



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:28 PM UTC

PDB ID : 5W3Y / pdb_00005w3y
Title : Crystal structure of PopP2 C321A in complex with IP6 and AcCoA
Authors : Zhang, Z.M.; Gao, L.; Song, J.
Deposited on : 2017-06-08
Resolution : 2.20 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

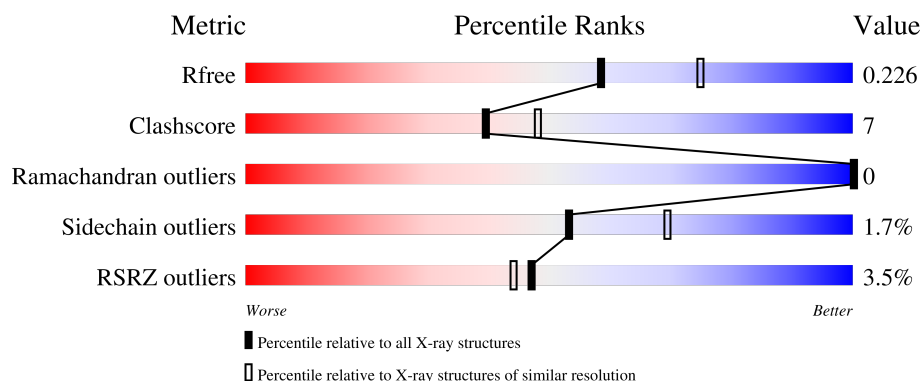
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	352	2% 83% 12% 5%
1	B	352	9% 77% 15% 7%
1	C	352	% 83% 12% 5%
1	D	352	% 81% 14% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10739 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 PopP2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2538	1570	475	481	12			
1	B	327	Total	C	N	O	S	0	0	0
			2401	1486	451	454	10			
1	C	335	Total	C	N	O	S	0	0	0
			2536	1567	474	483	12			
1	D	334	Total	C	N	O	S	0	0	0
			2536	1569	472	483	12			

There are 52 discrepancies between the modelled and reference sequences:

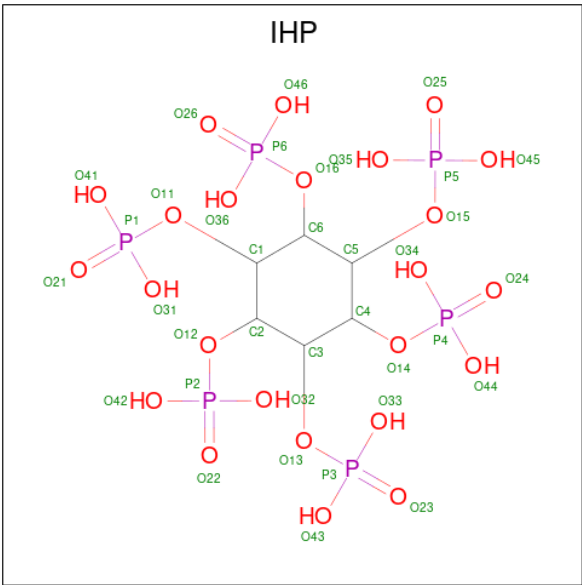
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	SER	-	expression tag	UNP A0A0S4VB05
A	138	GLU	-	expression tag	UNP A0A0S4VB05
A	139	PHE	-	expression tag	UNP A0A0S4VB05
A	140	GLU	-	expression tag	UNP A0A0S4VB05
A	141	LEU	-	expression tag	UNP A0A0S4VB05
A	142	GLY	-	expression tag	UNP A0A0S4VB05
A	143	ALA	-	expression tag	UNP A0A0S4VB05
A	144	PRO	-	expression tag	UNP A0A0S4VB05
A	145	ALA	-	expression tag	UNP A0A0S4VB05
A	146	GLY	-	expression tag	UNP A0A0S4VB05
A	147	ARG	-	expression tag	UNP A0A0S4VB05
A	148	GLN	-	expression tag	UNP A0A0S4VB05
A	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05
B	137	SER	-	expression tag	UNP A0A0S4VB05
B	138	GLU	-	expression tag	UNP A0A0S4VB05
B	139	PHE	-	expression tag	UNP A0A0S4VB05
B	140	GLU	-	expression tag	UNP A0A0S4VB05
B	141	LEU	-	expression tag	UNP A0A0S4VB05
B	142	GLY	-	expression tag	UNP A0A0S4VB05
B	143	ALA	-	expression tag	UNP A0A0S4VB05
B	144	PRO	-	expression tag	UNP A0A0S4VB05

Continued on next page...

Continued from previous page...

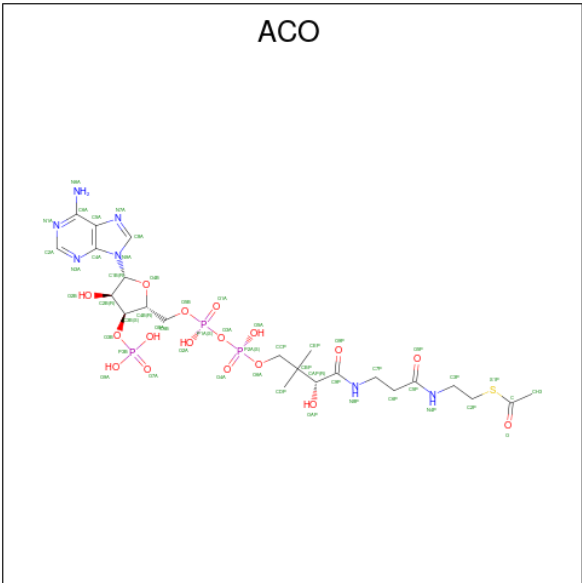
Chain	Residue	Modelled	Actual	Comment	Reference
B	145	ALA	-	expression tag	UNP A0A0S4VB05
B	146	GLY	-	expression tag	UNP A0A0S4VB05
B	147	ARG	-	expression tag	UNP A0A0S4VB05
B	148	GLN	-	expression tag	UNP A0A0S4VB05
B	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05
C	137	SER	-	expression tag	UNP A0A0S4VB05
C	138	GLU	-	expression tag	UNP A0A0S4VB05
C	139	PHE	-	expression tag	UNP A0A0S4VB05
C	140	GLU	-	expression tag	UNP A0A0S4VB05
C	141	LEU	-	expression tag	UNP A0A0S4VB05
C	142	GLY	-	expression tag	UNP A0A0S4VB05
C	143	ALA	-	expression tag	UNP A0A0S4VB05
C	144	PRO	-	expression tag	UNP A0A0S4VB05
C	145	ALA	-	expression tag	UNP A0A0S4VB05
C	146	GLY	-	expression tag	UNP A0A0S4VB05
C	147	ARG	-	expression tag	UNP A0A0S4VB05
C	148	GLN	-	expression tag	UNP A0A0S4VB05
C	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05
D	137	SER	-	expression tag	UNP A0A0S4VB05
D	138	GLU	-	expression tag	UNP A0A0S4VB05
D	139	PHE	-	expression tag	UNP A0A0S4VB05
D	140	GLU	-	expression tag	UNP A0A0S4VB05
D	141	LEU	-	expression tag	UNP A0A0S4VB05
D	142	GLY	-	expression tag	UNP A0A0S4VB05
D	143	ALA	-	expression tag	UNP A0A0S4VB05
D	144	PRO	-	expression tag	UNP A0A0S4VB05
D	145	ALA	-	expression tag	UNP A0A0S4VB05
D	146	GLY	-	expression tag	UNP A0A0S4VB05
D	147	ARG	-	expression tag	UNP A0A0S4VB05
D	148	GLN	-	expression tag	UNP A0A0S4VB05
D	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

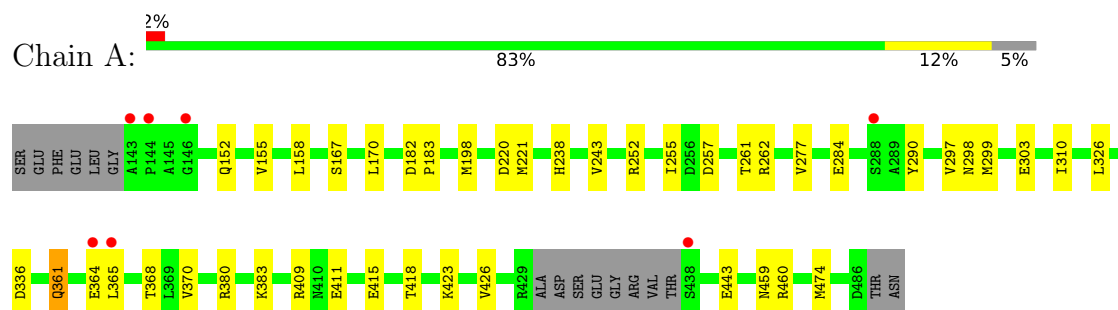
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	92	Total	O	0	0
			92	92		
4	C	119	Total	O	0	0
			119	119		
4	D	143	Total	O	0	0
			143	143		

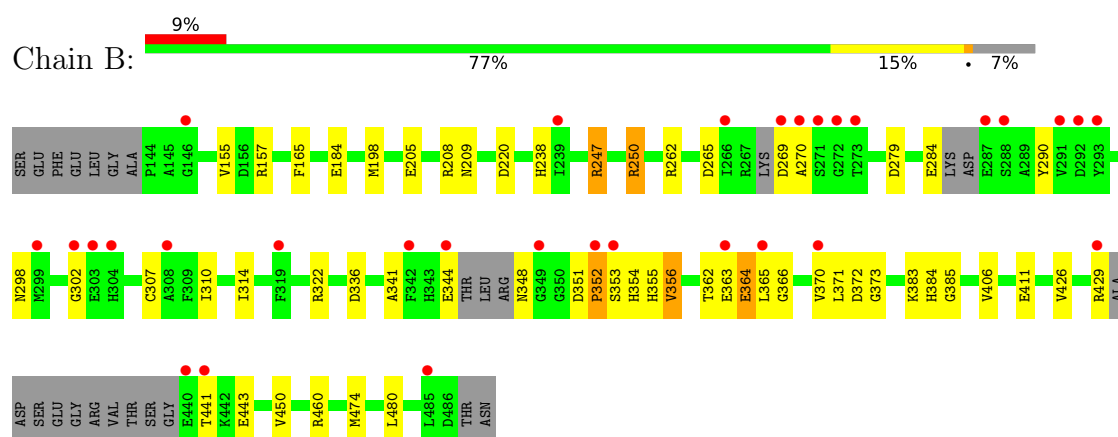
3 Residue-property plots [i](#)

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.

