



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:54 AM UTC

PDB ID : 5KLQ / pdb_00005klq
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

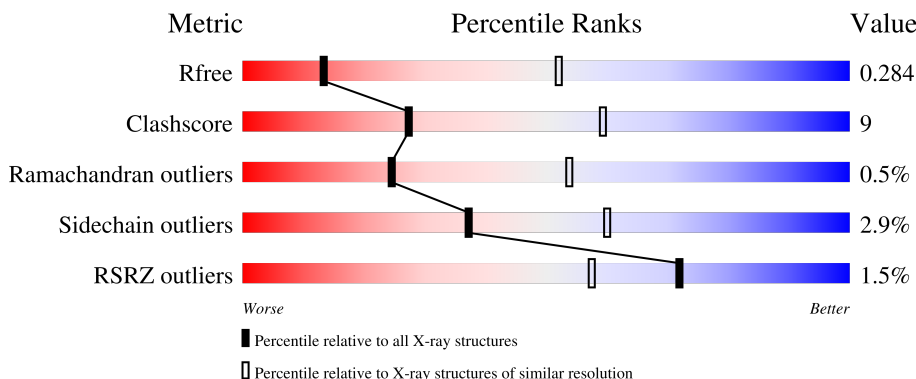
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

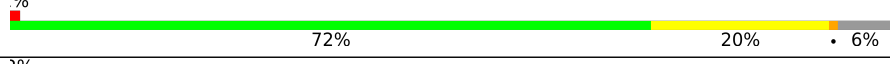
The reported resolution of this entry is 3.40 Å.

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 ≥ 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	
1	B	342	
1	C	342	

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:

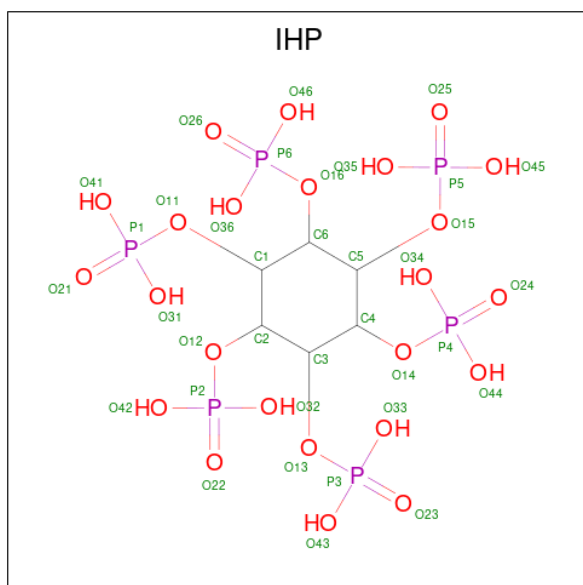
Chain	Residue	Modelled	Actual	Comment	Reference
C	28	SER	-	expression tag	UNP Q6VE93
C	82	ALA	LYS	engineered mutation	UNP Q6VE93
C	83	ALA	LYS	engineered mutation	UNP Q6VE93
C	119	TYR	LYS	engineered mutation	UNP Q6VE93
C	120	TYR	GLU	engineered mutation	UNP Q6VE93
C	298	TYR	LYS	engineered mutation	UNP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

Continued on next page...

Continued from previous page...

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 (CCD ID: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$).



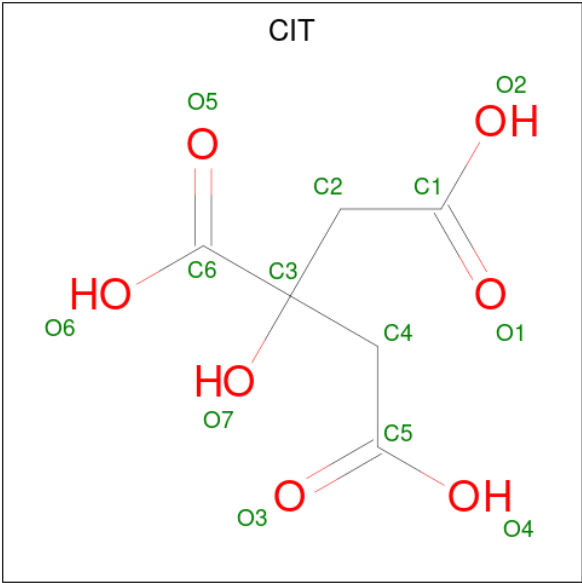
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 36	C 6	O 24	P 6	0	0
2	A	1	Total 36	C 6	O 24	P 6	0	0
2	B	1	Total 36	C 6	O 24	P 6	0	0

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $\text{C}_{21}\text{H}_{36}\text{N}_7\text{O}_{16}\text{P}_3\text{S}$).



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 (CCD ID: CIT) (formula: C₆H₈O₇).

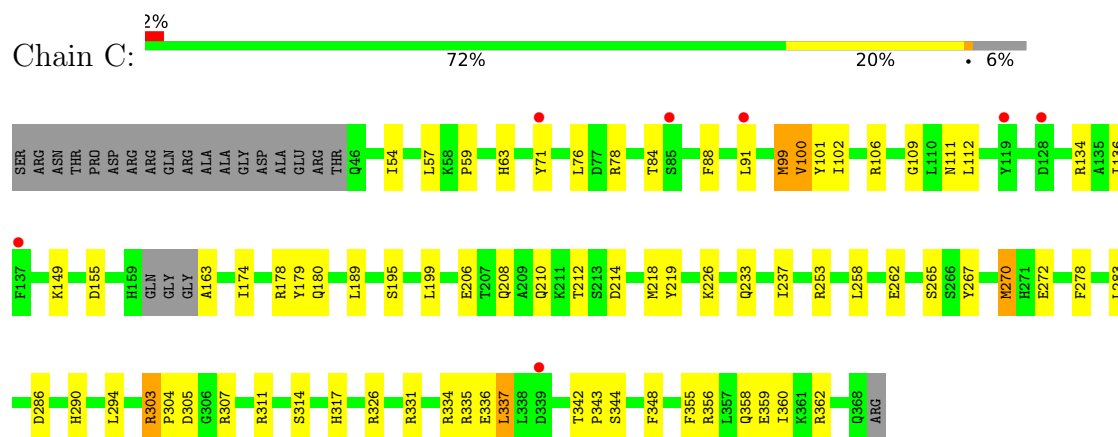


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

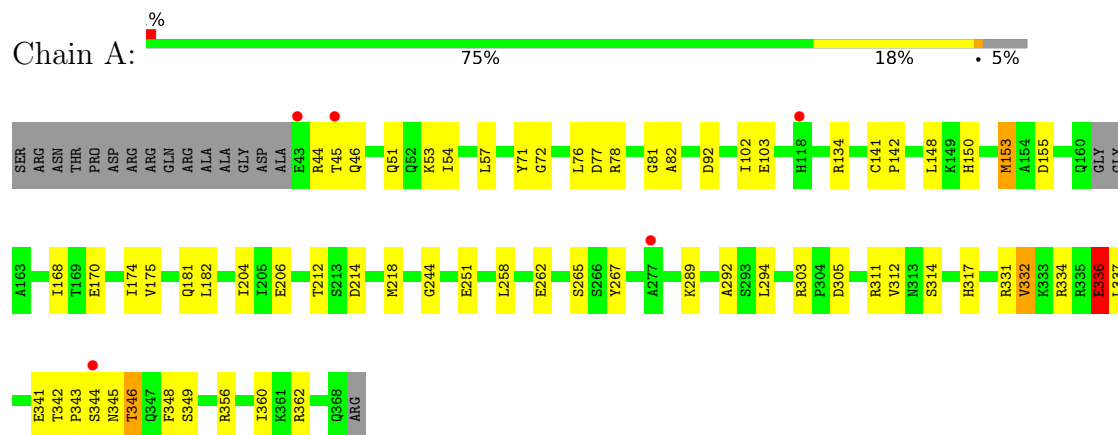
3 Residue-property plots [i](#)

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.

