A
3	C	402	COA	CEP-CBP-CCP-O6A
3	A	402	COA	CEP-CBP-CCP-O6A
2	B	401	IHP	C5-C6-O16-P6
4	B	403	CIT	C1-C2-C3-O7
3	B	402	COA	O4B-C4B-C5B-O5B
2	B	401	IHP	C4-C3-O13-P3
4	B	403	CIT	C4-C3-C6-O5
3	A	402	COA	N8P-C9P-CAP-OAP
3	B	402	COA	C3B-O3B-P3B-O7A
2	C	401	IHP	C5-C4-O14-P4
2	A	401	IHP	C5-C4-O14-P4
2	B	401	IHP	C2-C3-O13-P3
3	C	402	COA	CCP-O6A-P2A-O4A
3	C	402	COA	CCP-O6A-P2A-O5A
3	A	402	COA	CCP-O6A-P2A-O4A
3	A	402	COA	CCP-O6A-P2A-O5A
4	B	403	CIT	C4-C3-C6-O6
4	B	403	CIT	C1-C2-C3-C4
2	A	401	IHP	C3-C2-O12-P2
3	A	402	COA	P1A-O3A-P2A-O5A
3	B	402	COA	P2A-O3A-P1A-O1A
3	A	402	COA	O9P-C9P-CAP-CBP
3	A	402	COA	N8P-C9P-CAP-CBP
3	A	402	COA	P1A-O3A-P2A-O4A
3	B	402	COA	P2A-O3A-P1A-O5B
3	C	402	COA	O9P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
2	C	401	IHP	C2-O12-P2-O22
2	C	401	IHP	C5-O15-P5-O25
2	A	401	IHP	C4-O14-P4-O24
2	A	401	IHP	C6-O16-P6-O26
2	B	401	IHP	C4-O14-P4-O24
2	B	401	IHP	C5-O15-P5-O25
3	C	402	COA	C2P-C3P-N4P-C5P
2	C	401	IHP	C2-O12-P2-O32
2	C	401	IHP	C3-O13-P3-O43
2	C	401	IHP	C5-O15-P5-O35
2	A	401	IHP	C4-O14-P4-O34
2	A	401	IHP	C6-O16-P6-O46
2	B	401	IHP	C1-O11-P1-O41
2	B	401	IHP	C5-O15-P5-O35
2	B	401	IHP	C5-O15-P5-O45
3	A	402	COA	CBP-CCP-O6A-P2A

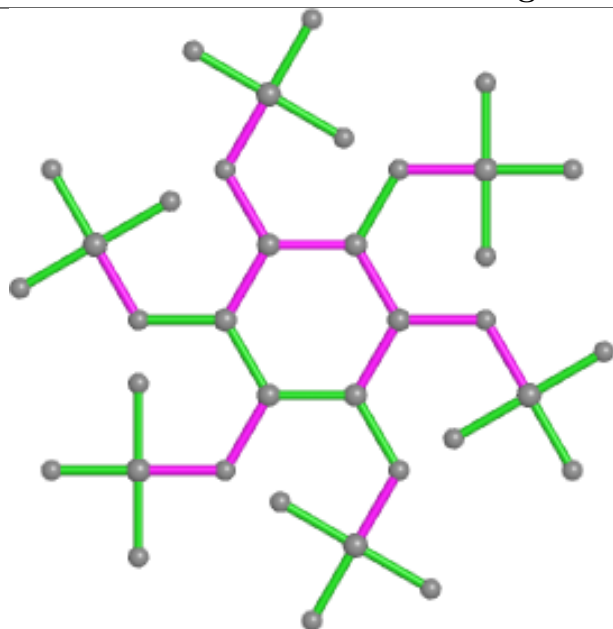
There are no ring outliers.

5 monomers are involved in 18 short contacts:

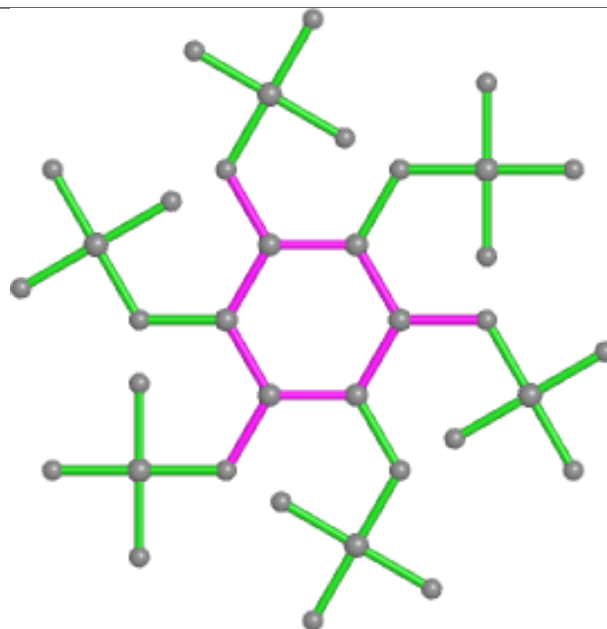
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	IHP	1	0
3	A	402	COA	5	0
3	C	402	COA	3	0
2	C	401	IHP	7	0
2	B	401	IHP	2	0

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.