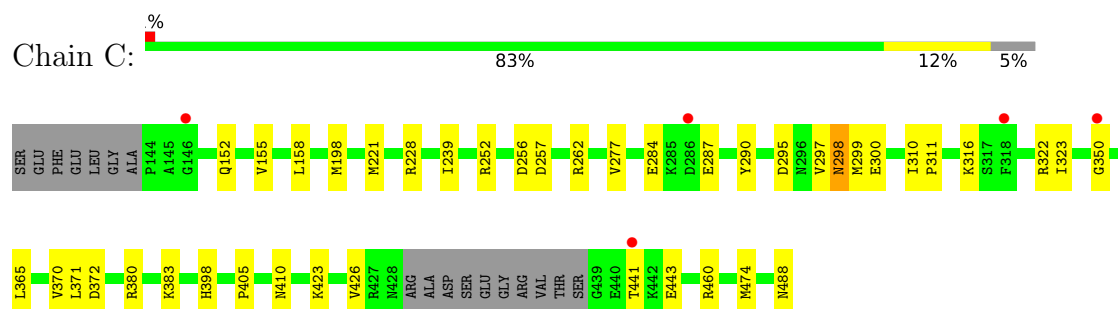
• Molecule 1: PopP2 protein



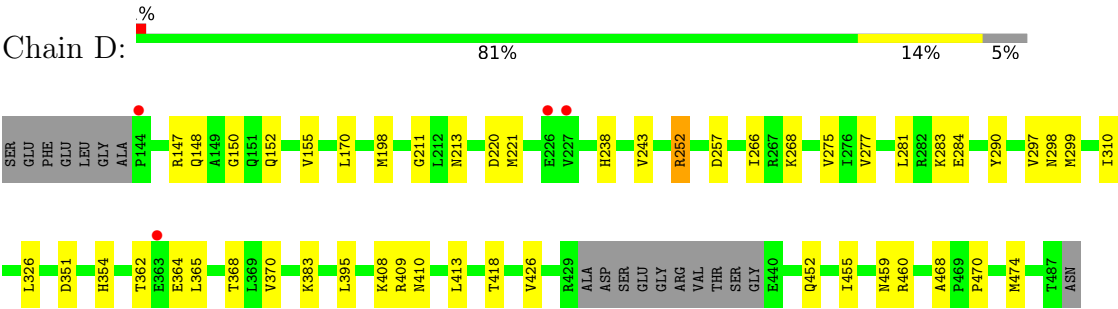
• Molecule 1: PopP2 protein



• Molecule 1: PopP2 protein



• Molecule 1: PopP2 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.39Å 79.88Å 77.75Å 112.33° 111.65° 103.39°	Depositor
Resolution (Å)	39.09 – 2.20 39.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.09-2.20) 97.7 (39.09-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.225 0.186 , 0.226	Depositor DCC
R_{free} test set	2027 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.186 for -l,h+k+l,-k 0.186 for h+k+l,-l,-h 0.016 for l,-h-k-l,h 0.012 for -h-k-l,l,k 0.126 for k,h,-h-k-l 0.013 for -k,-h,-l 0.010 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10739	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, 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	0.44	0/2579	0.84	1/3493 (0.0%)
1	B	0.44	0/2436	0.87	2/3301 (0.1%)
1	C	0.44	0/2576	0.83	4/3487 (0.1%)
1	D	0.45	0/2577	0.84	5/3488 (0.1%)
All	All	0.44	0/10168	0.84	12/13769 (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	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	GLU	N-CA-C	6.98	122.23	113.43
1	B	302	GLY	N-CA-C	6.52	121.94	112.55
1	A	364	GLU	N-CA-C	-5.80	105.29	112.72
1	D	468	ALA	CA-C-N	5.50	123.68	119.66
1	D	468	ALA	C-N-CA	5.50	123.68	119.66
1	C	398	HIS	CA-C-N	5.50	125.33	119.28
1	C	398	HIS	C-N-CA	5.50	125.33	119.28
1	D	364	GLU	N-CA-C	-5.42	106.72	113.55
1	D	362	THR	N-CA-C	-5.41	102.87	110.50
1	C	350	GLY	N-CA-C	-5.32	106.71	112.08
1	C	316	LYS	N-CA-C	-5.11	107.70	114.04
1	D	354	HIS	N-CA-C	-5.05	107.12	113.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	352	PRO	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	2538	0	2492	32	0
1	B	2401	0	2310	42	0
1	C	2536	0	2502	27	0
1	D	2536	0	2495	33	0
2	A	36	0	6	3	0
2	B	36	0	6	3	0
2	C	36	0	6	2	0
2	D	36	0	6	4	0
3	A	31	0	11	0	0
3	B	31	0	11	1	0
3	C	31	0	11	0	0
3	D	31	0	11	1	0
4	A	106	0	0	7	0
4	B	92	0	0	5	1
4	C	119	0	0	3	1
4	D	143	0	0	8	0
All	All	10739	0	9867	134	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 7.

All (134) 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:152:GLN:O	4:A:601:HOH:O	1.93	0.86
1:C:256:ASP:OD2	4:C:601:HOH:O	1.92	0.86
1:D:252:ARG:NH2	4:D:602:HOH:O	2.09	0.85
1:D:452:GLN:NE2	4:D:603:HOH:O	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASP:OD1	1:B:270:ALA:N	2.15	0.77
1:D:351:ASP:OD2	4:D:601:HOH:O	2.03	0.75
1:B:362:THR:OG1	1:B:366:GLY:N	2.17	0.74
1:C:299:MET:HG2	1:C:365:LEU:HD21	1.69	0.74
1:A:361:GLN:O	4:A:603:HOH:O	2.05	0.73
1:A:220:ASP:OD1	1:A:238:HIS:NE2	2.22	0.73
1:D:409:ARG:NH1	4:D:604:HOH:O	2.15	0.73
1:C:155:VAL:HG22	1:C:474:MET:HE3	1.72	0.72
1:D:155:VAL:HG22	1:D:474:MET:HE3	1.71	0.72
1:B:155:VAL:HG22	1:B:474:MET:HE3	1.72	0.72
1:A:252:ARG:NH2	1:A:336:ASP:OD2	2.22	0.71
1:A:415:GLU:OE1	4:A:604:HOH:O	2.11	0.69
3:B:502:ACO:H51A	3:B:502:ACO:H8A	1.74	0.68
1:B:209:ASN:OD1	4:B:601:HOH:O	2.11	0.68
1:A:155:VAL:HG22	1:A:474:MET:HE3	1.76	0.67
1:B:250:ARG:NH2	1:B:336:ASP:O	2.29	0.66
1:D:221:MET:HE3	1:D:257:ASP:HB2	1.78	0.66
1:A:243:VAL:O	4:A:605:HOH:O	2.13	0.65
1:D:299:MET:HG2	1:D:365:LEU:HD21	1.79	0.64
1:C:311:PRO:O	4:C:602:HOH:O	2.15	0.63
1:B:365:LEU:HD12	1:B:366:GLY:HA3	1.80	0.63
1:B:351:ASP:HB3	1:B:352:PRO:C	2.24	0.63
1:D:277:VAL:HG21	1:D:297:VAL:HG11	1.81	0.63
1:D:211:GLY:O	1:D:252:ARG:NH1	2.32	0.62
1:B:184:GLU:OE1	1:B:429:ARG:NH1	2.33	0.61
1:A:198:MET:HE1	1:A:326:LEU:HB2	1.81	0.61
1:B:205:GLU:OE1	1:B:208:ARG:NH1	2.33	0.61
1:B:250:ARG:NH2	1:B:336:ASP:OD1	2.33	0.61
1:B:370:VAL:HG12	1:B:372:ASP:H	1.66	0.61
1:D:368:THR:HG23	4:D:626:HOH:O	2.02	0.60
1:B:355:HIS:CD2	4:B:613:HOH:O	2.55	0.59
1:C:310:ILE:HG12	1:C:370:VAL:HG21	1.84	0.58
1:A:262:ARG:NH1	4:A:610:HOH:O	2.31	0.58
1:A:409:ARG:HG3	1:A:411:GLU:HG3	1.85	0.58
1:B:344:GLU:O	1:B:348:ASN:N	2.37	0.57
1:A:277:VAL:HG21	1:A:297:VAL:HG11	1.85	0.57
1:B:356:VAL:HG22	1:B:373:GLY:HA2	1.84	0.57
1:C:284:GLU:HB2	1:C:290:TYR:CZ	2.40	0.57
1:D:152:GLN:NE2	4:D:606:HOH:O	2.20	0.56
1:B:364:GLU:H	1:B:366:GLY:N	2.04	0.55
1:A:299:MET:HE1	1:A:303:GLU:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLU:HG2	1:C:290:TYR:HE2	1.72	0.54
1:C:383:LYS:HE3	2:C:501:IHP:O35	2.06	0.54
1:B:363:GLU:H	1:B:366:GLY:HA2	1.71	0.54
1:C:460:ARG:NH2	2:C:501:IHP:O44	2.26	0.54
1:B:450:VAL:HG23	4:B:634:HOH:O	2.07	0.53
1:C:198:MET:HE3	1:C:322:ARG:HB3	1.89	0.53
1:D:266:ILE:HG12	1:D:275:VAL:HG13	1.90	0.53
1:D:281:LEU:HD21	1:D:283:LYS:HE3	1.91	0.52
1:C:262:ARG:NH1	4:C:612:HOH:O	2.43	0.52
1:B:220:ASP:OD1	1:B:238:HIS:NE2	2.39	0.52
1:B:184:GLU:OE1	4:B:602:HOH:O	2.19	0.51
1:A:299:MET:HG2	1:A:365:LEU:HD11	1.93	0.51
1:C:298:ASN:HB3	1:C:365:LEU:HD23	1.92	0.51
1:B:310:ILE:HG12	1:B:370:VAL:HG21	1.93	0.51
1:D:198:MET:HE1	1:D:326:LEU:HB2	1.93	0.51
1:A:298:ASN:HB3	1:A:365:LEU:HD13	1.92	0.50
1:A:170:LEU:HD21	1:A:459:ASN:OD1	2.12	0.50
1:A:221:MET:HG3	1:A:257:ASP:O	2.12	0.50
1:B:262:ARG:NE	1:B:279:ASP:OD2	2.43	0.50
1:D:170:LEU:HD21	1:D:459:ASN:OD1	2.12	0.50
1:D:220:ASP:OD1	1:D:238:HIS:NE2	2.45	0.50
1:A:460:ARG:HH12	2:A:501:IHP:P3	2.35	0.49
1:D:152:GLN:H	1:D:152:GLN:CD	2.20	0.49
1:C:221:MET:HG3	1:C:257:ASP:O	2.13	0.49
1:D:284:GLU:HB2	1:D:290:TYR:CZ	2.48	0.49
1:D:395:LEU:HD21	1:D:413:LEU:HD23	1.94	0.49
1:B:383:LYS:NZ	2:B:501:IHP:O23	2.46	0.49
1:A:310:ILE:HG12	1:A:370:VAL:HB	1.95	0.48
1:B:284:GLU:HB2	1:B:290:TYR:CE2	2.48	0.48
1:B:364:GLU:H	1:B:365:LEU:C	2.22	0.48
1:C:152:GLN:H	1:C:152:GLN:CD	2.21	0.48
1:A:299:MET:HE3	1:A:365:LEU:HD21	1.95	0.48
1:B:460:ARG:NH2	2:B:501:IHP:O35	2.35	0.47
1:B:460:ARG:HH22	2:B:501:IHP:P5	2.37	0.47
1:D:460:ARG:NH2	2:D:501:IHP:H3	2.30	0.47
1:C:370:VAL:O	1:C:371:LEU:HB2	2.15	0.47
1:C:410:ASN:HB2	1:D:418:THR:OG1	2.14	0.47
1:A:252:ARG:N	1:A:252:ARG:HD2	2.29	0.47
1:C:287:GLU:HG2	1:C:290:TYR:CE2	2.49	0.47
1:B:384:HIS:HB3	1:B:450:VAL:HG22	1.96	0.47
1:A:299:MET:HA	1:A:299:MET:HE2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:VAL:HG12	1:C:372:ASP:H	1.80	0.46
1:C:380:ARG:NH2	1:C:405:PRO:O	2.47	0.46
1:B:365:LEU:HA	1:B:366:GLY:HA3	1.70	0.46
1:B:370:VAL:O	1:B:371:LEU:HB2	2.15	0.46
1:C:228:ARG:HH21	1:C:488:ASN:C	2.23	0.46
1:A:423:LYS:HE2	1:A:443:GLU:OE1	2.16	0.46
1:B:250:ARG:NH1	1:B:265:ASP:OD1	2.48	0.46
1:B:198:MET:HE3	1:B:322:ARG:HB3	1.98	0.45
1:D:150:GLY:HA2	1:D:152:GLN:HE22	1.82	0.45
1:B:247:ARG:NH2	4:B:603:HOH:O	2.23	0.45
1:A:418:THR:OG1	1:D:410:ASN:HB2	2.17	0.45
1:D:170:LEU:HD11	1:D:455:ILE:HG23	1.99	0.45
1:D:460:ARG:HH22	2:D:501:IHP:H3	1.81	0.44
1:B:352:PRO:C	1:B:354:HIS:H	2.26	0.44
1:D:148:GLN:HB2	4:D:606:HOH:O	2.17	0.44
1:A:284:GLU:HB2	1:A:290:TYR:CZ	2.53	0.44
1:B:406:VAL:HG22	1:B:411:GLU:O	2.18	0.44
1:C:298:ASN:HB3	1:C:365:LEU:CD2	2.48	0.44
1:B:352:PRO:HG2	1:B:353:SER:HA	2.00	0.44
1:C:198:MET:HE1	1:C:323:ILE:HD13	1.99	0.44
1:A:158:LEU:HD12	1:A:474:MET:HE1	2.00	0.44
1:D:213:ASN:ND2	4:D:615:HOH:O	2.50	0.44
1:D:298:ASN:C	1:D:298:ASN:HD22	2.26	0.43
1:B:355:HIS:CD2	1:B:355:HIS:N	2.86	0.43
1:A:383:LYS:NZ	2:A:501:IHP:O21	2.52	0.43
1:A:368:THR:HG23	4:A:642:HOH:O	2.19	0.43
1:B:284:GLU:HB2	1:B:290:TYR:CZ	2.53	0.43
1:D:243:VAL:O	1:D:268:LYS:NZ	2.34	0.43
1:C:423:LYS:HE2	1:C:443:GLU:OE2	2.19	0.43
1:D:147:ARG:O	1:D:470:PRO:HG2	2.18	0.42
3:D:502:ACO:O5B	3:D:502:ACO:H8A	2.18	0.42
1:D:310:ILE:HG12	1:D:370:VAL:HB	2.02	0.42
1:A:182:ASP:HA	1:A:183:PRO:HD3	1.87	0.42
1:B:298:ASN:HD22	1:B:298:ASN:C	2.26	0.42
1:C:277:VAL:HG21	1:C:297:VAL:HG11	2.00	0.42
1:C:295:ASP:OD1	1:C:365:LEU:HB2	2.20	0.42
1:B:352:PRO:HB2	1:B:354:HIS:H	1.85	0.42
1:B:314:ILE:HG23	1:B:385:GLY:HA2	2.02	0.42
1:B:165:PHE:CD2	1:B:480:LEU:HD11	2.55	0.41
1:B:341:ALA:O	1:B:344:GLU:HB2	2.20	0.41
1:D:383:LYS:HE3	2:D:501:IHP:O24	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:O	1:A:261:THR:HA	2.20	0.41
1:A:460:ARG:NH1	2:A:501:IHP:O33	2.44	0.41
1:C:239:ILE:HD12	1:C:300:GLU:HG2	2.02	0.40
1:A:158:LEU:HD12	1:A:474:MET:CE	2.51	0.40
1:A:361:GLN:NE2	4:A:602:HOH:O	2.02	0.40
1:C:158:LEU:HD23	1:C:158:LEU:HA	1.91	0.40
1:D:408:LYS:HB2	2:D:501:IHP:O46	2.21	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)
4:B:624:HOH:O	4:C:699:HOH:O[1_454]	2.13	0.07