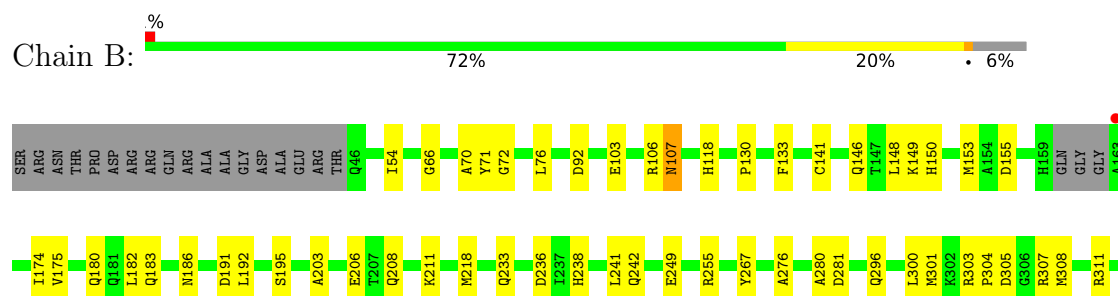
• Molecule 1: Orf34



• Molecule 1: Orf34



• Molecule 1: Orf34





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.13Å 82.30Å 86.27Å 64.20° 76.69° 89.35°	Depositor
Resolution (Å)	47.57 – 3.40 47.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.57-3.40) 98.4 (47.57-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.281 0.237 , 0.284	Depositor DCC
R_{free} test set	1609 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: COA, IHP, CIT

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	0.36	0/2518	0.82	2/3416 (0.1%)
1	B	0.36	0/2478	0.79	0/3362
1	C	0.37	0/2486	0.81	5/3375 (0.1%)
All	All	0.37	0/7482	0.81	7/10153 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ARG	CA-C-N	5.81	125.50	119.05
1	C	303	ARG	C-N-CA	5.81	125.50	119.05
1	A	336	GLU	CA-C-N	5.60	131.78	121.70
1	A	336	GLU	C-N-CA	5.60	131.78	121.70
1	C	149	LYS	CB-CA-C	-5.55	110.16	116.54
1	C	163	ALA	CA-C-N	5.12	125.02	119.85
1	C	163	ALA	C-N-CA	5.12	125.02	119.85

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	45	0
1	B	2427	0	2323	40	0
1	C	2434	0	2331	53	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	133	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 9.

All (133) 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:99:MET:HE3	1:C:359:GLU:CB	1.96	0.95
1:C:99:MET:HE3	1:C:359:GLU:HB2	1.66	0.76
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:C:99:MET:HE3	1:C:359:GLU:HB3	1.69	0.72
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:218:MET:HE2	1:B:356:ARG:HA	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:MET:HE2	1:C:356:ARG:HA	1.79	0.64
1:A:292:ALA:HA	1:A:349:SER:HB3	1.79	0.63
1:B:301:MET:HE3	1:B:324:VAL:H	1.63	0.63
1:A:343:PRO:C	1:A:345:ASN:HA	2.24	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:218:MET:HE2	1:A:356:ARG:HA	1.81	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:C:99:MET:O	1:C:100:VAL:C	2.43	0.60
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: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
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:A:289:LYS:NZ	1:A:312:VAL:O	2.35	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: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:A:103:GLU:OE2	1:A:362:ARG:NH1	2.36	0.54
1:C:99:MET:CE	1:C:218:MET:HE1	2.37	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:B:71:TYR:OH	1:B:92:ASP:OD1	2.24	0.53
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:B:280:ALA:HA	1:B:308:MET:HE3	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:174:ILE:HG13	1:A:206:GLU:HB2	1.93	0.51
1:C:99:MET:HE1	1:C:218:MET:HE1	1.93	0.50
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: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:A:134:ARG:HB3	1:A:153:MET:HE1	1.94	0.49
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
1:C:109:GLY:O	1:C:111:ASN:ND2	2.45	0.48
1:C:258:LEU:HD22	1:C:270:MET:HE3	1.96	0.47
1:A:170:GLU:OE2	1:A:181:GLN:NE2	2.47	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: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:B:301:MET:HE1	1:B:322:ASN:CG	2.39	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:343:PRO:O	1:C:344:SER:OG	2.25	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:A:71:TYR:OH	1:A:92:ASP:OD1	2.31	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
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

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	321/342 (94%)	305 (95%)	16 (5%)	0	100	100
1	B	317/342 (93%)	299 (94%)	13 (4%)	5 (2%)	7	29
1	C	317/342 (93%)	300 (95%)	16 (5%)	1 (0%)	36	65
All	All	955/1026 (93%)	904 (95%)	45 (5%)	6 (1%)	24	50

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%)	34	58
1	B	244/279 (88%)	238 (98%)	6 (2%)	42	62
1	C	246/279 (88%)	239 (97%)	7 (3%)	38	60
All	All	739/837 (88%)	718 (97%)	21 (3%)	37	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	99	MET
1	C	195	SER
1	C	212	THR
1	C	270	MET
1	C	331	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
1	B	107	ASN
1	B	146	GLN
1	B	153	MET
1	B	242	GLN
1	B	267	TYR
1	B	345	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	201	GLN
1	C	208	GLN
1	A	208	GLN
1	A	271	HIS
1	B	63	HIS
1	B	183	GLN
1	B	230	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 [i](#)

There are no oligosaccharides 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
4	CIT	B	403	-	12,12,12	1.02	0	17,17,17	1.52	2 (11%)
2	IHP	C	401	-	36,36,36	3.52	16 (44%)	60,60,60	1.78	10 (16%)
3	COA	A	402	-	47,50,50	2.88	9 (19%)	69,75,75	1.62	14 (20%)
2	IHP	A	401	-	36,36,36	3.42	13 (36%)	60,60,60	1.62	11 (18%)
3	COA	C	402	-	47,50,50	2.86	9 (19%)	69,75,75	1.61	14 (20%)
3	COA	B	402	-	32,33,50	3.55	7 (21%)	50,52,75	1.62	12 (24%)
2	IHP	B	401	-	36,36,36	3.80	14 (38%)	60,60,60	2.30	19 (31%)

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
4	CIT	B	403	-	-	4/16/16/16	-
2	IHP	C	401	-	-	6/30/54/54	0/1/1/1
3	COA	A	402	-	-	19/48/64/64	0/3/3/3
2	IHP	A	401	-	-	3/30/54/54	0/1/1/1
3	COA	C	402	-	-	20/48/64/64	0/3/3/3
3	COA	B	402	-	-	7/21/37/64	0/3/3/3
2	IHP	B	401	-	-	13/30/54/54	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	COA	P3B-O3B	15.59	1.86	1.59
3	A	402	COA	P3B-O3B	14.34	1.84	1.59
3	C	402	COA	P3B-O3B	14.32	1.84	1.59
2	B	401	IHP	P1-O11	11.07	1.78	1.59
3	B	402	COA	P1A-O3A	9.10	1.69	1.59
3	C	402	COA	P1A-O3A	8.91	1.69	1.59
3	A	402	COA	P1A-O3A	8.91	1.69	1.59
2	C	401	IHP	P1-O11	8.86	1.75	1.59
2	C	401	IHP	P5-O15	8.49	1.74	1.59
2	B	401	IHP	P5-O15	8.10	1.73	1.59
2	B	401	IHP	P3-O13	8.06	1.73	1.59
2	A	401	IHP	P3-O13	7.98	1.73	1.59
2	A	401	IHP	P5-O15	7.44	1.72	1.59
2	B	401	IHP	C2-C1	7.31	1.67	1.52
2	B	401	IHP	P4-O14	7.21	1.72	1.59
2	C	401	IHP	P2-O12	6.93	1.71	1.59
2	A	401	IHP	C5-C4	6.80	1.66	1.52
2	A	401	IHP	P4-O14	6.64	1.71	1.59
2	B	401	IHP	P6-O16	6.58	1.71	1.59
2	C	401	IHP	P3-O13	6.58	1.71	1.59
2	C	401	IHP	C3-C2	6.56	1.65	1.52
2	A	401	IHP	P1-O11	6.41	1.70	1.59
2	A	401	IHP	P6-O16	6.27	1.70	1.59
3	B	402	COA	P2A-O6A	5.78	1.76	1.54
2	A	401	IHP	P2-O12	5.65	1.69	1.59
2	A	401	IHP	C4-C3	5.51	1.63	1.52
2	C	401	IHP	P4-O14	5.42	1.69	1.59
2	C	401	IHP	C2-C1	5.38	1.63	1.52
2	B	401	IHP	C3-C2	5.32	1.63	1.52
2	B	401	IHP	P2-O12	4.90	1.68	1.59
3	A	402	COA	P2A-O6A	4.78	1.78	1.59
2	A	401	IHP	C6-C5	4.54	1.61	1.52
3	C	402	COA	P2A-O6A	4.52	1.77	1.59
2	C	401	IHP	P6-O16	4.42	1.67	1.59
2	C	401	IHP	C4-C3	4.07	1.60	1.52
2	B	401	IHP	C5-C4	4.00	1.60	1.52
2	C	401	IHP	C5-C4	3.84	1.60	1.52
2	C	401	IHP	C6-C1	3.73	1.59	1.52
2	B	401	IHP	C6-C5	3.56	1.59	1.52
2	A	401	IHP	C3-C2	3.30	1.59	1.52
3	A	402	COA	C5P-N4P	3.10	1.40	1.33
3	C	402	COA	C5P-N4P	2.93	1.40	1.33
3	C	402	COA	O3B-C3B	-2.93	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	COA	O3B-C3B	-2.84	1.34	1.44
3	B	402	COA	O3B-C3B	-2.83	1.34	1.44
3	C	402	COA	C9P-N8P	2.81	1.40	1.33
3	A	402	COA	C9P-N8P	2.76	1.40	1.33
3	A	402	COA	C5A-C4A	2.74	1.44	1.39
3	A	402	COA	C2A-N1A	2.71	1.38	1.33
3	C	402	COA	C5A-C4A	2.61	1.43	1.39
2	A	401	IHP	O11-C1	-2.55	1.35	1.44
2	C	401	IHP	O13-C3	-2.54	1.35	1.44
3	A	402	COA	C4A-N3A	2.42	1.38	1.34
2	B	401	IHP	O13-C3	-2.41	1.35	1.44
2	C	401	IHP	C6-C5	2.39	1.57	1.52
2	C	401	IHP	O15-C5	-2.34	1.36	1.44
3	B	402	COA	C5A-C4A	2.30	1.43	1.39
2	C	401	IHP	O16-C6	-2.28	1.36	1.44
3	C	402	COA	C2A-N1A	2.24	1.37	1.33
2	A	401	IHP	O15-C5	-2.20	1.36	1.44
2	A	401	IHP	O13-C3	-2.18	1.36	1.44
3	C	402	COA	C4A-N3A	2.13	1.38	1.34
2	C	401	IHP	O11-C1	-2.12	1.36	1.44
3	B	402	COA	C4A-N3A	2.12	1.38	1.34
3	B	402	COA	C2A-N1A	2.09	1.37	1.33
2	B	401	IHP	O16-C6	-2.07	1.37	1.44
2	B	401	IHP	O12-C2	-2.05	1.37	1.44
2	B	401	IHP	O15-C5	-2.01	1.37	1.44