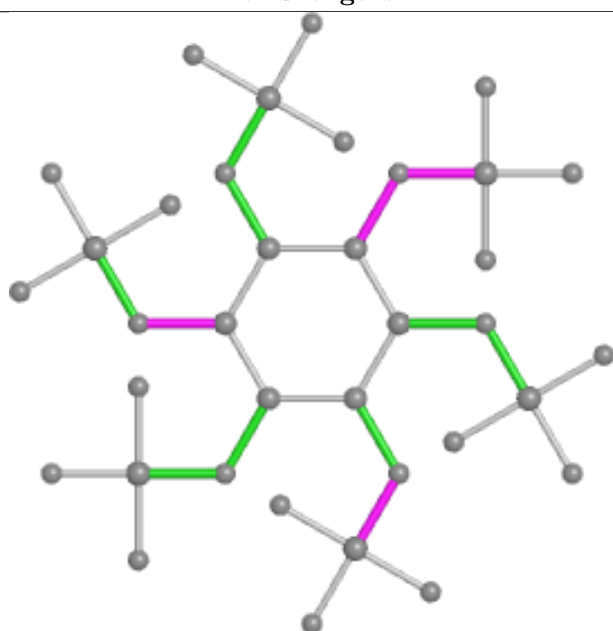
## Ligand IHP A 401



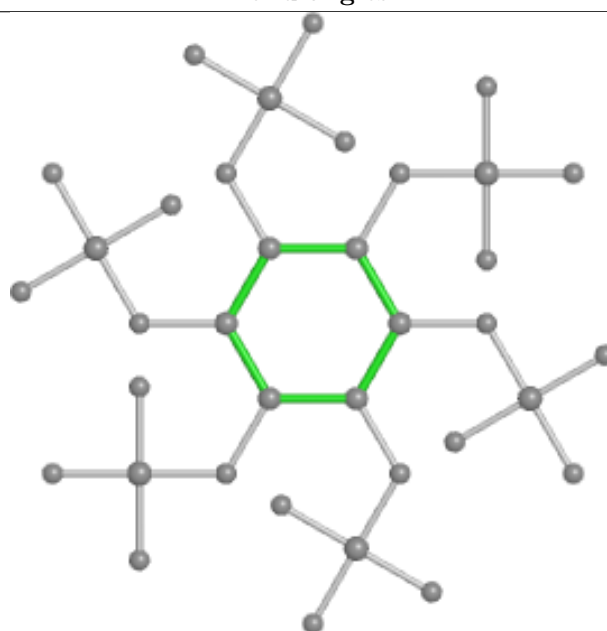
Bond lengths



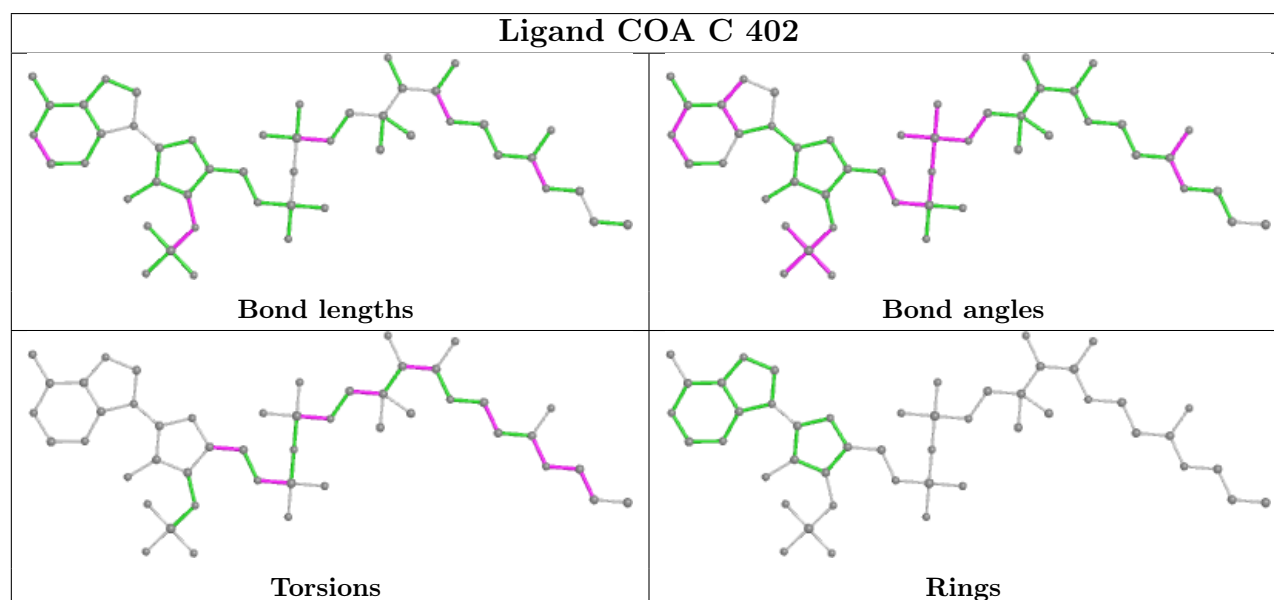
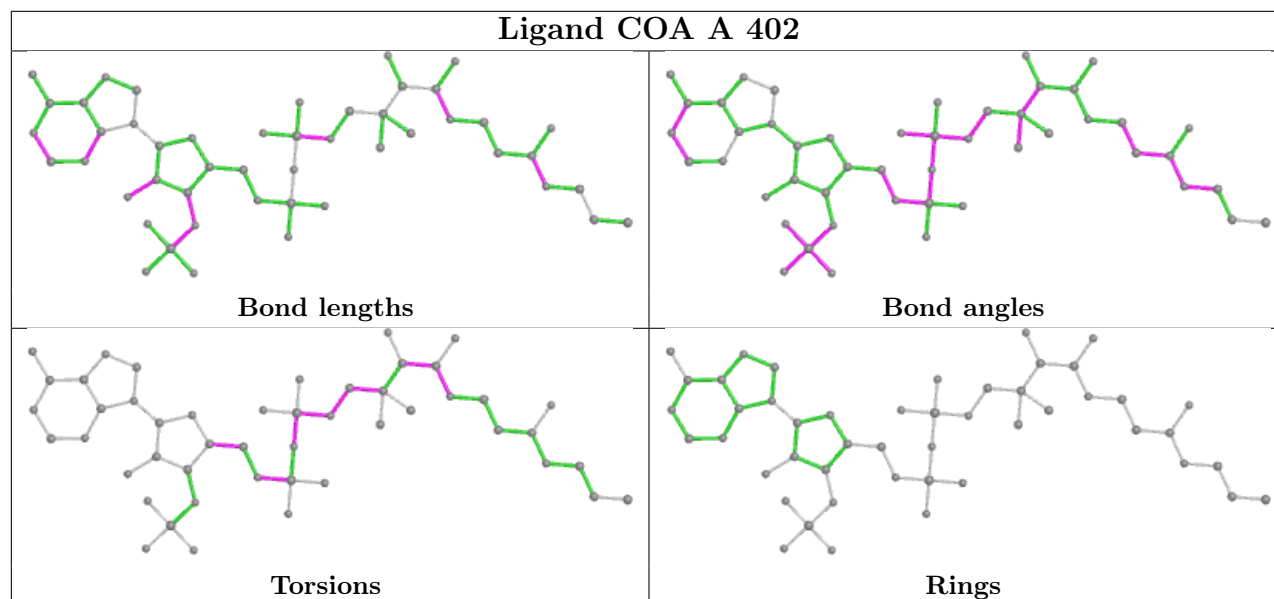
Bond angles