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	332/352 (94%)	325 (98%)	7 (2%)	0	100	100
1	B	317/352 (90%)	310 (98%)	7 (2%)	0	100	100
1	C	331/352 (94%)	323 (98%)	8 (2%)	0	100	100
1	D	330/352 (94%)	324 (98%)	6 (2%)	0	100	100
All	All	1310/1408 (93%)	1282 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	262/290 (90%)	258 (98%)	4 (2%)	57	73
1	B	238/290 (82%)	230 (97%)	8 (3%)	32	44
1	C	265/290 (91%)	261 (98%)	4 (2%)	57	73
1	D	264/290 (91%)	262 (99%)	2 (1%)	73	85
All	All	1029/1160 (89%)	1011 (98%)	18 (2%)	53	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	SER
1	A	361	GLN
1	A	380	ARG
1	A	426	VAL
1	B	157	ARG
1	B	247	ARG
1	B	250	ARG
1	B	307	CYS
1	B	356	VAL
1	B	426	VAL
1	B	441	THR
1	B	443	GLU
1	C	252	ARG
1	C	298	ASN
1	C	426	VAL
1	C	441	THR
1	D	252	ARG
1	D	426	VAL

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

Mol	Chain	Res	Type
1	A	179	GLN
1	A	209	ASN
1	B	213	ASN
1	B	355	HIS
1	D	161	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	398	HIS
1	D	481	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	C	501	-	36,36,36	2.72	14 (38%)	60,60,60	1.53	9 (15%)
2	IHP	D	501	-	36,36,36	2.65	14 (38%)	60,60,60	1.65	11 (18%)
3	ACO	A	502	-	32,33,53	3.44	8 (25%)	50,52,79	1.69	9 (18%)
2	IHP	A	501	-	36,36,36	2.71	14 (38%)	60,60,60	1.89	13 (21%)
3	ACO	B	502	-	32,33,53	3.49	6 (18%)	50,52,79	1.64	13 (26%)
3	ACO	D	502	-	32,33,53	3.27	5 (15%)	50,52,79	1.63	12 (24%)
3	ACO	C	502	-	32,33,53	3.66	8 (25%)	50,52,79	1.59	11 (22%)
2	IHP	B	501	-	36,36,36	2.90	16 (44%)	60,60,60	1.76	11 (18%)

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	C	501	-	-	3/30/54/54	0/1/1/1
2	IHP	D	501	-	-	1/30/54/54	0/1/1/1
3	ACO	A	502	-	-	6/21/37/67	0/3/3/3
2	IHP	A	501	-	-	2/30/54/54	0/1/1/1
3	ACO	B	502	-	-	6/21/37/67	0/3/3/3
3	ACO	D	502	-	-	4/21/37/67	0/3/3/3
3	ACO	C	502	-	-	4/21/37/67	0/3/3/3
2	IHP	B	501	-	-	1/30/54/54	0/1/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	ACO	P3B-O3B	16.65	1.88	1.59
3	B	502	ACO	P3B-O3B	15.32	1.86	1.59
3	A	502	ACO	P3B-O3B	15.13	1.86	1.59
3	D	502	ACO	P3B-O3B	14.38	1.84	1.59
3	B	502	ACO	P1A-O3A	8.71	1.68	1.59
2	A	501	IHP	P5-O15	8.66	1.74	1.59
2	B	501	IHP	P1-O11	8.62	1.74	1.59
3	A	502	ACO	P1A-O3A	8.52	1.68	1.59
3	C	502	ACO	P1A-O3A	8.30	1.68	1.59
2	C	501	IHP	P3-O13	8.03	1.73	1.59
2	D	501	IHP	P2-O12	7.78	1.73	1.59
3	D	502	ACO	P1A-O3A	7.69	1.67	1.59
2	B	501	IHP	P3-O13	6.16	1.70	1.59
2	C	501	IHP	P1-O11	5.96	1.70	1.59
2	B	501	IHP	P5-O15	5.91	1.69	1.59
3	D	502	ACO	P2A-O6A	5.55	1.75	1.54
3	A	502	ACO	P2A-O6A	5.41	1.74	1.54
3	B	502	ACO	P2A-O6A	5.41	1.74	1.54
3	C	502	ACO	P2A-O6A	5.33	1.74	1.54
2	C	501	IHP	P6-O16	5.32	1.68	1.59
2	D	501	IHP	P6-O16	5.18	1.68	1.59
2	D	501	IHP	P5-O15	4.89	1.68	1.59
2	A	501	IHP	P2-O12	4.89	1.68	1.59
2	A	501	IHP	P3-O13	4.85	1.68	1.59
2	A	501	IHP	O11-C1	-4.66	1.28	1.44
2	C	501	IHP	O15-C5	-4.61	1.28	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	IHP	P6-O16	4.50	1.67	1.59
2	D	501	IHP	O14-C4	-4.32	1.29	1.44
2	C	501	IHP	P5-O15	4.23	1.66	1.59
2	B	501	IHP	O13-C3	-4.22	1.29	1.44
2	A	501	IHP	O13-C3	-4.19	1.29	1.44
2	A	501	IHP	P1-O11	4.19	1.66	1.59
2	D	501	IHP	C5-C4	4.18	1.60	1.52
2	D	501	IHP	P3-O13	4.16	1.66	1.59
2	B	501	IHP	C3-C2	4.15	1.60	1.52
2	B	501	IHP	C6-C5	3.88	1.60	1.52
2	B	501	IHP	P2-O12	3.77	1.66	1.59
2	D	501	IHP	O13-C3	-3.76	1.31	1.44
2	C	501	IHP	O11-C1	-3.66	1.31	1.44
2	D	501	IHP	P1-O11	3.62	1.65	1.59
2	C	501	IHP	C6-C5	3.48	1.59	1.52
2	B	501	IHP	P4-O14	3.45	1.65	1.59
2	C	501	IHP	P2-O12	3.42	1.65	1.59
2	C	501	IHP	C5-C4	3.40	1.59	1.52
2	A	501	IHP	C6-C1	3.36	1.59	1.52
2	A	501	IHP	C2-C1	3.27	1.59	1.52
3	D	502	ACO	O3B-C3B	-3.27	1.32	1.44
2	D	501	IHP	P4-O14	3.26	1.65	1.59
2	B	501	IHP	O15-C5	-3.23	1.33	1.44
2	A	501	IHP	O16-C6	-3.16	1.33	1.44
2	D	501	IHP	O11-C1	-3.12	1.33	1.44
2	C	501	IHP	P4-O14	3.04	1.64	1.59
3	B	502	ACO	O3B-C3B	-2.99	1.33	1.44
2	A	501	IHP	P4-O14	2.99	1.64	1.59
2	D	501	IHP	C6-C5	2.99	1.58	1.52
2	C	501	IHP	C6-C1	2.87	1.58	1.52
2	D	501	IHP	O16-C6	-2.87	1.34	1.44
2	C	501	IHP	O14-C4	-2.86	1.34	1.44
2	A	501	IHP	C4-C3	2.84	1.58	1.52
3	C	502	ACO	C5A-C4A	2.84	1.44	1.39
2	A	501	IHP	O14-C4	-2.83	1.34	1.44
2	B	501	IHP	C4-C3	2.79	1.58	1.52
3	B	502	ACO	C5A-C4A	2.76	1.44	1.39
3	C	502	ACO	O3B-C3B	-2.75	1.34	1.44
2	A	501	IHP	O15-C5	-2.70	1.34	1.44
3	A	502	ACO	O3B-C3B	-2.70	1.34	1.44
2	B	501	IHP	O11-C1	-2.69	1.34	1.44
2	B	501	IHP	O12-C2	-2.67	1.35	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	IHP	O12-C2	-2.59	1.35	1.44
2	D	501	IHP	O15-C5	-2.57	1.35	1.44
2	A	501	IHP	P6-O16	2.52	1.63	1.59
2	B	501	IHP	C5-C4	2.50	1.57	1.52
3	B	502	ACO	C2A-N1A	2.42	1.38	1.33
3	A	502	ACO	C5A-C4A	2.39	1.43	1.39
2	B	501	IHP	O14-C4	-2.35	1.36	1.44
3	C	502	ACO	C4A-N3A	2.32	1.38	1.34
3	D	502	ACO	C5A-C4A	2.30	1.43	1.39
2	D	501	IHP	C4-C3	2.24	1.56	1.52
2	C	501	IHP	O13-C3	-2.24	1.36	1.44
3	A	502	ACO	C2A-N1A	2.18	1.37	1.33
3	A	502	ACO	O2B-C2B	-2.11	1.37	1.43
3	A	502	ACO	C4A-N3A	2.09	1.38	1.34
3	C	502	ACO	C8A-N9A	2.08	1.41	1.37
2	B	501	IHP	C6-C1	2.02	1.56	1.52
3	C	502	ACO	C2A-N1A	2.01	1.37	1.33