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	IHP	O11-C1-C2	6.53	122.64	108.76
2	B	401	IHP	C6-C5-C4	-6.04	97.17	110.43
2	B	401	IHP	O13-C3-C2	5.49	120.43	108.76
2	B	401	IHP	O16-C6-C5	5.24	119.91	108.76
2	B	401	IHP	C6-C1-C2	-4.94	99.59	110.43
3	A	402	COA	P3B-O3B-C3B	-4.82	110.56	123.43
2	C	401	IHP	C3-C2-C1	4.77	120.90	110.43
3	C	402	COA	P3B-O3B-C3B	-4.72	110.83	123.43
3	B	402	COA	P3B-O3B-C3B	-4.47	111.49	123.43
2	C	401	IHP	O15-C5-C4	4.41	118.14	108.76
2	B	401	IHP	O14-C4-C5	4.29	117.89	108.76
2	A	401	IHP	C5-C4-C3	4.21	119.66	110.43
4	B	403	CIT	O6-C6-C3	4.07	120.94	113.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	O3B-P3B-O7A	-4.06	94.86	109.33
2	B	401	IHP	O12-C2-C1	3.75	116.74	108.76
2	C	401	IHP	O15-C5-C6	3.74	116.72	108.76
3	C	402	COA	O3B-P3B-O7A	-3.71	96.10	109.33
2	C	401	IHP	O13-C3-C2	3.69	116.61	108.76
2	C	401	IHP	O11-C1-C2	3.67	116.58	108.76
2	A	401	IHP	O15-C5-C4	3.58	116.37	108.76
3	C	402	COA	O3A-P1A-O1A	-3.57	99.95	110.70
2	B	401	IHP	C4-C3-C2	-3.54	102.66	110.43
2	B	401	IHP	O15-C5-C4	3.48	116.17	108.76
2	A	401	IHP	O13-C3-C2	3.42	116.03	108.76
2	A	401	IHP	O11-C1-C2	3.35	115.89	108.76
2	B	401	IHP	C3-C2-C1	3.31	117.69	110.43
3	A	402	COA	O5A-P2A-O3A	3.26	116.08	107.27
2	C	401	IHP	O11-C1-C6	3.22	115.60	108.76
3	A	402	COA	O3A-P1A-O1A	-3.12	101.33	110.70
2	C	401	IHP	C5-C4-C3	3.00	117.02	110.43
3	C	402	COA	P1A-O5B-C5B	-2.98	104.25	121.35
3	A	402	COA	C7P-C6P-C5P	-2.98	107.43	112.39
3	B	402	COA	O5A-P2A-O3A	2.97	114.59	104.64
3	C	402	COA	O9A-P3B-O8A	2.93	118.79	107.80
3	B	402	COA	P1A-O5B-C5B	-2.92	104.64	121.35
2	A	401	IHP	O13-C3-C4	2.86	114.84	108.76
2	A	401	IHP	O15-C5-C6	2.85	114.83	108.76
3	A	402	COA	O9A-P3B-O8A	2.81	118.34	107.80
3	B	402	COA	O5A-P2A-O4A	2.80	121.74	110.83
3	B	402	COA	O2A-P1A-O3A	-2.79	99.72	107.27
2	A	401	IHP	O11-C1-C6	2.77	114.66	108.76
3	A	402	COA	P1A-O5B-C5B	-2.74	105.63	121.35
3	C	402	COA	P2A-O6A-CCP	-2.70	106.42	121.12
3	B	402	COA	O8A-P3B-O3B	-2.64	95.55	105.85
3	C	402	COA	N3A-C4A-N9A	2.61	131.61	127.17
2	A	401	IHP	C6-C1-C2	-2.58	104.77	110.43
2	A	401	IHP	P6-O16-C6	2.52	130.16	123.43
2	B	401	IHP	O12-C2-C3	2.52	114.12	108.76
3	C	402	COA	O5A-P2A-O3A	2.50	114.03	107.27
3	A	402	COA	P2A-O6A-CCP	-2.50	107.53	121.12
3	C	402	COA	C4B-O4B-C1B	-2.49	103.97	109.47
2	C	401	IHP	C5-C6-C1	2.49	115.88	110.43
2	B	401	IHP	P5-O15-C5	2.48	130.05	123.43
2	C	401	IHP	C6-C5-C4	-2.44	105.07	110.43
3	A	402	COA	CEP-CBP-CAP	2.41	112.87	108.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	IHP	P4-O14-C4	2.37	129.77	123.43
2	C	401	IHP	O13-C3-C4	2.37	113.80	108.76
3	C	402	COA	C2A-N1A-C6A	-2.36	114.86	118.73
3	B	402	COA	N3A-C4A-N9A	2.34	131.15	127.17
3	C	402	COA	O6A-P2A-O4A	-2.34	99.66	108.94
3	C	402	COA	C5A-C4A-N3A	-2.34	123.50	126.72
3	C	402	COA	O5A-P2A-O4A	2.30	123.13	112.44
3	A	402	COA	C2A-N1A-C6A	-2.28	114.98	118.73
3	B	402	COA	O6A-P2A-O4A	-2.27	101.97	110.83
2	B	401	IHP	O15-C5-C6	2.26	113.57	108.76
3	B	402	COA	C2A-N1A-C6A	-2.25	115.03	118.73
3	C	402	COA	O5P-C5P-N4P	-2.22	118.67	123.03
2	B	401	IHP	O11-C1-C6	2.22	113.48	108.76
2	B	401	IHP	O13-C3-C4	2.20	113.44	108.76
2	B	401	IHP	O41-P1-O11	2.17	114.29	105.85
3	B	402	COA	C2B-C3B-C4B	-2.16	99.45	103.24
3	A	402	COA	N3A-C4A-N9A	2.16	130.84	127.17
2	B	401	IHP	O43-P3-O13	2.16	114.26	105.85
3	B	402	COA	C5A-C4A-N3A	-2.14	123.78	126.72
3	A	402	COA	O6A-P2A-O4A	-2.13	100.49	108.94
4	B	403	CIT	O2-C1-C2	2.11	121.04	114.35
2	B	401	IHP	O42-P2-O12	2.10	114.03	105.85
3	A	402	COA	O5A-P2A-O4A	2.06	122.03	112.44
2	B	401	IHP	P1-O11-C1	2.06	128.93	123.43
3	B	402	COA	O9A-P3B-O7A	2.05	118.84	110.83
3	A	402	COA	C3P-N4P-C5P	-2.05	119.02	122.82
2	A	401	IHP	O45-P5-O15	2.01	113.66	105.85