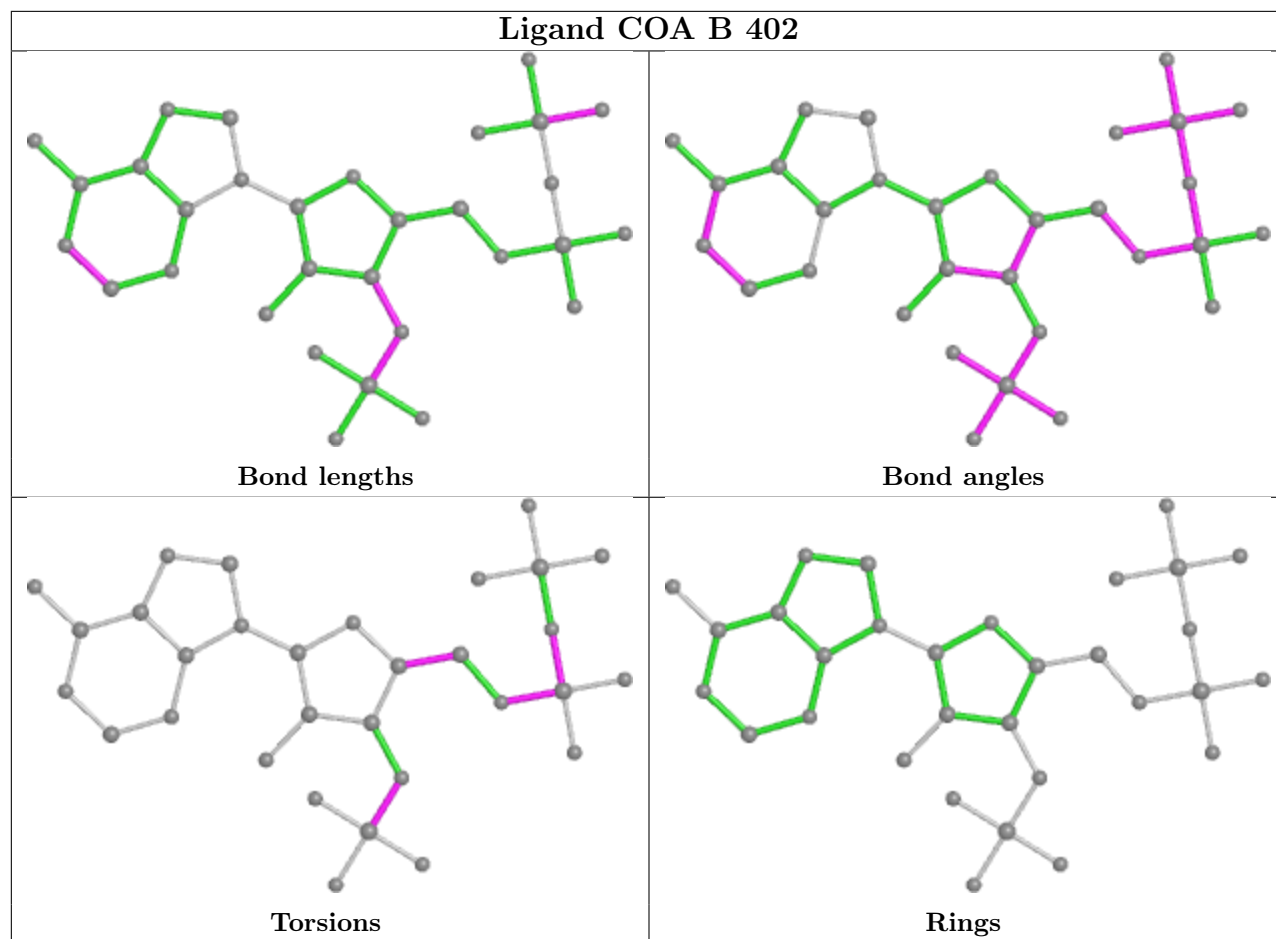


Torsions



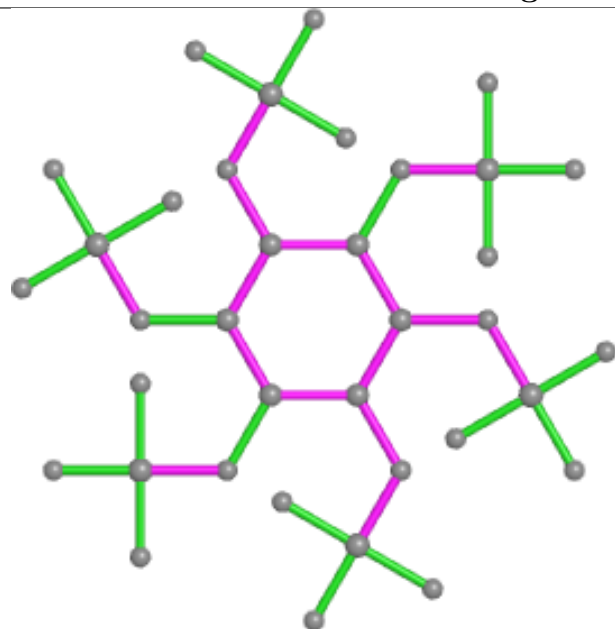
Rings



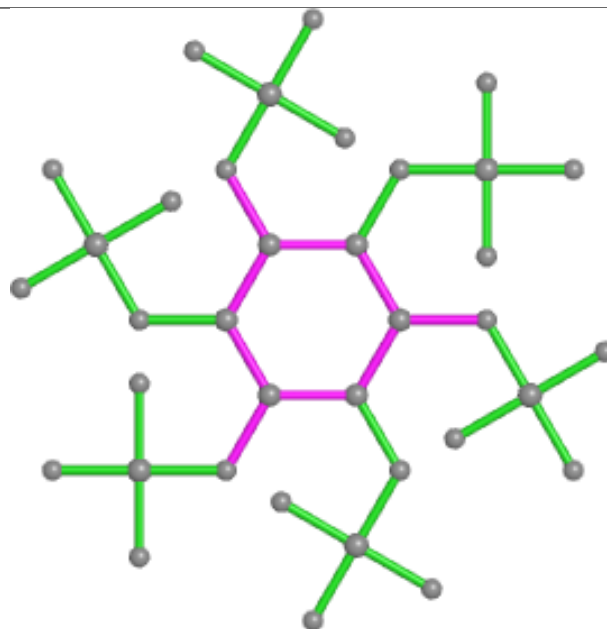




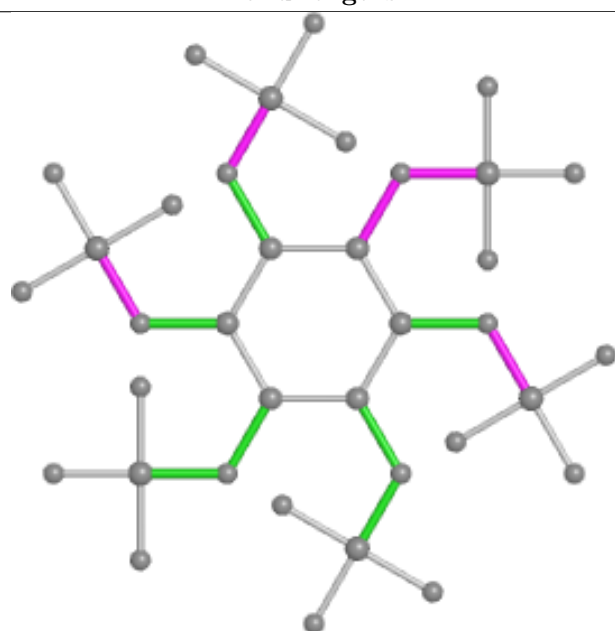
## Ligand IHP C 401



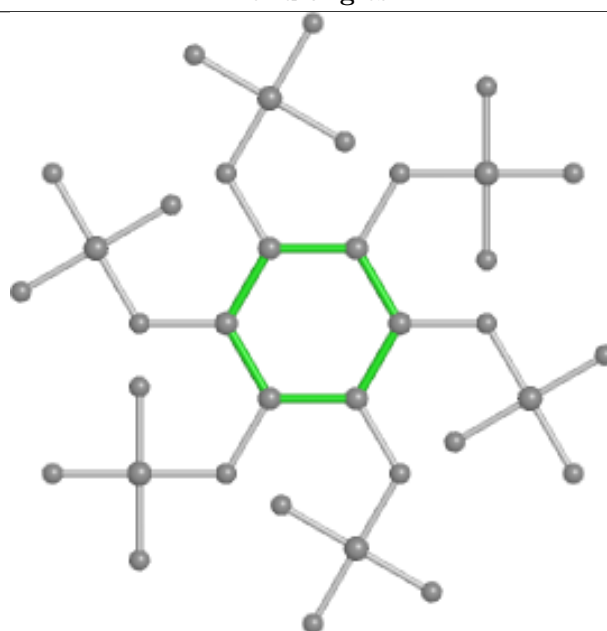
Bond lengths