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IHP	O15-C5-C4	5.71	120.91	108.76
2	C	501	IHP	C5-C6-C1	5.43	122.34	110.43
2	B	501	IHP	C5-C4-C3	5.12	121.66	110.43
2	A	501	IHP	C3-C2-C1	5.07	121.55	110.43
2	A	501	IHP	C5-C6-C1	5.01	121.41	110.43
2	B	501	IHP	C3-C2-C1	4.75	120.85	110.43
3	A	502	ACO	P3B-O3B-C3B	-4.70	110.87	123.43
2	D	501	IHP	C5-C4-C3	4.59	120.49	110.43
3	D	502	ACO	P3B-O3B-C3B	-4.54	111.32	123.43
2	B	501	IHP	O11-C1-C6	4.50	118.34	108.76
2	C	501	IHP	O13-C3-C2	4.24	117.78	108.76
2	D	501	IHP	P4-O14-C4	4.10	134.37	123.43
2	D	501	IHP	O12-C2-C1	4.08	117.45	108.76
3	A	502	ACO	O3A-P1A-O1A	-3.97	98.76	110.70
3	A	502	ACO	O3B-P3B-O7A	-3.85	95.60	109.33
3	B	502	ACO	P3B-O3B-C3B	-3.85	113.15	123.43
2	A	501	IHP	O15-C5-C6	3.83	116.91	108.76
2	B	501	IHP	O15-C5-C6	3.77	116.78	108.76
3	C	502	ACO	P3B-O3B-C3B	-3.67	113.62	123.43
2	D	501	IHP	C5-C6-C1	3.67	118.48	110.43
3	D	502	ACO	O3A-P1A-O1A	-3.66	99.69	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IHP	C6-C5-C4	-3.55	102.63	110.43
2	C	501	IHP	C5-C4-C3	3.55	118.22	110.43
3	B	502	ACO	O3A-P1A-O1A	-3.46	100.30	110.70
2	A	501	IHP	P1-O11-C1	3.43	132.59	123.43
2	C	501	IHP	P5-O15-C5	3.32	132.31	123.43
2	A	501	IHP	O13-C3-C4	3.29	115.76	108.76
3	C	502	ACO	P1A-O5B-C5B	-3.28	102.56	121.35
2	D	501	IHP	P6-O16-C6	3.28	132.18	123.43
3	B	502	ACO	P1A-O5B-C5B	-3.27	102.59	121.35
3	D	502	ACO	O5A-P2A-O4A	3.24	123.45	110.83
3	B	502	ACO	O5A-P2A-O4A	3.23	123.42	110.83
3	C	502	ACO	O5A-P2A-O4A	3.19	123.28	110.83
2	B	501	IHP	O11-C1-C2	3.19	115.55	108.76
2	A	501	IHP	C5-C4-C3	3.17	117.38	110.43
2	B	501	IHP	C6-C1-C2	-3.16	103.49	110.43
3	A	502	ACO	P1A-O5B-C5B	-3.00	104.14	121.35
3	A	502	ACO	O5A-P2A-O4A	2.98	122.46	110.83
3	B	502	ACO	O3B-P3B-O7A	-2.98	98.72	109.33
3	A	502	ACO	O9A-P3B-O8A	2.97	118.96	107.80
3	C	502	ACO	O8A-P3B-O3B	-2.94	94.39	105.85
2	D	501	IHP	O14-P4-O24	-2.90	98.99	109.33
2	D	501	IHP	O44-P4-O14	2.89	117.09	105.85
3	B	502	ACO	O9A-P3B-O3B	-2.82	94.85	105.85
3	D	502	ACO	P1A-O5B-C5B	-2.79	105.39	121.35
2	C	501	IHP	C4-C3-C2	-2.73	104.43	110.43
3	C	502	ACO	O2A-P1A-O3A	-2.71	99.95	107.27
2	B	501	IHP	O15-C5-C4	2.69	114.48	108.76
3	B	502	ACO	O9A-P3B-O8A	2.62	117.62	107.80
3	B	502	ACO	O6A-P2A-O4A	-2.52	101.02	110.83
2	D	501	IHP	O12-C2-C3	2.52	114.11	108.76
2	C	501	IHP	O13-C3-C4	2.49	114.06	108.76
2	D	501	IHP	O34-P4-O14	2.49	115.55	105.85
3	D	502	ACO	O8A-P3B-O3B	-2.42	96.41	105.85
3	A	502	ACO	N3A-C4A-N9A	2.41	131.27	127.17
2	A	501	IHP	O14-C4-C3	2.40	113.87	108.76
3	A	502	ACO	O6A-P2A-O4A	-2.37	101.59	110.83
3	D	502	ACO	O6A-P2A-O4A	-2.36	101.62	110.83
3	C	502	ACO	C2B-C3B-C4B	-2.36	99.10	103.24
2	A	501	IHP	P2-O12-C2	-2.35	117.15	123.43
3	C	502	ACO	O6A-P2A-O4A	-2.32	101.78	110.83
2	C	501	IHP	O45-P5-O15	2.32	114.87	105.85
3	A	502	ACO	C2A-N1A-C6A	-2.28	114.98	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	IHP	O11-C1-C2	2.27	113.60	108.76
3	D	502	ACO	C2A-N1A-C6A	-2.27	115.00	118.73
2	C	501	IHP	P1-O11-C1	2.26	129.48	123.43
3	D	502	ACO	O9A-P3B-O7A	2.26	119.65	110.83
3	B	502	ACO	N3A-C4A-N9A	2.26	131.01	127.17
3	B	502	ACO	O6A-P2A-O5A	-2.26	99.35	107.80
3	C	502	ACO	O9A-P3B-O8A	2.25	116.26	107.80
3	B	502	ACO	C2A-N1A-C6A	-2.21	115.10	118.73
2	B	501	IHP	O16-C6-C5	2.20	113.44	108.76
3	C	502	ACO	O9A-P3B-O7A	2.19	119.38	110.83
3	B	502	ACO	O8A-P3B-O7A	2.17	119.29	110.83
2	B	501	IHP	C5-C6-C1	2.17	115.18	110.43
3	C	502	ACO	N3A-C4A-N9A	2.17	130.85	127.17
3	D	502	ACO	N3A-C4A-N9A	2.14	130.81	127.17
3	D	502	ACO	O9A-P3B-O3B	-2.12	97.59	105.85
2	A	501	IHP	O16-C6-C5	2.12	113.27	108.76
3	B	502	ACO	C2B-C3B-C4B	-2.12	99.53	103.24
2	B	501	IHP	O13-C3-C2	2.11	113.25	108.76
2	A	501	IHP	O14-C4-C5	2.08	113.19	108.76
3	D	502	ACO	C2B-C1B-N9A	-2.08	108.14	113.30
3	D	502	ACO	C5A-C4A-N3A	-2.07	123.87	126.72
3	C	502	ACO	C2A-N1A-C6A	-2.07	115.34	118.73
2	A	501	IHP	O45-P5-O15	2.06	113.88	105.85
2	B	501	IHP	C4-C3-C2	2.04	114.90	110.43
2	D	501	IHP	O15-C5-C6	2.03	113.08	108.76
2	C	501	IHP	O41-P1-O11	2.00	113.66	105.85

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	ACO	C5B-O5B-P1A-O1A
3	A	502	ACO	C5B-O5B-P1A-O2A
3	A	502	ACO	C5B-O5B-P1A-O3A
3	B	502	ACO	C3B-C4B-C5B-O5B
3	B	502	ACO	O4B-C4B-C5B-O5B
3	B	502	ACO	C5B-O5B-P1A-O2A
3	B	502	ACO	P2A-O3A-P1A-O5B
3	D	502	ACO	C5B-O5B-P1A-O1A
3	D	502	ACO	C5B-O5B-P1A-O3A
3	A	502	ACO	O4B-C4B-C5B-O5B
3	D	502	ACO	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	502	ACO	C3B-C4B-C5B-O5B
3	D	502	ACO	C3B-C4B-C5B-O5B
3	A	502	ACO	P2A-O3A-P1A-O5B
3	C	502	ACO	P2A-O3A-P1A-O5B
3	C	502	ACO	C3B-C4B-C5B-O5B
2	C	501	IHP	C3-O13-P3-O23
3	B	502	ACO	C5B-O5B-P1A-O3A
2	D	501	IHP	C4-O14-P4-O34
3	B	502	ACO	C3B-O3B-P3B-O9A
3	C	502	ACO	O4B-C4B-C5B-O5B
3	C	502	ACO	P1A-O3A-P2A-O6A
2	C	501	IHP	C4-O14-P4-O44
2	C	501	IHP	C5-O15-P5-O45
2	A	501	IHP	C1-O11-P1-O21
2	A	501	IHP	C2-O12-P2-O22
2	B	501	IHP	C4-O14-P4-O24

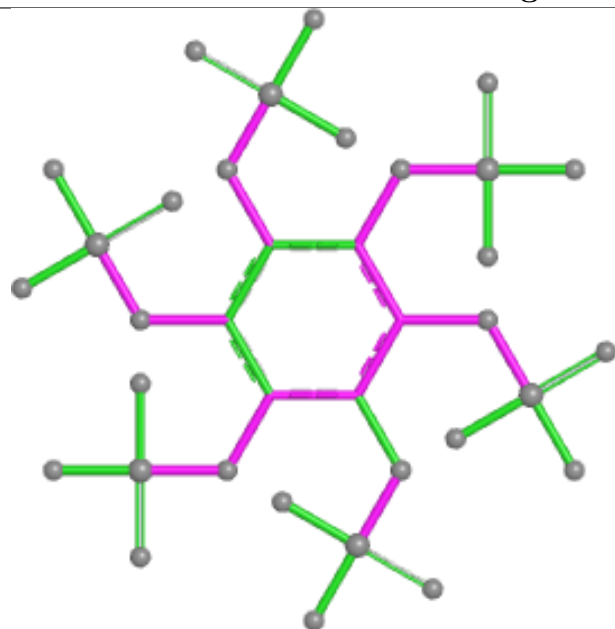
There are no ring outliers.

6 monomers are involved in 14 short contacts:

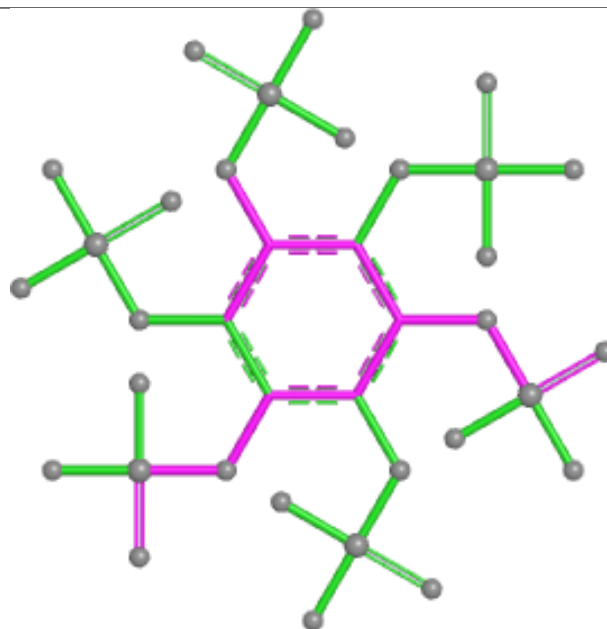
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	IHP	2	0
2	D	501	IHP	4	0
2	A	501	IHP	3	0
3	B	502	ACO	1	0
3	D	502	ACO	1	0
2	B	501	IHP	3	0

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.