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
3	C	402	COA	O4B-C1B-N9A-C4A
3	C	402	COA	O4B-C1B-N9A-C8A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	402	COA	CDP-CBP-CCP-O6A
3	C	402	COA	CEP-CBP-CCP-O6A
3	C	402	COA	CAP-CBP-CCP-O6A
3	C	402	COA	C5P-C6P-C7P-N8P
3	C	402	COA	S1P-C2P-C3P-N4P
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	CDP-CBP-CCP-O6A
3	A	402	COA	CEP-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	C	402	COA	C3B-C4B-C5B-O5B
3	A	402	COA	C3B-C4B-C5B-O5B
3	C	402	COA	O5P-C5P-N4P-C3P
3	B	402	COA	C3B-C4B-C5B-O5B
3	B	402	COA	O4B-C4B-C5B-O5B
2	B	401	IHP	C5-C6-O16-P6
2	C	401	IHP	C4-O14-P4-O24
2	B	401	IHP	C4-C3-O13-P3
3	A	402	COA	N8P-C9P-CAP-OAP
2	C	401	IHP	C5-C4-O14-P4
2	A	401	IHP	C5-C4-O14-P4
2	B	401	IHP	C2-C3-O13-P3
2	C	401	IHP	C5-O15-P5-O25
4	B	403	CIT	C1-C2-C3-O7
3	C	402	COA	CCP-O6A-P2A-O3A
3	C	402	COA	CCP-O6A-P2A-O4A
3	C	402	COA	CCP-O6A-P2A-O5A
3	A	402	COA	CCP-O6A-P2A-O3A
3	A	402	COA	CCP-O6A-P2A-O4A
3	A	402	COA	CCP-O6A-P2A-O5A
3	A	402	COA	P1A-O3A-P2A-O5A
3	B	402	COA	P2A-O3A-P1A-O1A
4	B	403	CIT	C4-C3-C6-O5
3	A	402	COA	O9P-C9P-CAP-CBP
2	A	401	IHP	C3-C2-O12-P2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	401	IHP	C3-O13-P3-O43
3	A	402	COA	N8P-C9P-CAP-CBP
3	C	402	COA	O9P-C9P-CAP-OAP
2	C	401	IHP	C2-O12-P2-O22
2	A	401	IHP	C4-O14-P4-O24
2	B	401	IHP	C1-O11-P1-O21
2	B	401	IHP	C5-O15-P5-O25
3	A	402	COA	P1A-O3A-P2A-O4A
3	B	402	COA	P2A-O3A-P1A-O5B
4	B	403	CIT	C4-C3-C6-O6
3	C	402	COA	C2P-C3P-N4P-C5P
4	B	403	CIT	C1-C2-C3-C4
2	C	401	IHP	C2-O12-P2-O32
2	C	401	IHP	C3-O13-P3-O43
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
3	B	402	COA	C3B-O3B-P3B-O7A
3	C	402	COA	N8P-C9P-CAP-OAP

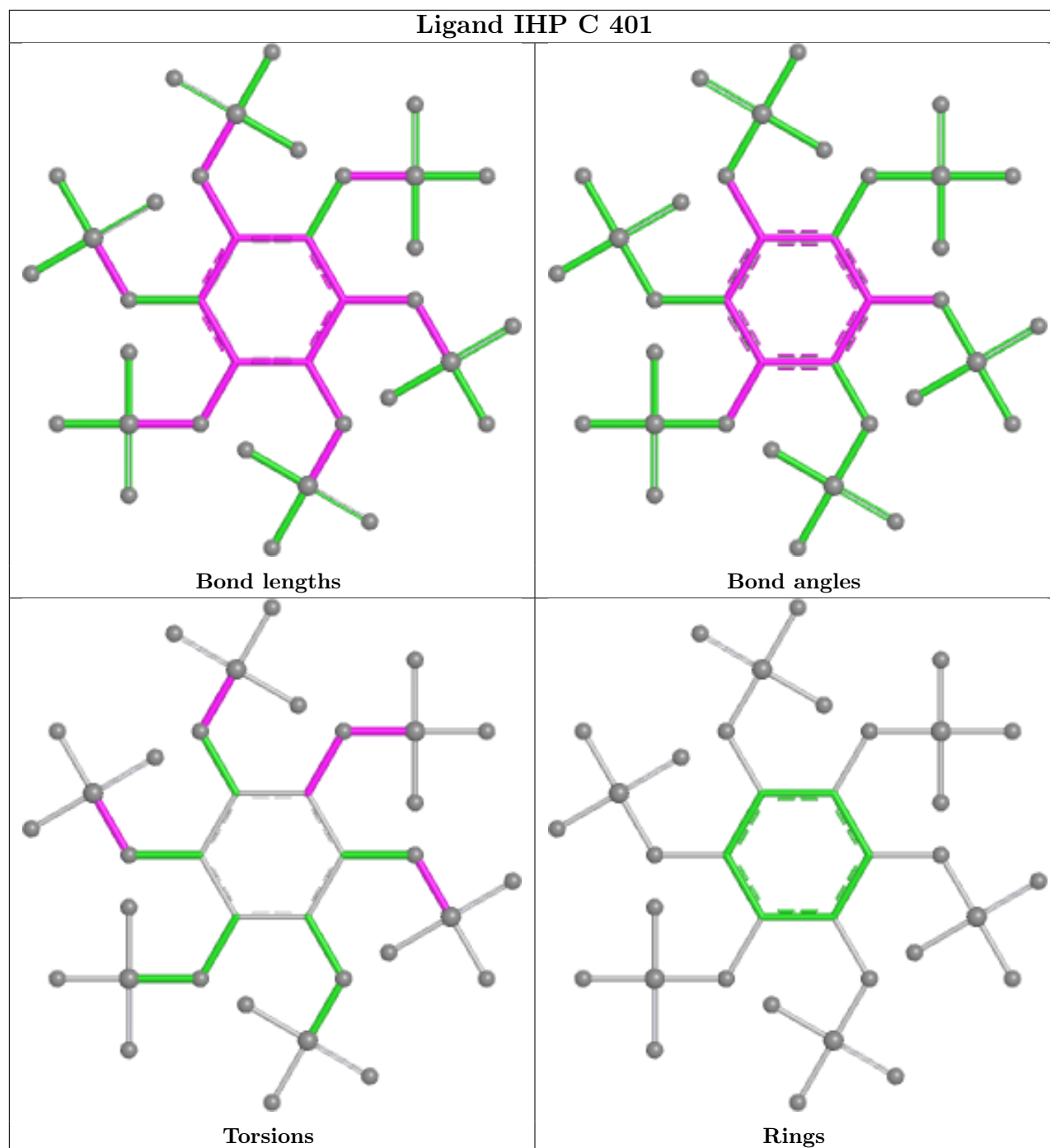
There are no ring outliers.