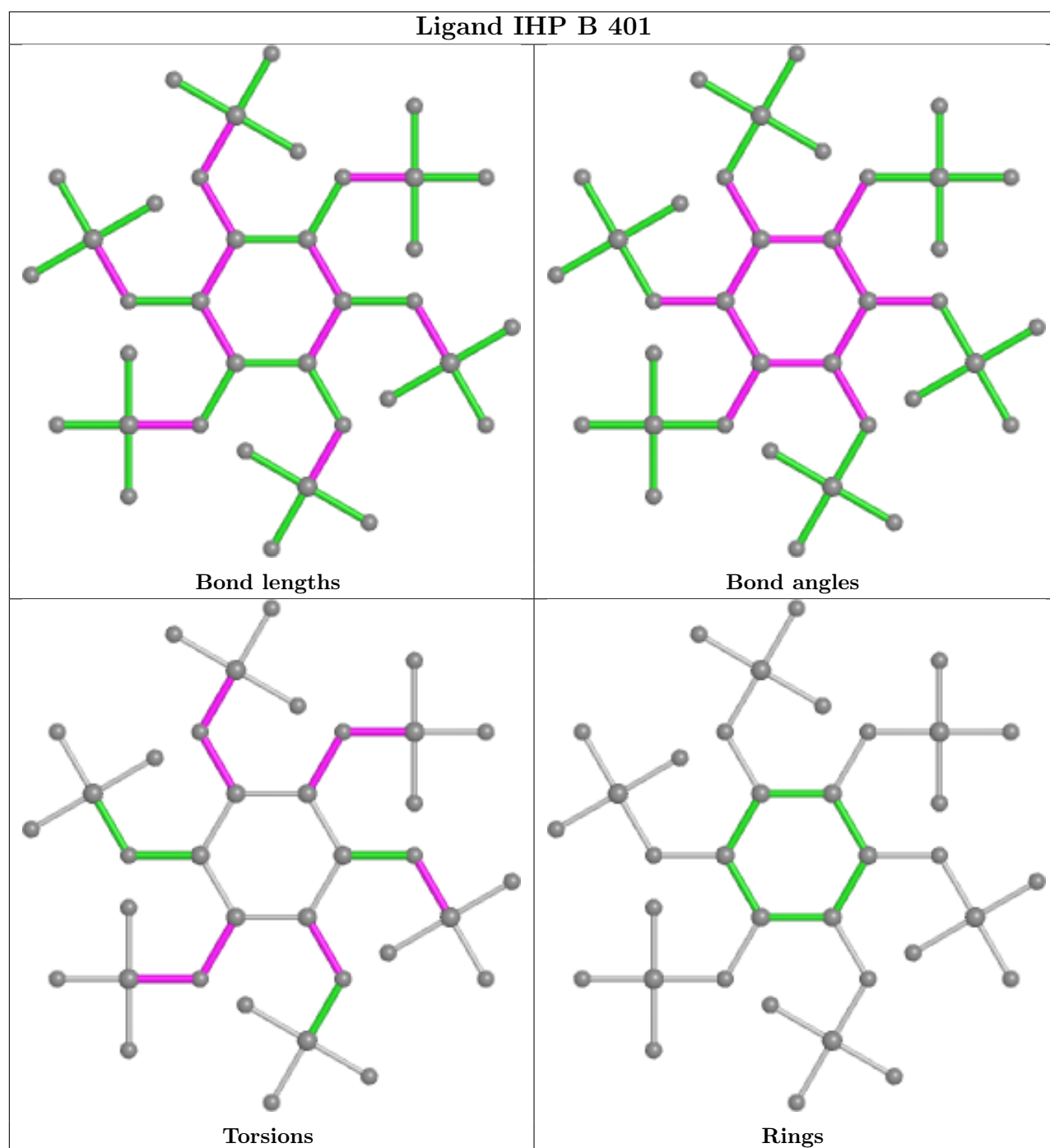
Bond angles



Torsions



Rings



## 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	324/342 (94%)	-0.07	6 (1%) 66 65	23, 31, 47, 58	0
1	B	320/342 (93%)	-0.12	0 100 100	22, 36, 53, 62	0
1	C	320/342 (93%)	-0.07	3 (0%) 84 83	23, 35, 52, 63	0
All	All	964/1026 (93%)	-0.09	9 (0%) 84 83	22, 34, 52, 63	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	GLU	4.8
1	C	85	SER	3.1
1	A	142	PRO	2.8
1	A	45	THR	2.4
1	A	368	GLN	2.2
1	C	81	GLY	2.1
1	C	71	TYR	2.1
1	A	52	GLN	2.0
1	A	277	ALA	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](#)