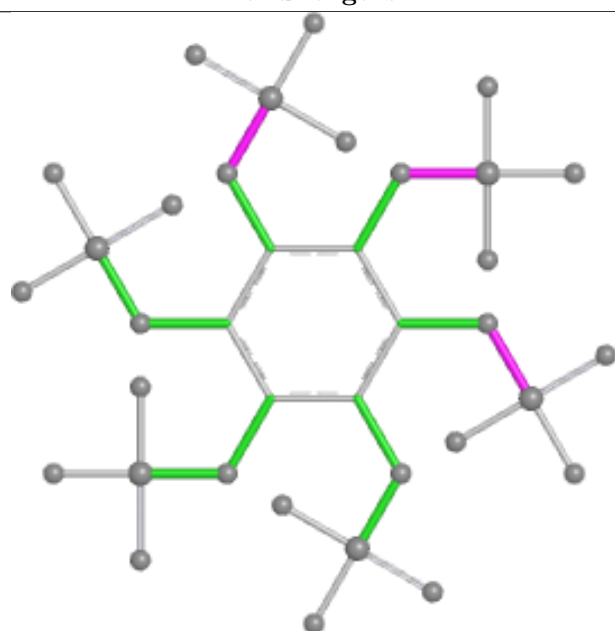
Ligand IHP C 501



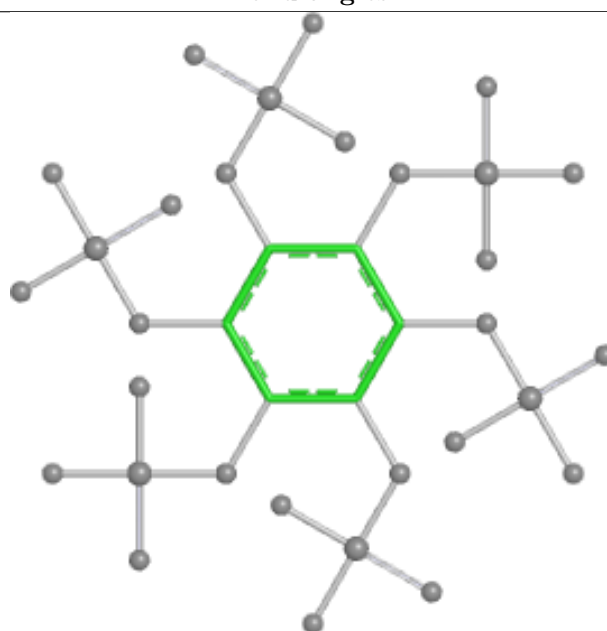
Bond lengths



Bond angles

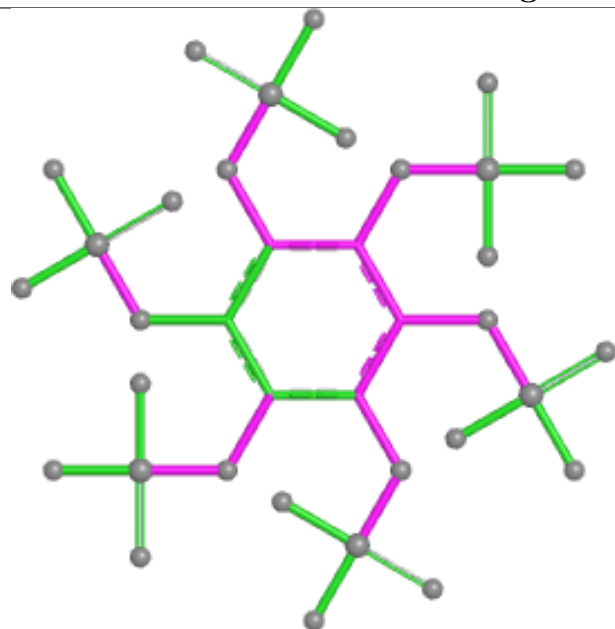


Torsions

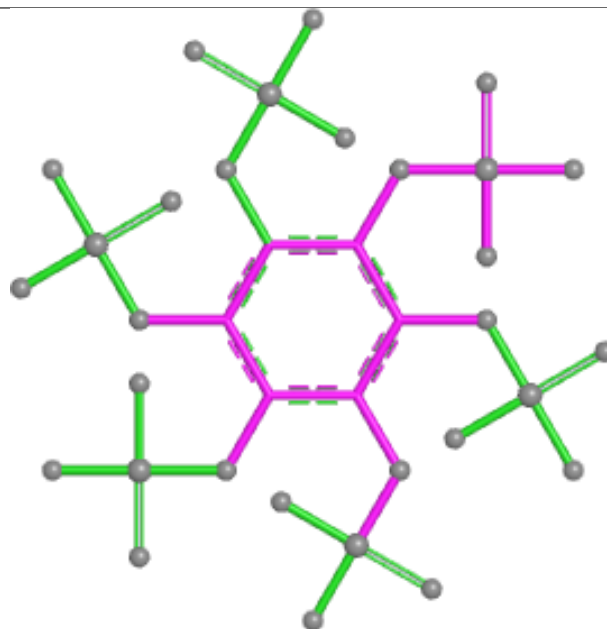


Rings

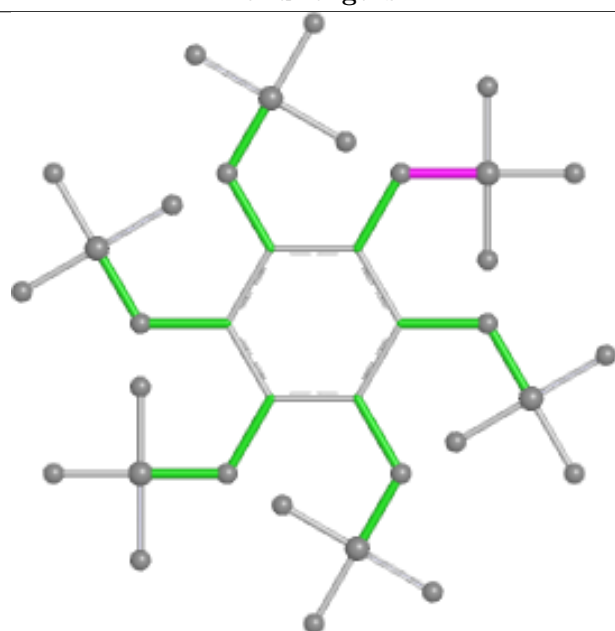
Ligand IHP D 501



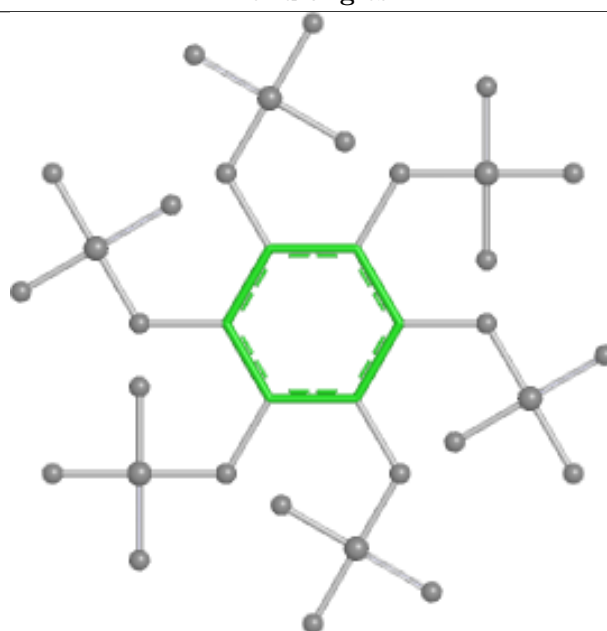
Bond lengths



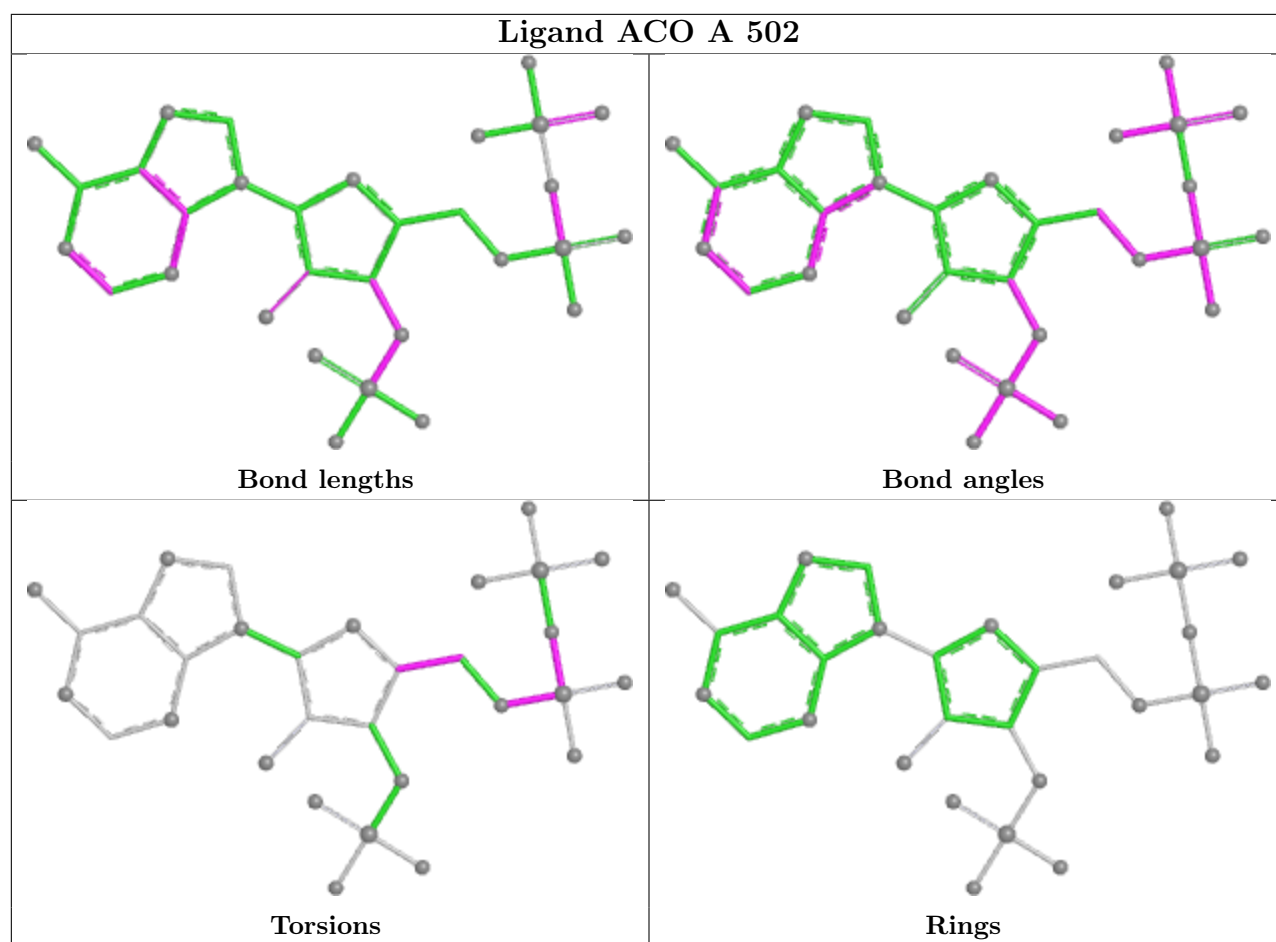
Bond angles



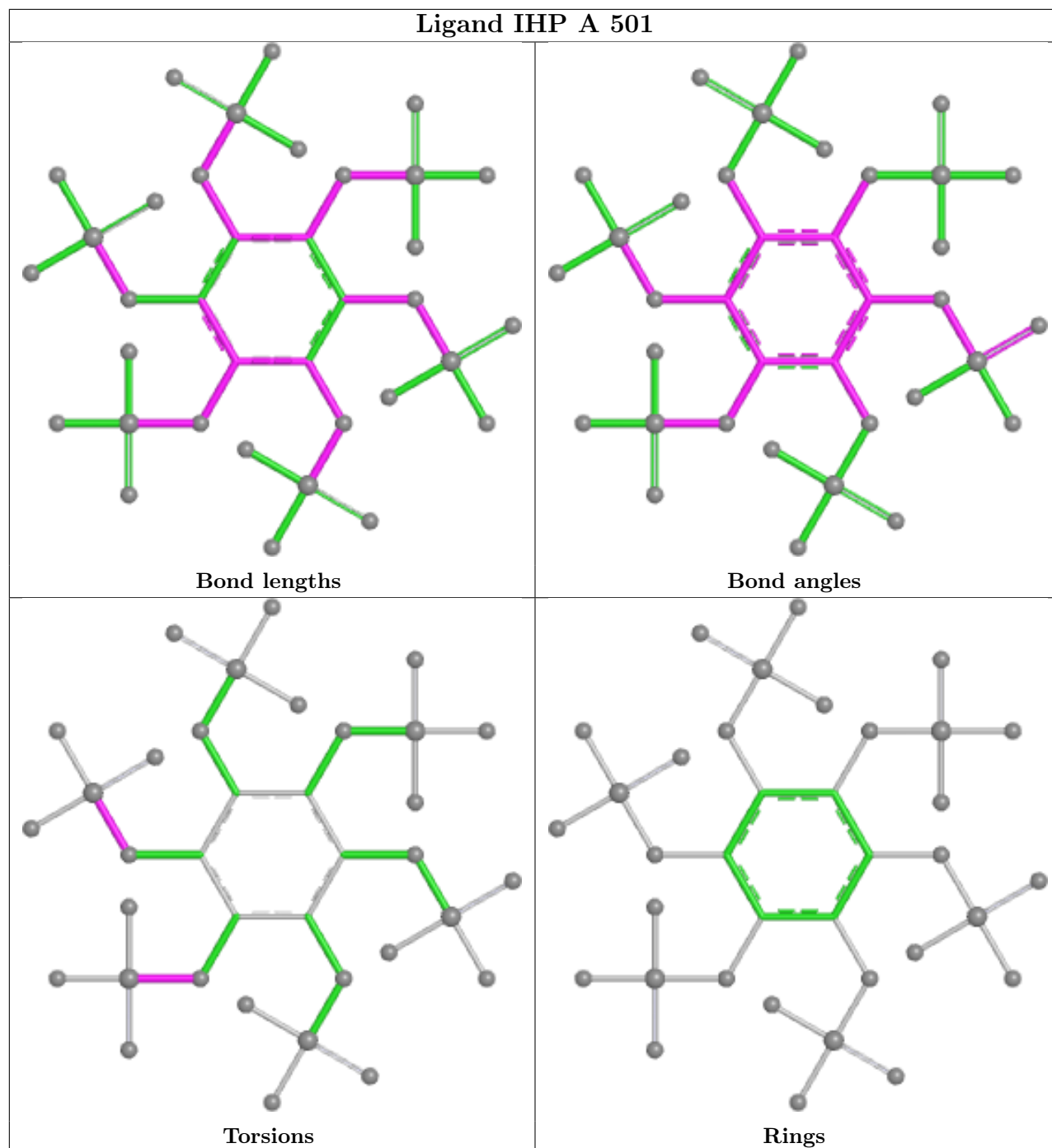
Torsions

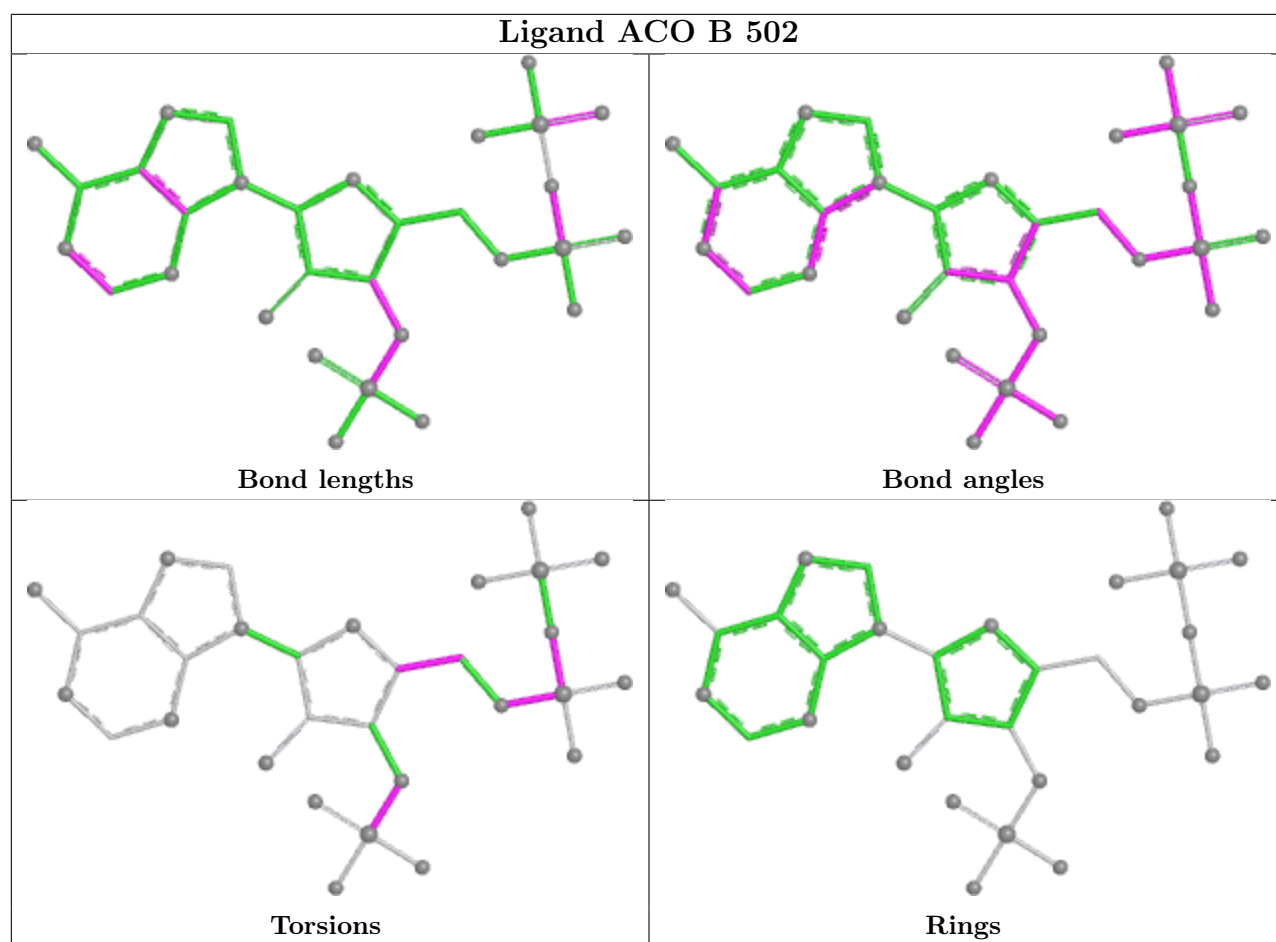


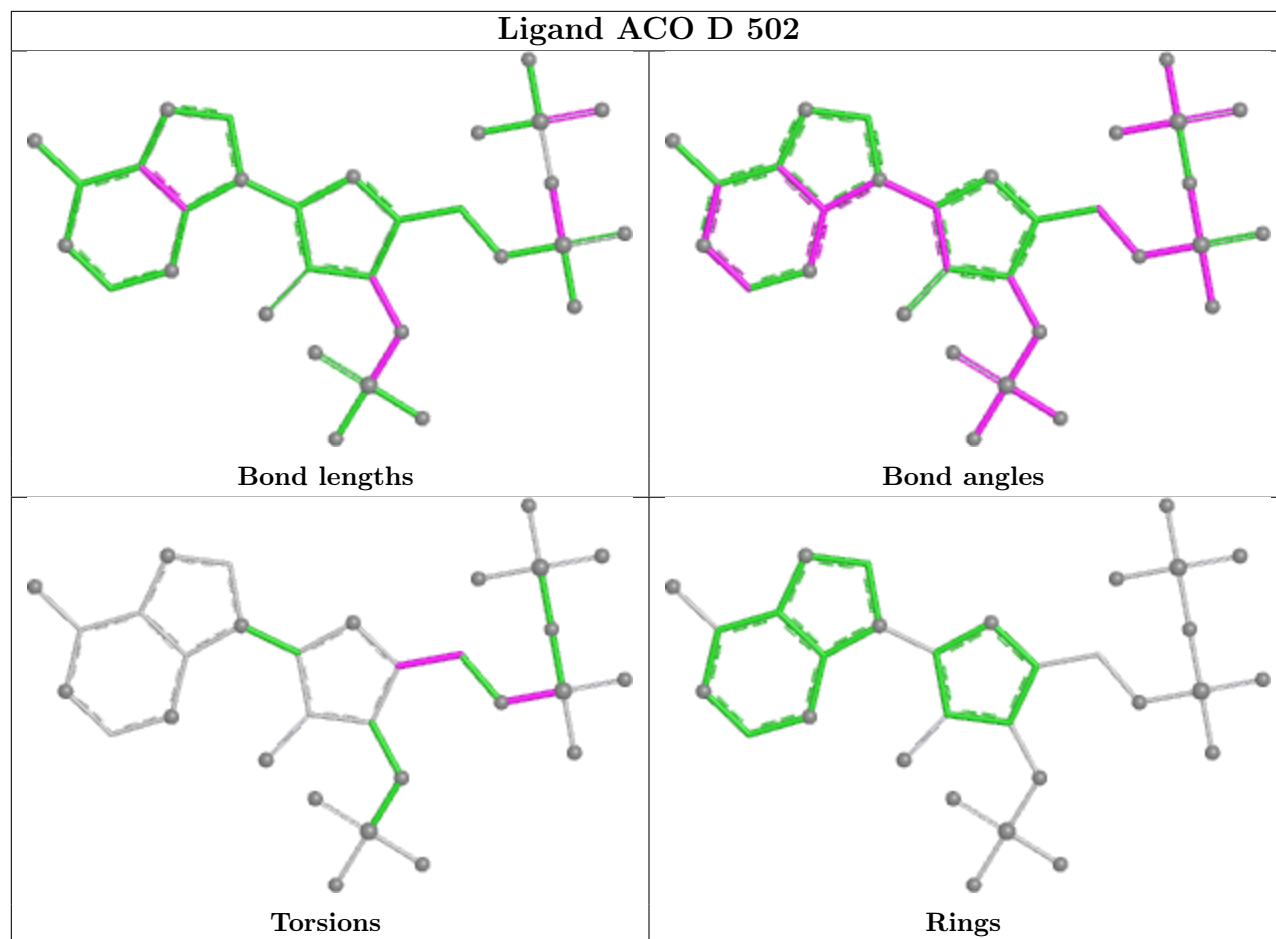
Rings

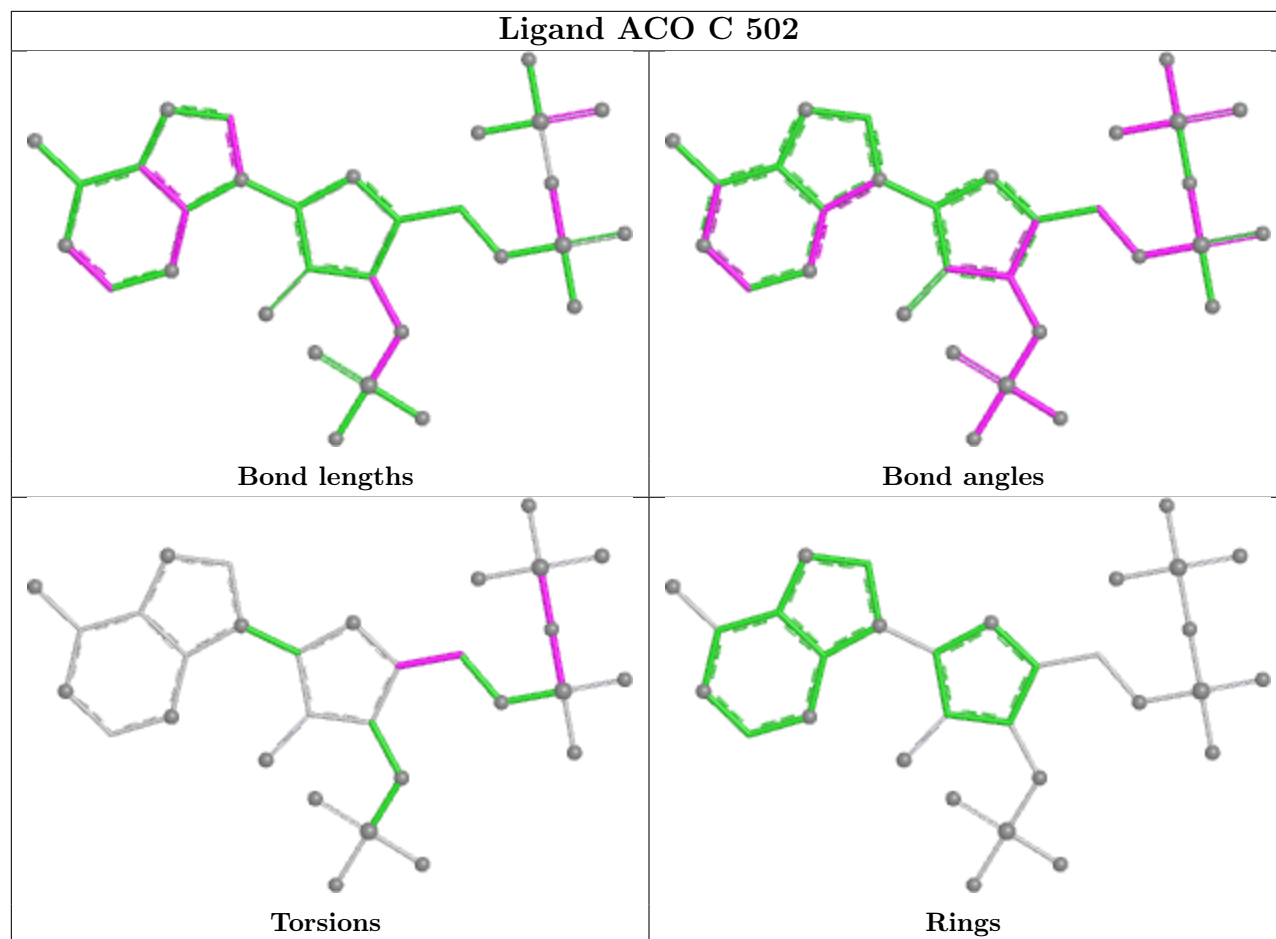


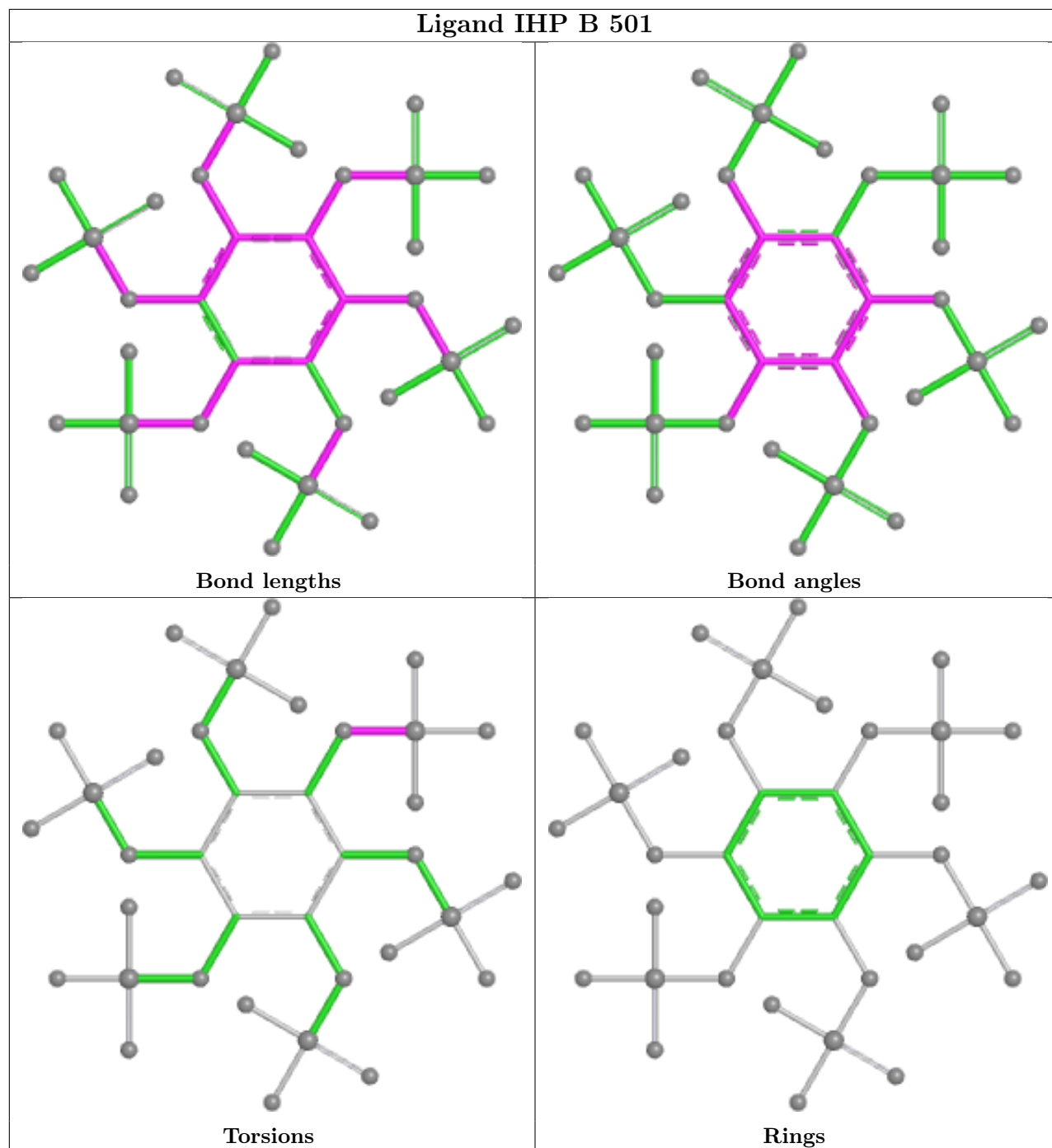
Ligand IHP A 501











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	336/352 (95%)	0.05	7 (2%) 63 60	33, 52, 87, 116	0
1	B	327/352 (92%)	0.42	31 (9%) 14 11	34, 63, 112, 127	0
1	C	335/352 (95%)	0.03	5 (1%) 72 69	31, 52, 88, 104	0
1	D	334/352 (94%)	-0.07	4 (1%) 76 74	32, 48, 80, 101	0