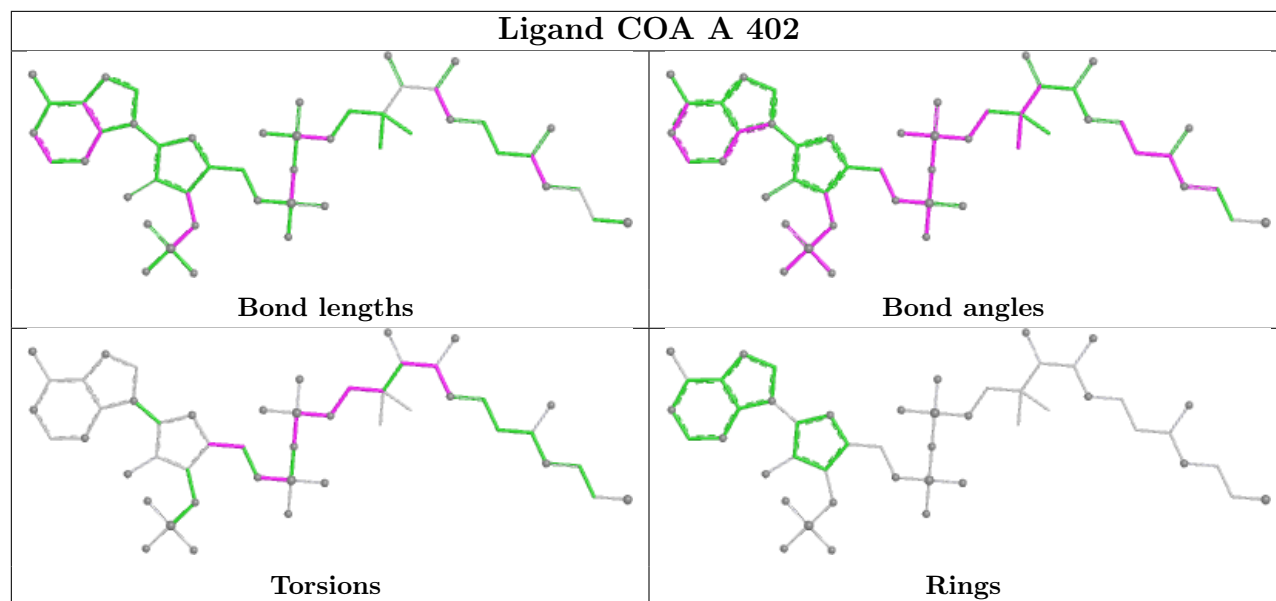
5 monomers are involved in 18 short contacts:

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

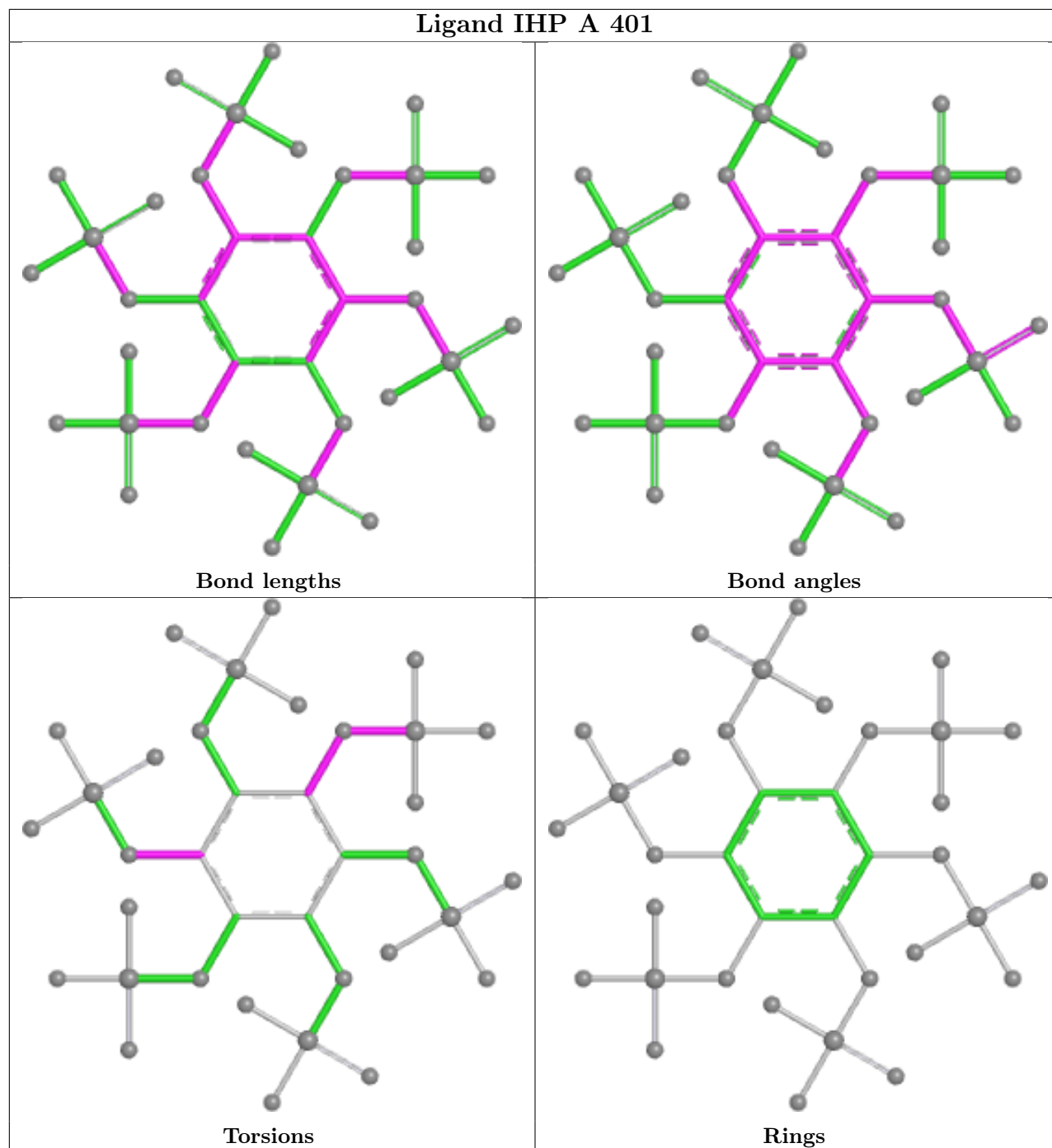
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