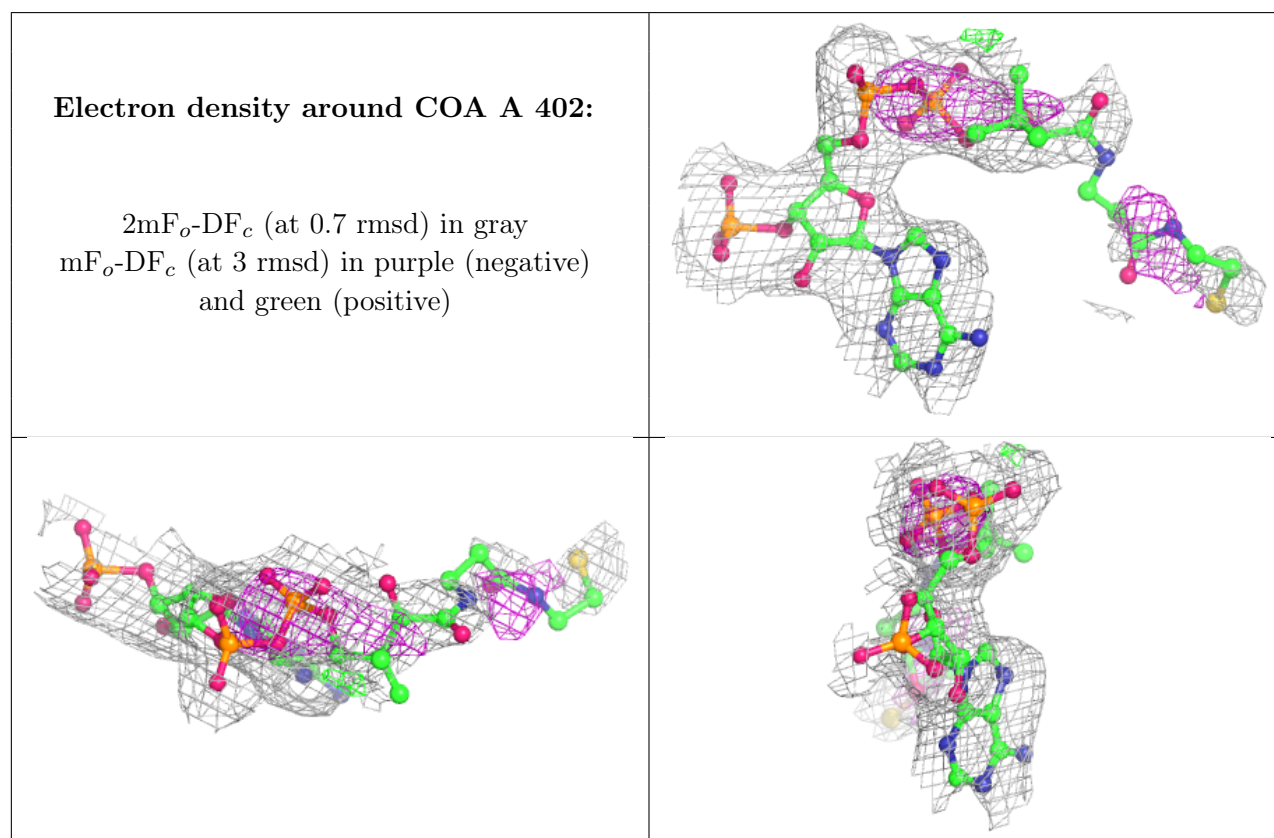
There are no monosaccharides in this entry.

## 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.

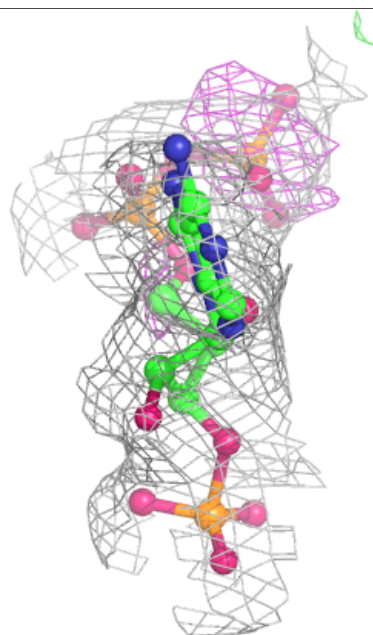
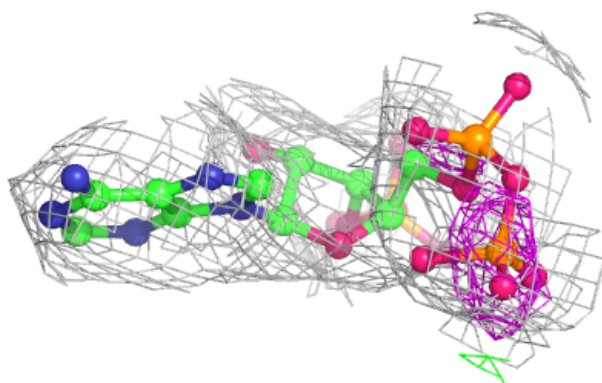
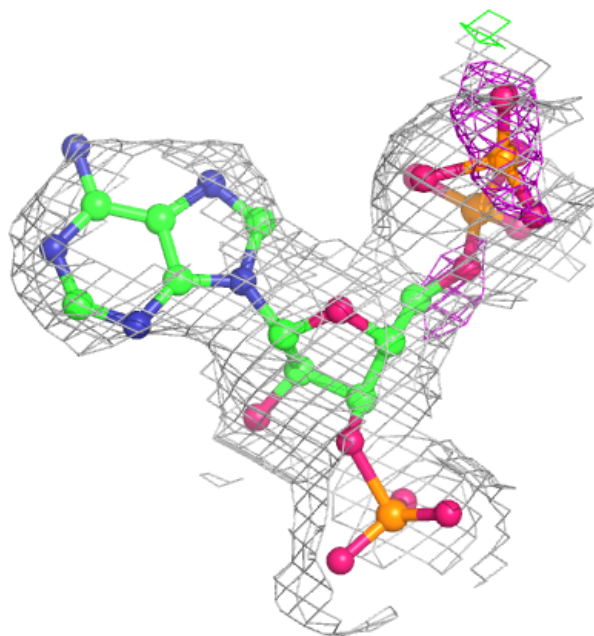
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CIT	B	403	13/13	0.77	0.24	40,40,40,40	0
3	COA	A	402	48/48	0.82	0.28	37,37,37,37	0
3	COA	B	402	31/48	0.86	0.19	43,43,43,43	0
3	COA	C	402	48/48	0.87	0.23	41,41,41,41	0
2	IHP	B	401	36/36	0.88	0.16	42,42,42,42	0
2	IHP	C	401	36/36	0.90	0.15	36,36,36,36	0
2	IHP	A	401	36/36	0.92	0.14	32,32,32,32	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.