All	All	1332/1408 (94%)	0.11	47 (3%) 47 44	31, 52, 98, 127	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	4.9
1	B	365	LEU	4.0
1	A	146	GLY	3.9
1	B	293	TYR	3.7
1	D	226	GLU	3.4
1	B	269	ASP	3.3
1	A	144	PRO	3.3
1	C	146	GLY	3.2
1	D	144	PRO	3.0
1	B	288	SER	2.9
1	B	342	PHE	2.9
1	B	302	GLY	2.9
1	B	291	VAL	2.8
1	C	286	ASP	2.7
1	B	304	HIS	2.7
1	B	287	GLU	2.7
1	B	344	GLU	2.7
1	B	349	GLY	2.6
1	B	308	ALA	2.6
1	B	146	GLY	2.5
1	B	303	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	288	SER	2.5
1	B	272	GLY	2.5
1	B	353	SER	2.4
1	B	266	ILE	2.4
1	C	350	GLY	2.3
1	B	352	PRO	2.2
1	D	363	GLU	2.2
1	A	365	LEU	2.2
1	B	441	THR	2.2
1	B	485	LEU	2.2
1	B	319	PHE	2.2
1	B	292	ASP	2.2
1	B	363	GLU	2.2
1	B	271	SER	2.2
1	C	441	THR	2.2
1	B	239	ILE	2.1
1	B	429	ARG	2.1
1	B	299	MET	2.1
1	B	370	VAL	2.1
1	D	227	VAL	2.1
1	A	438	SER	2.1
1	B	270	ALA	2.1
1	C	318	PHE	2.1
1	B	273	THR	2.0
1	A	364	GLU	2.0
1	B	440	GLU	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](#)