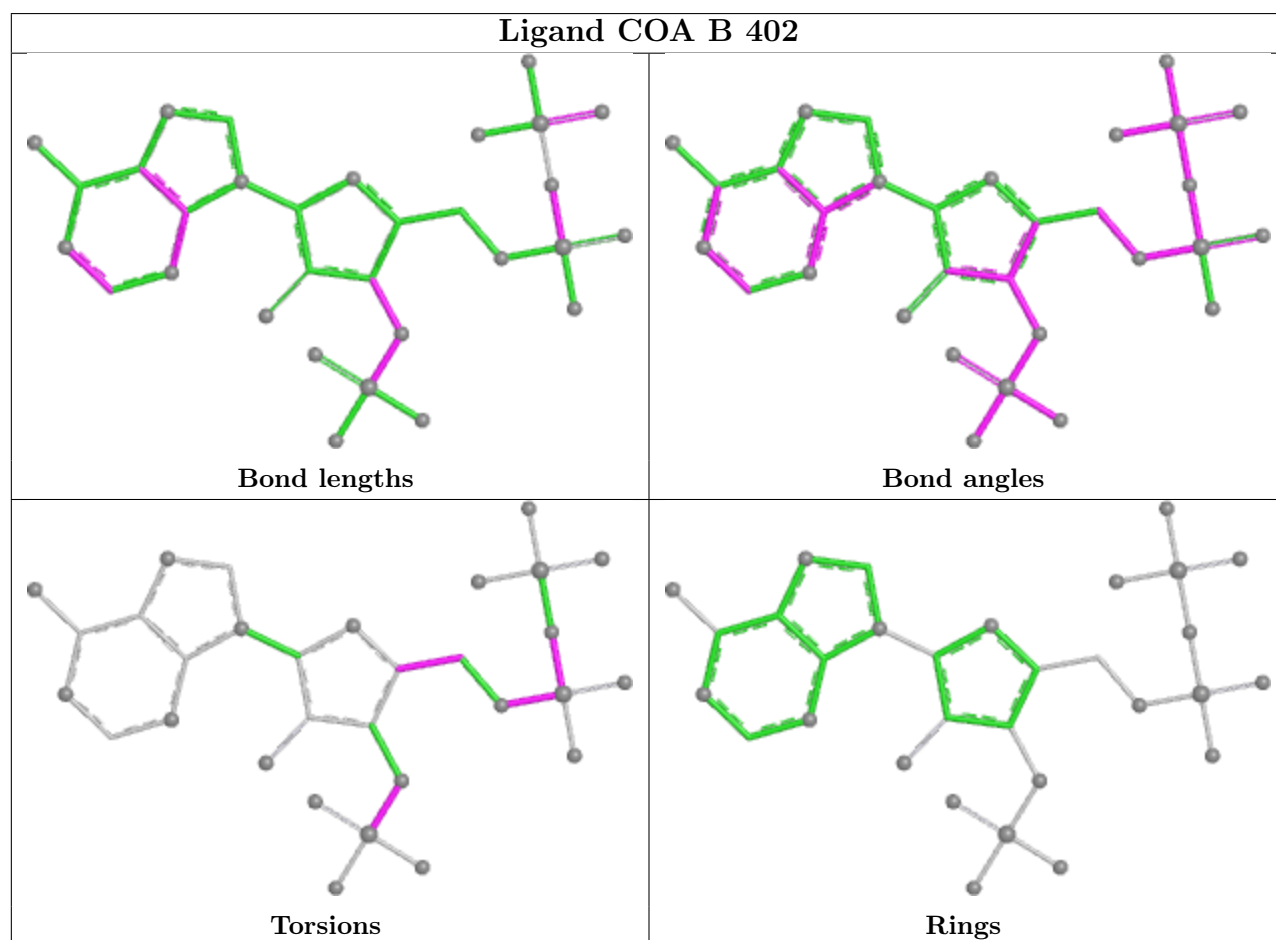
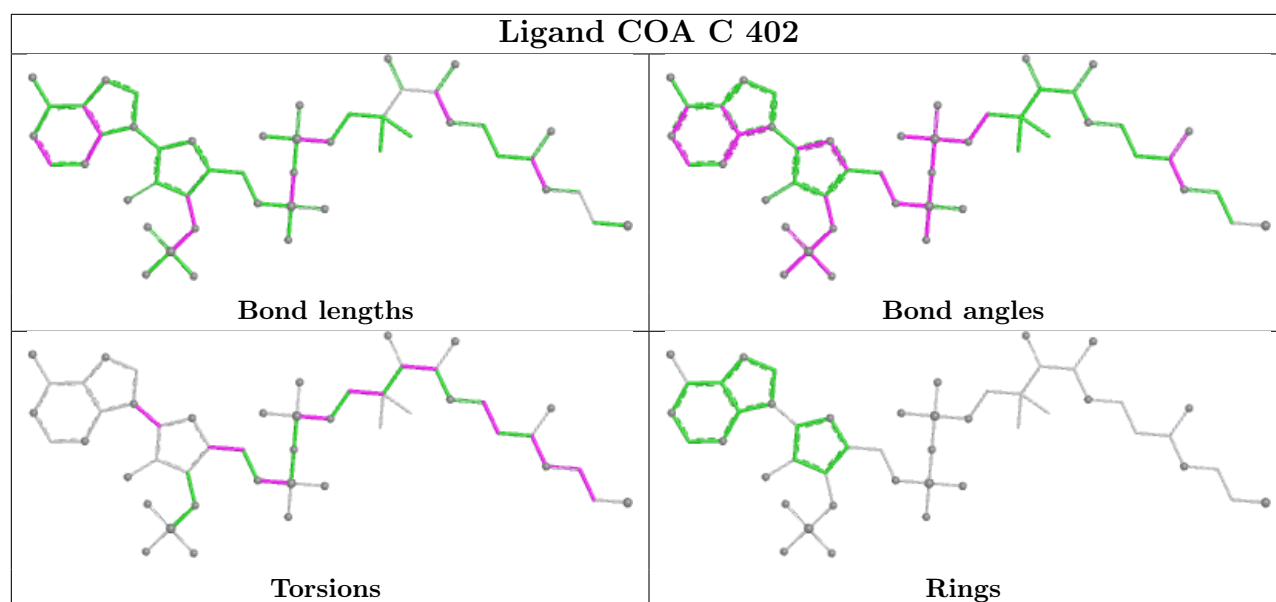
equivalents in the CSD to analyse the geometry.

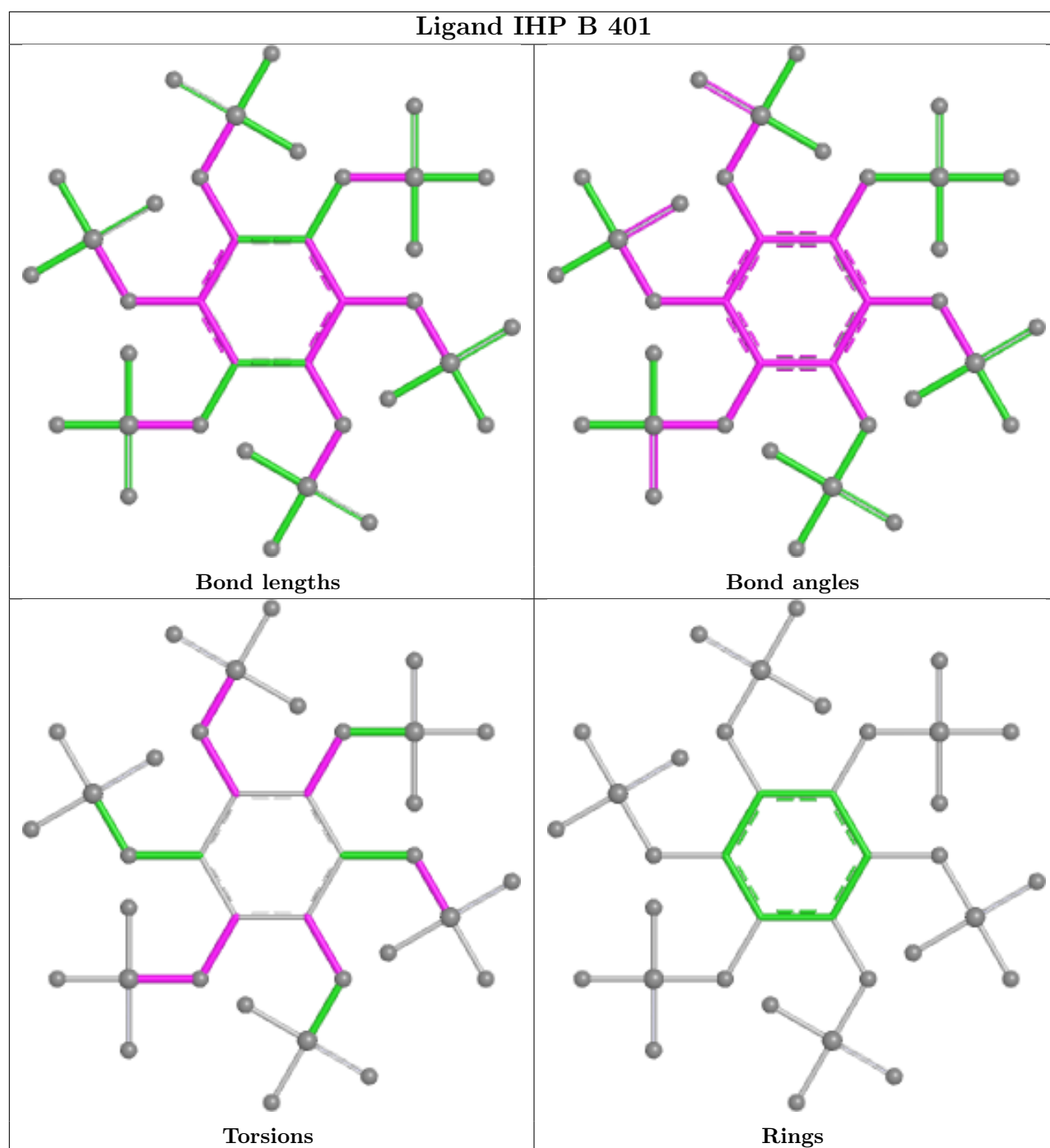




Ligand IHP A 401







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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	324/342 (94%)	0.20	5 (1%) 72 57	21, 31, 47, 58	1 (0%)
1	B	320/342 (93%)	0.16	2 (0%) 85 75	19, 36, 53, 62	1 (0%)
1	C	320/342 (93%)	0.22	7 (2%) 62 47	17, 35, 52, 63	1 (0%)
All	All	964/1026 (93%)	0.19	14 (1%) 72 57	17, 34, 52, 63	3 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119[A]	TYR	4.4
1	C	85	SER	4.2
1	C	71	TYR	3.5
1	A	43	GLU	3.4
1	C	128	ASP	2.7
1	B	343	PRO	2.4
1	A	118	HIS	2.4
1	A	45	THR	2.3
1	A	344	SER	2.3
1	B	163	ALA	2.3
1	C	137	PHE	2.3
1	A	277	ALA	2.2
1	C	339	ASP	2.2
1	C	91	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