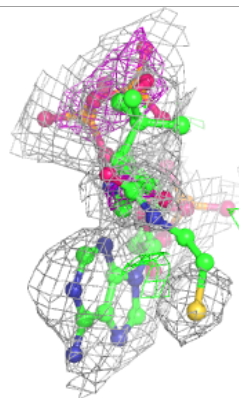
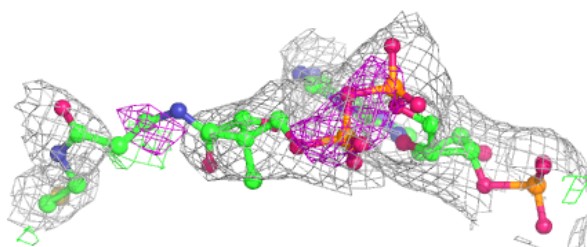
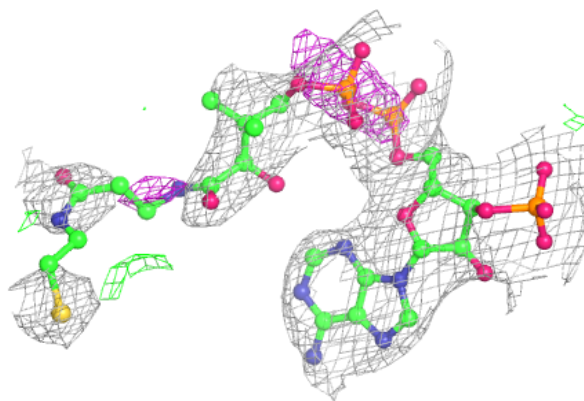
**Electron density around COA B 402:**

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



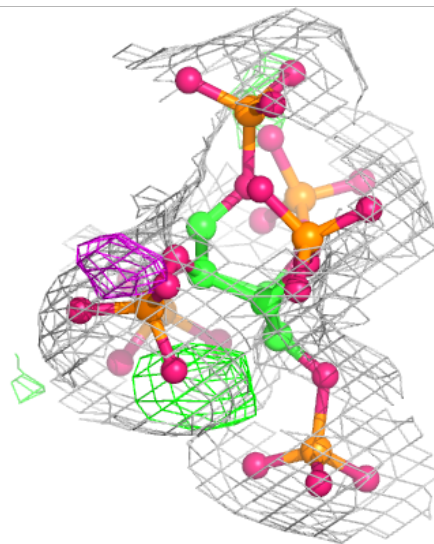
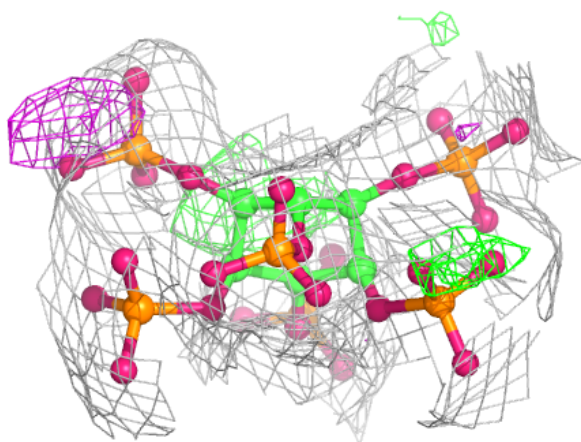
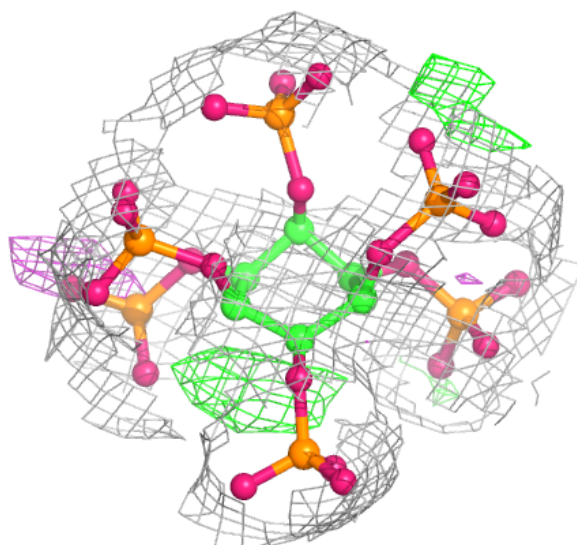
**Electron density around COA C 402:**