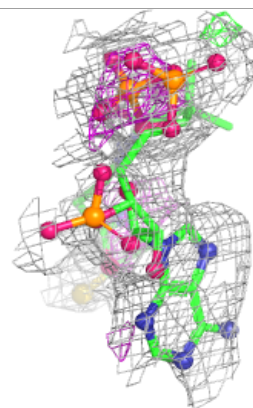
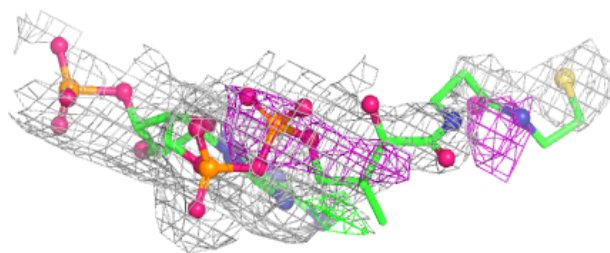
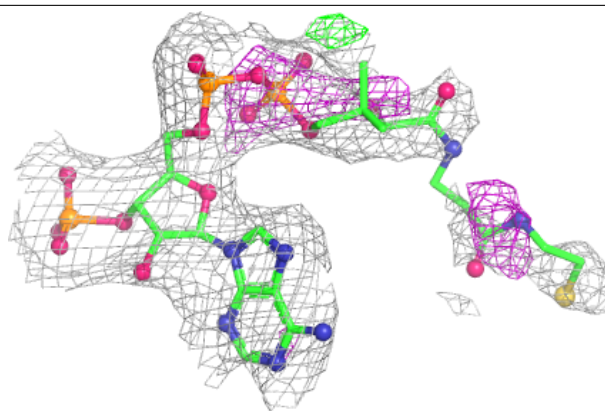
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	CIT	B	403	13/13	0.63	0.17	40,40,40,40	0
3	COA	A	402	48/48	0.81	0.14	37,37,37,37	0
2	IHP	B	401	36/36	0.83	0.11	42,42,42,42	0
3	COA	C	402	48/48	0.83	0.13	41,41,41,41	0
3	COA	B	402	31/48	0.85	0.12	43,43,43,43	0
2	IHP	C	401	36/36	0.90	0.09	36,36,36,36	0
2	IHP	A	401	36/36	0.91	0.08	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.

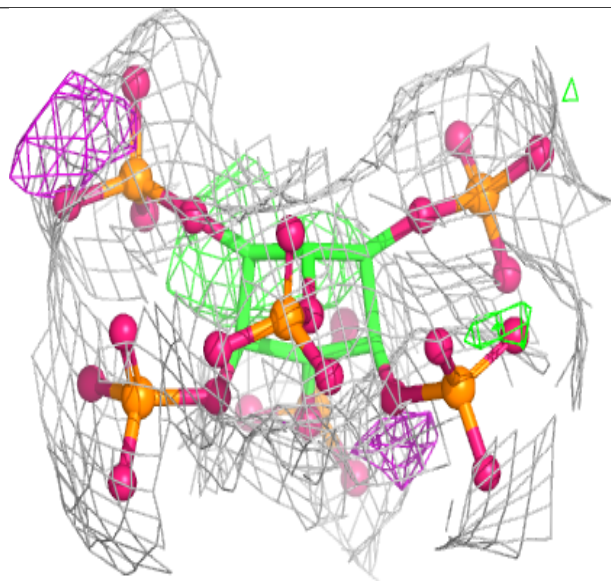
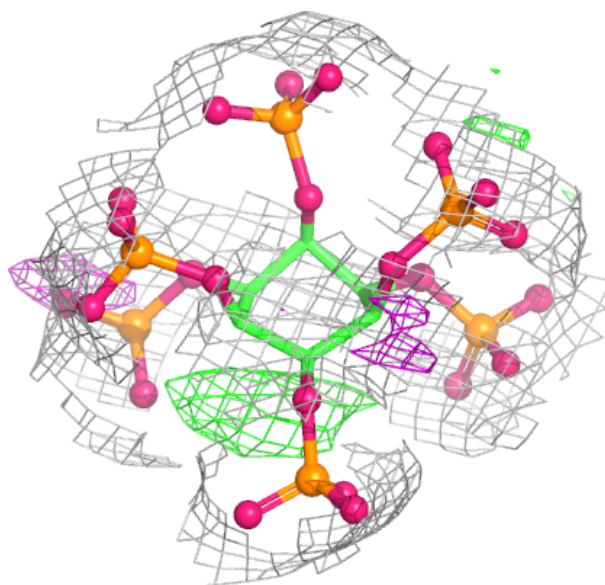
Electron density around COA A 402:

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



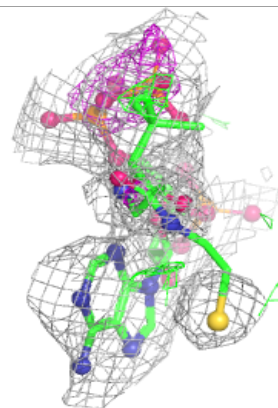
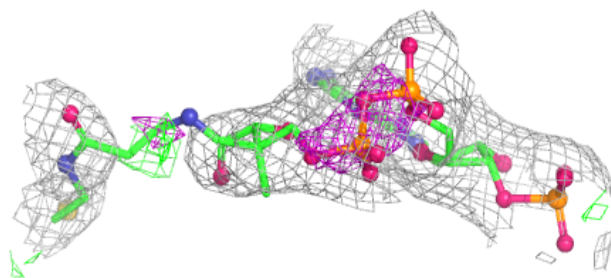
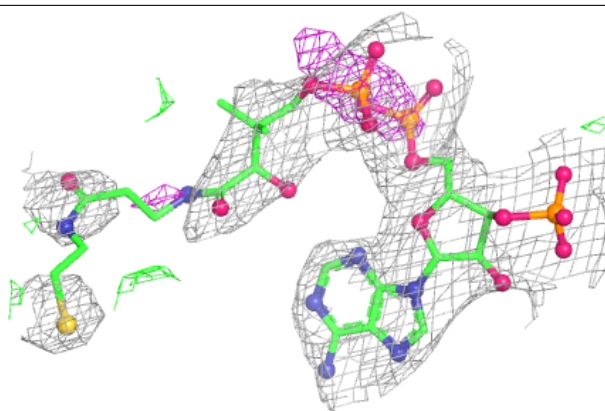
Electron density around IHP B 401:

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



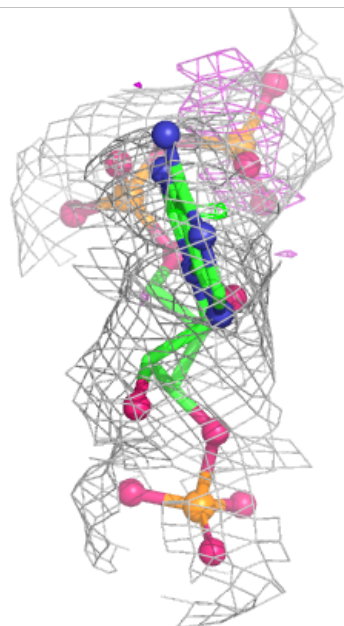
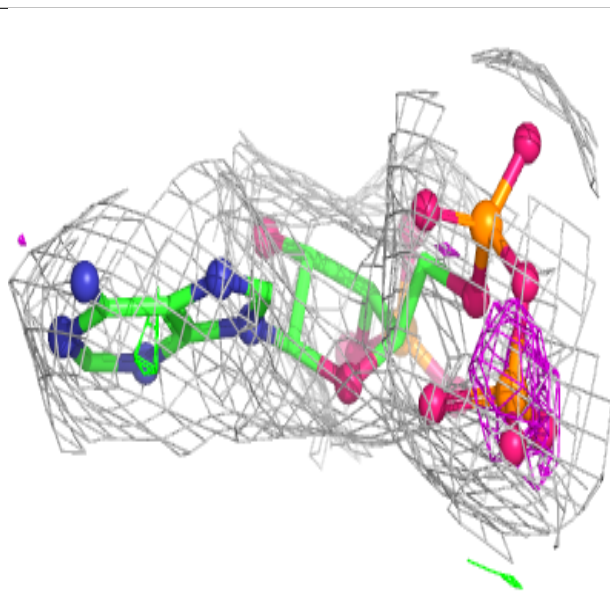
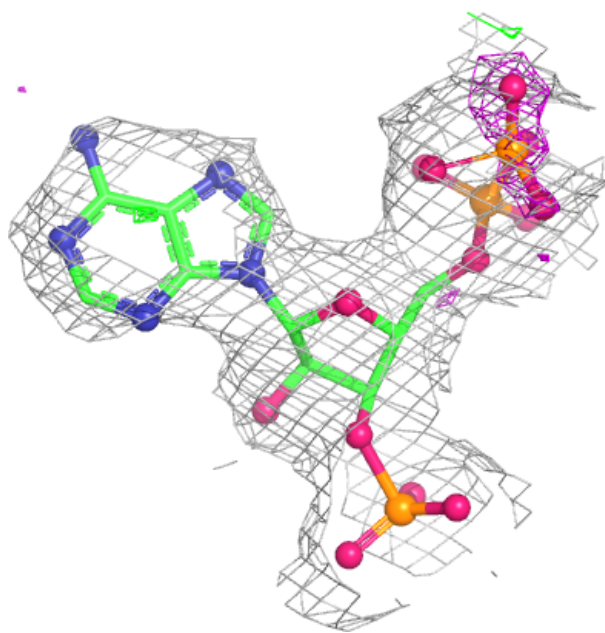
Electron density around COA C 402:

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



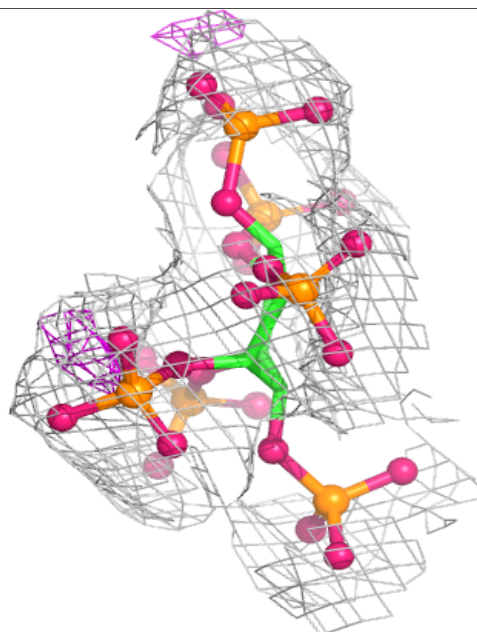
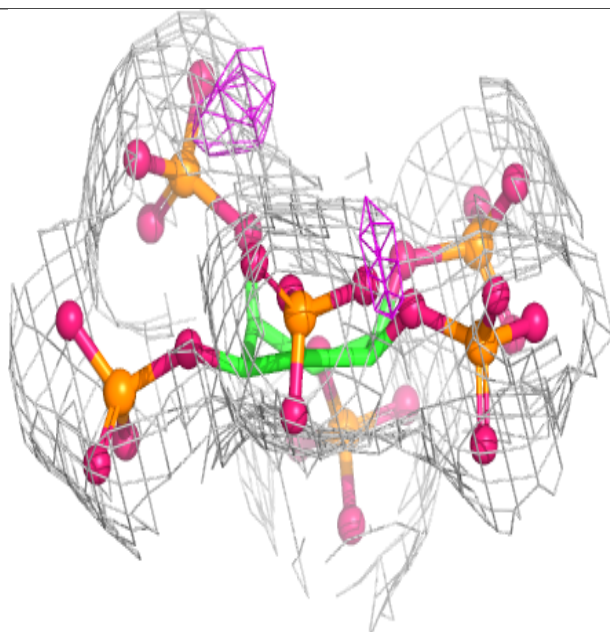
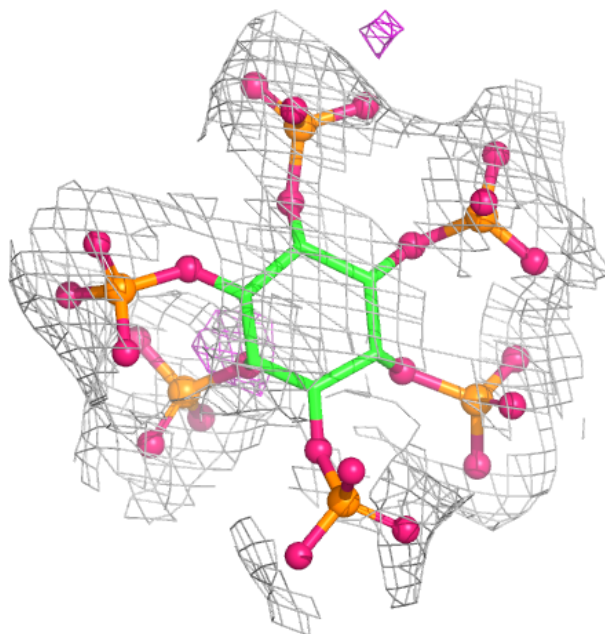
Electron density around COA B 402:

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



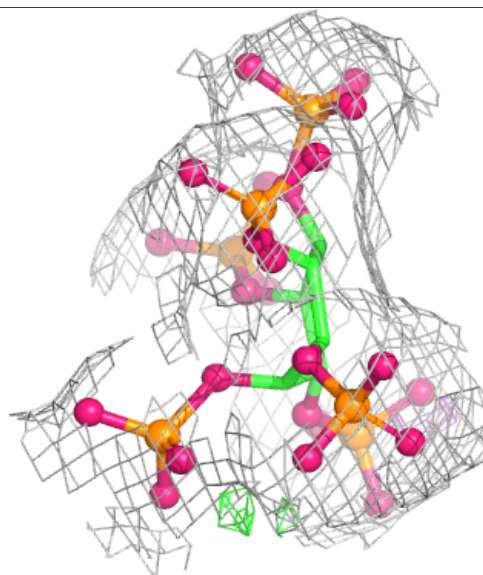
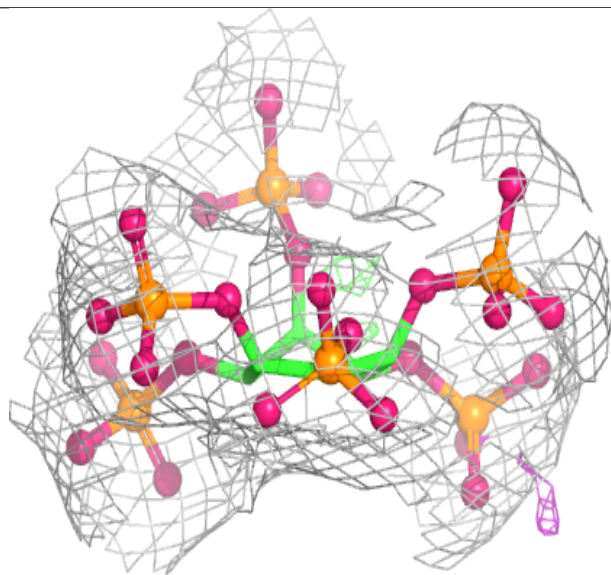
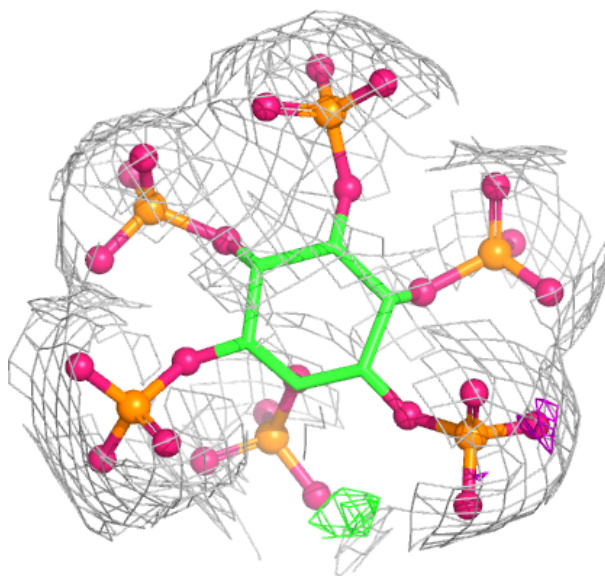
Electron density around IHP C 401:

$2mF_o-DF_c$ (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.