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



**Electron density around IHP B 401:**

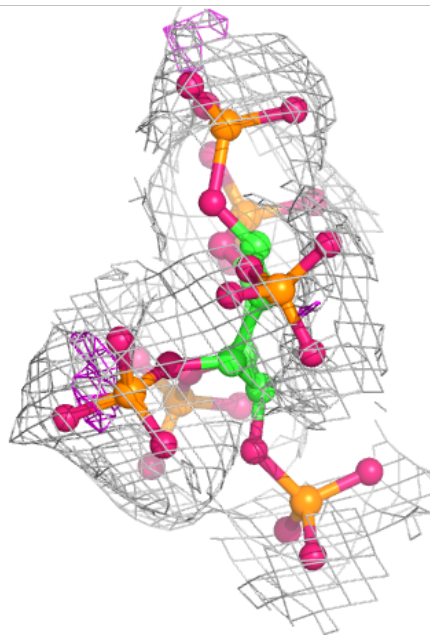
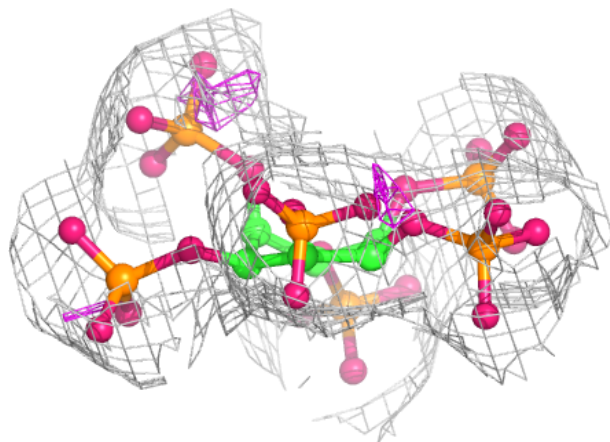
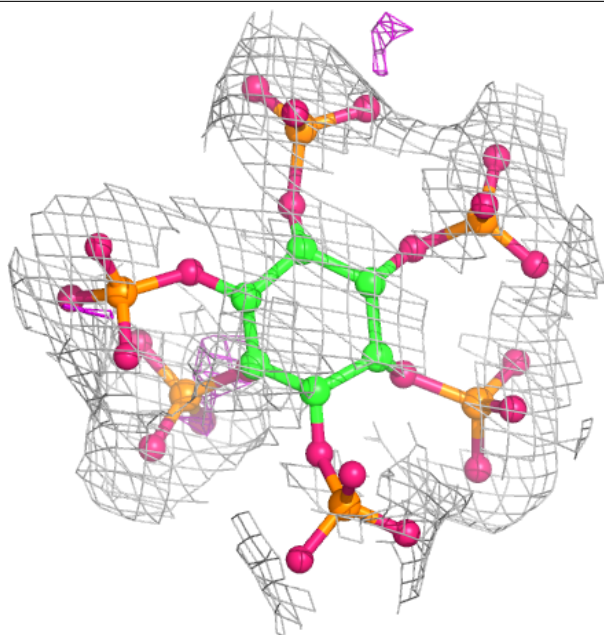
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around IHP C 401:**

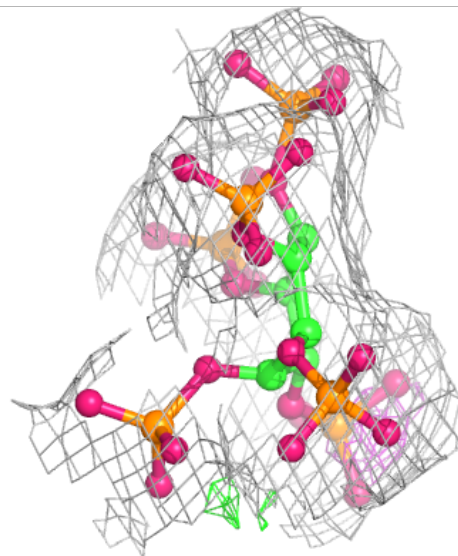
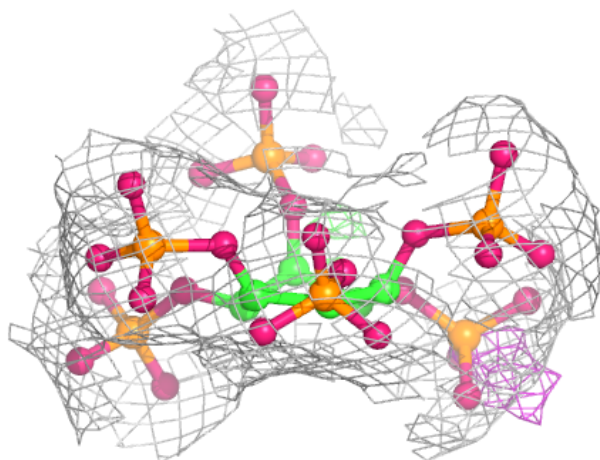
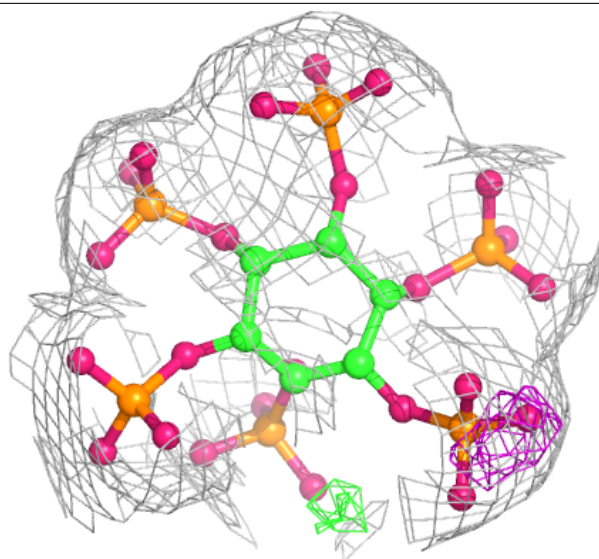
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around IHP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.