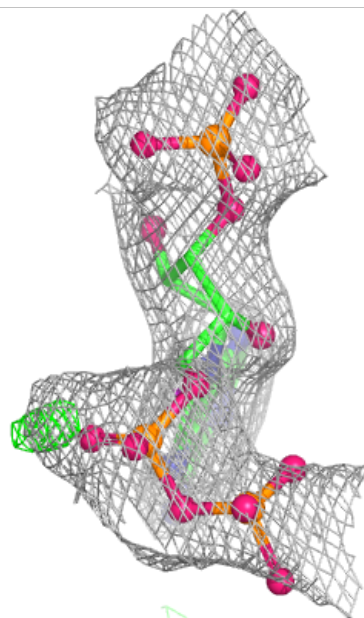
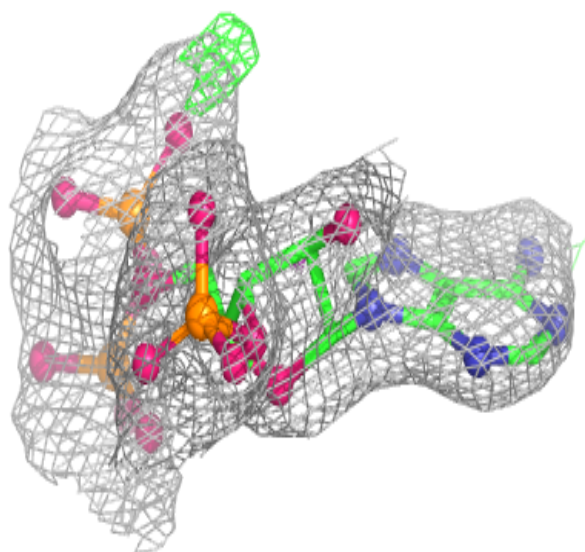
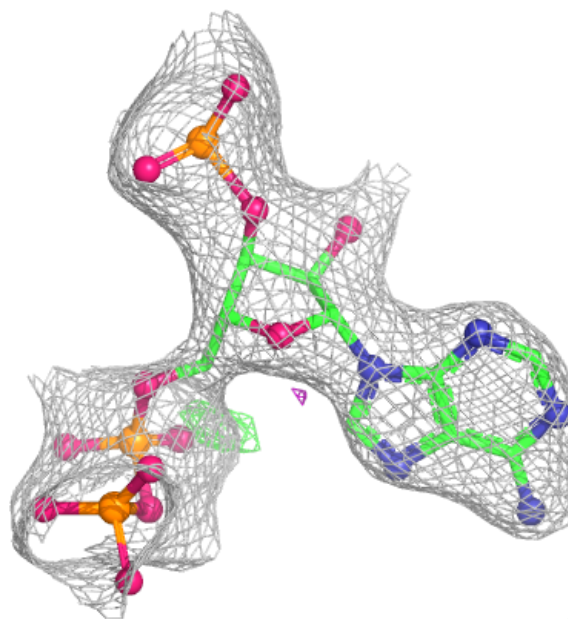
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ACO	B	502	31/51	0.90	0.09	57,72,145,150	0
3	ACO	A	502	31/51	0.91	0.09	47,59,118,119	0
3	ACO	C	502	31/51	0.93	0.08	41,62,173,174	0
2	IHP	B	501	36/36	0.94	0.11	32,53,124,132	0
2	IHP	A	501	36/36	0.94	0.10	35,54,94,95	0
3	ACO	D	502	31/51	0.94	0.09	40,46,131,135	0
2	IHP	C	501	36/36	0.95	0.09	30,52,77,87	0
2	IHP	D	501	36/36	0.96	0.08	31,53,75,87	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.

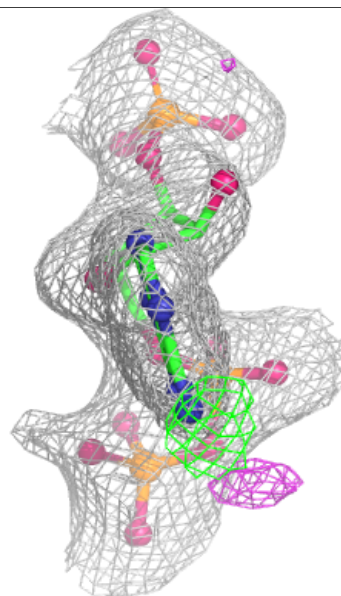
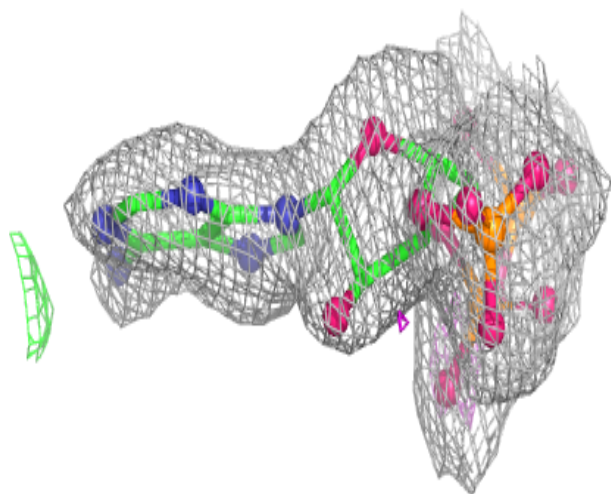
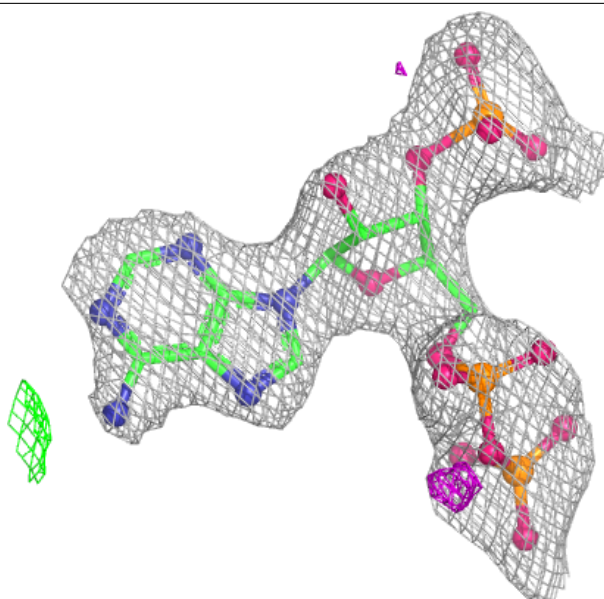
Electron density around ACO B 502:

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



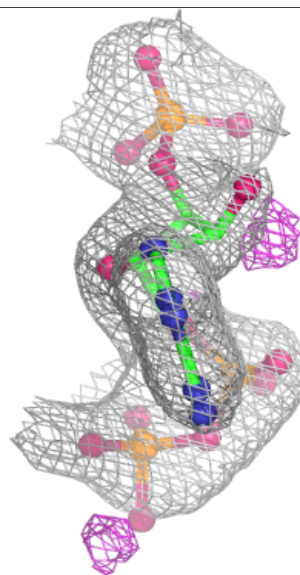
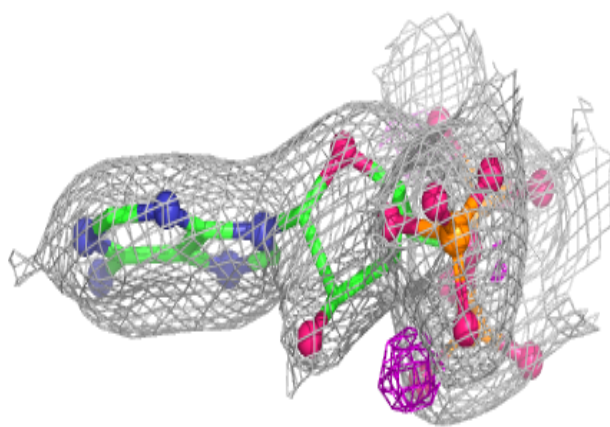
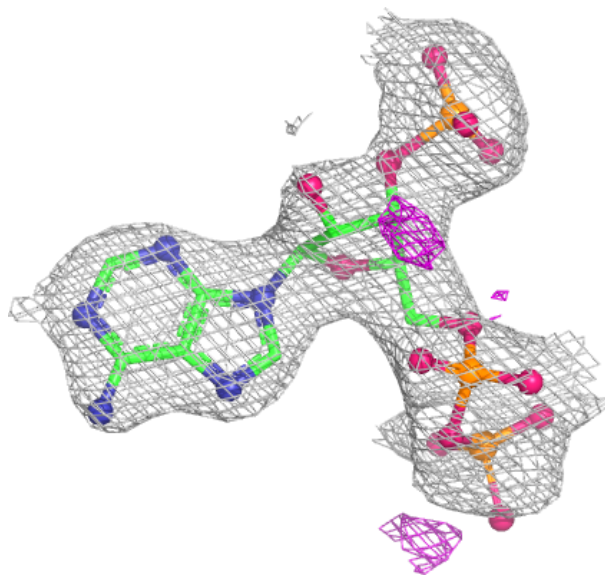
Electron density around ACO A 502:

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



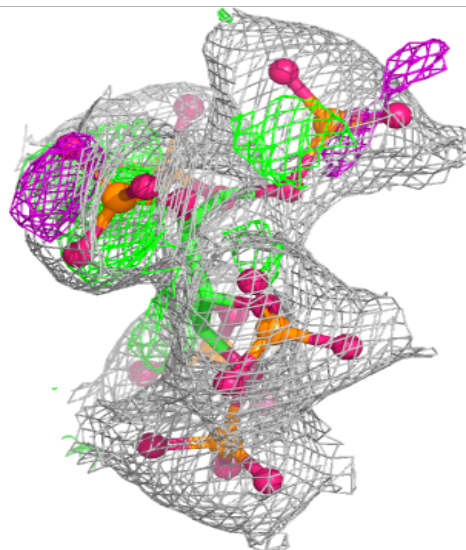
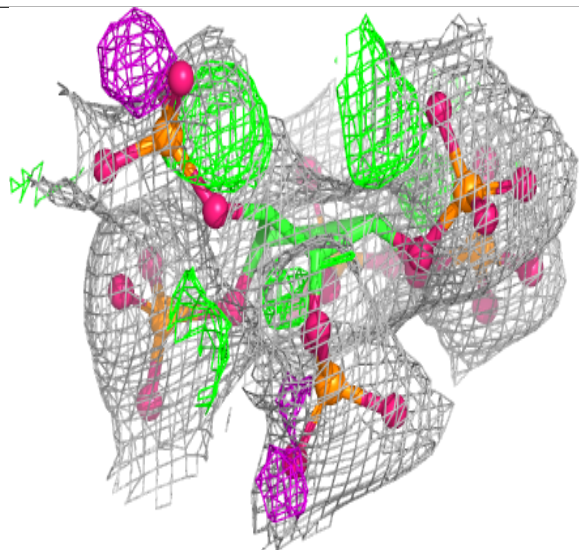
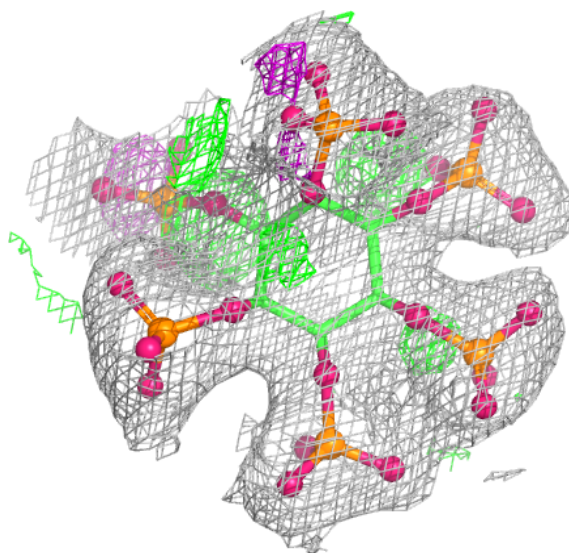
Electron density around ACO C 502:

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



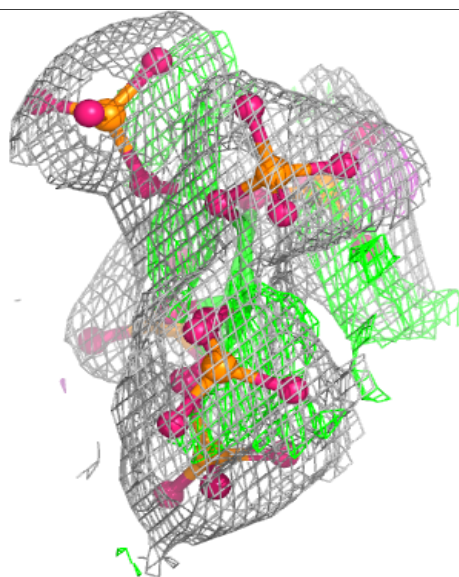
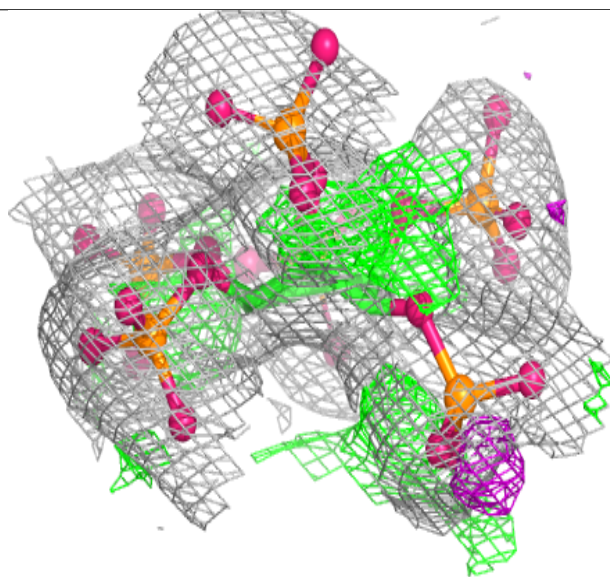
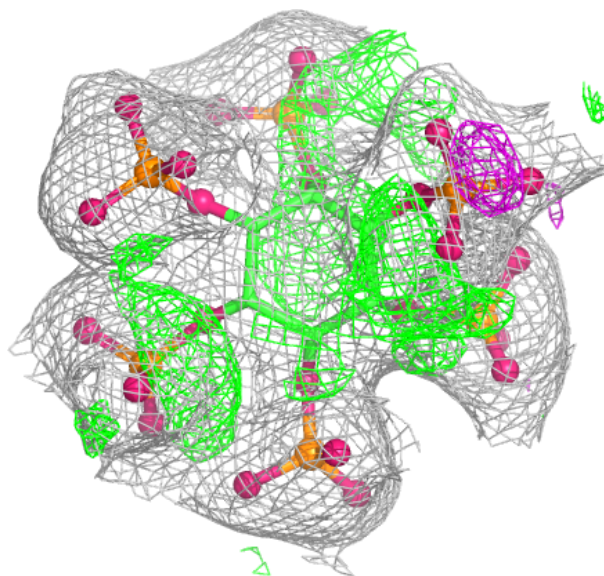
Electron density around IHP B 501:

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



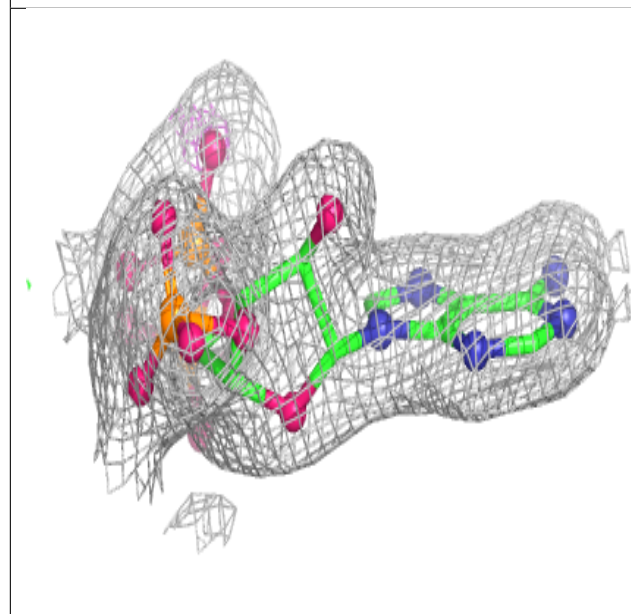
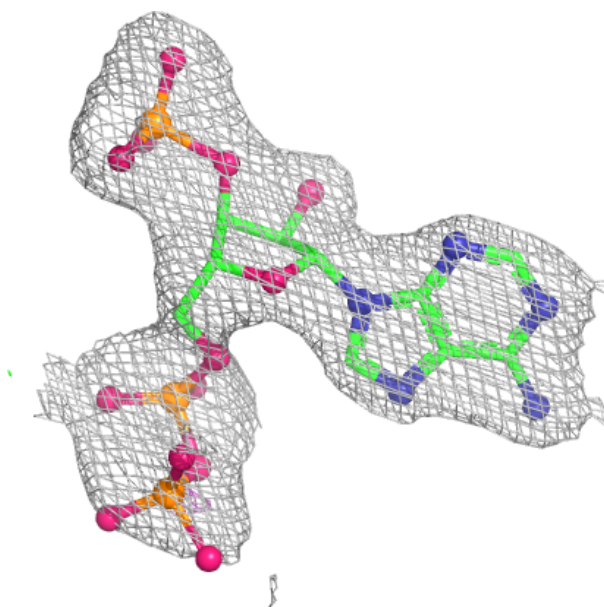
Electron density around IHP A 501:

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



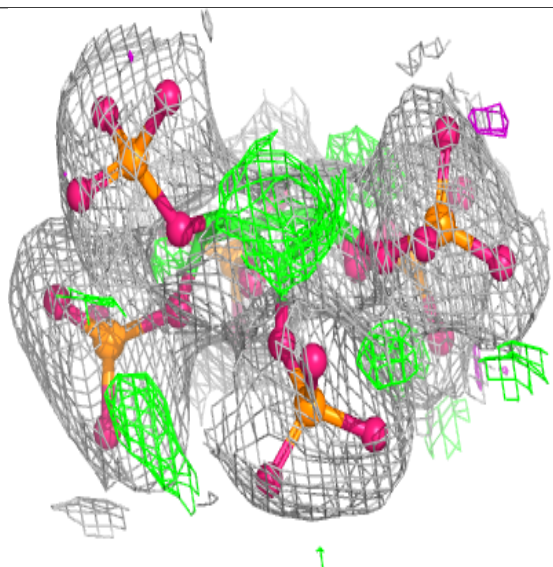
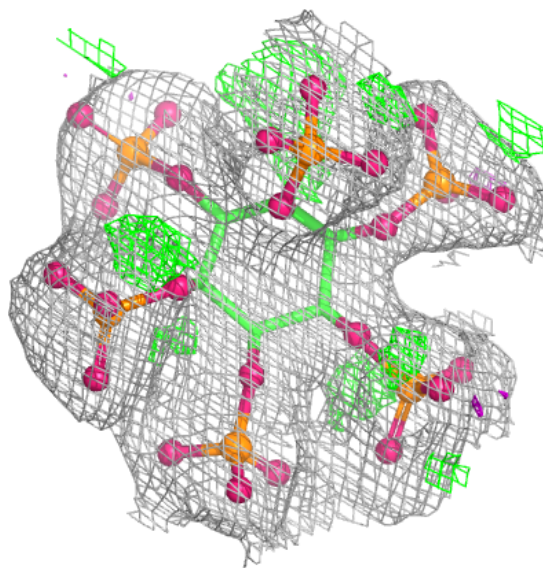
Electron density around ACO D 502:

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



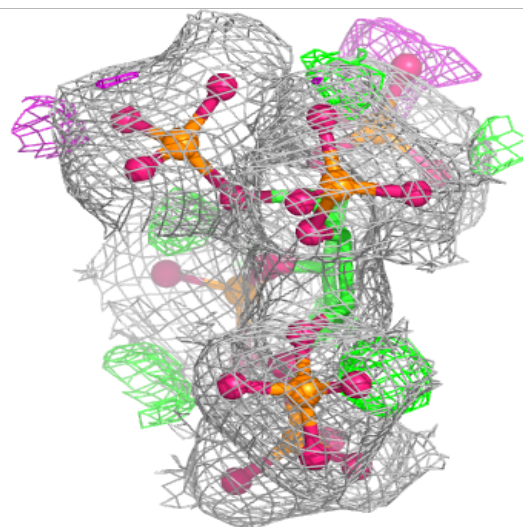
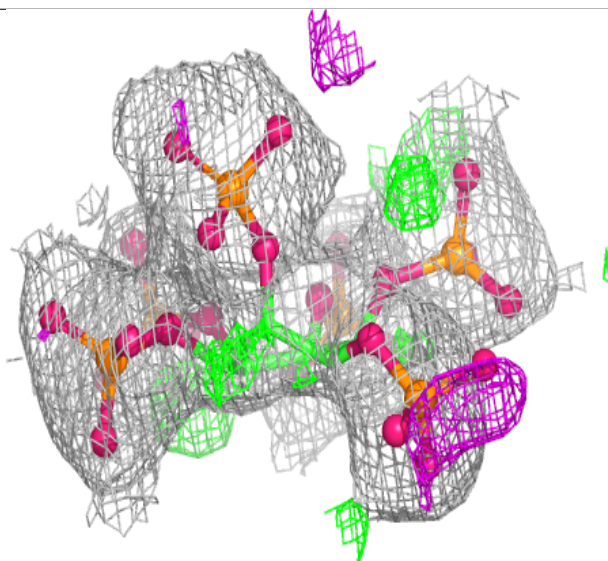
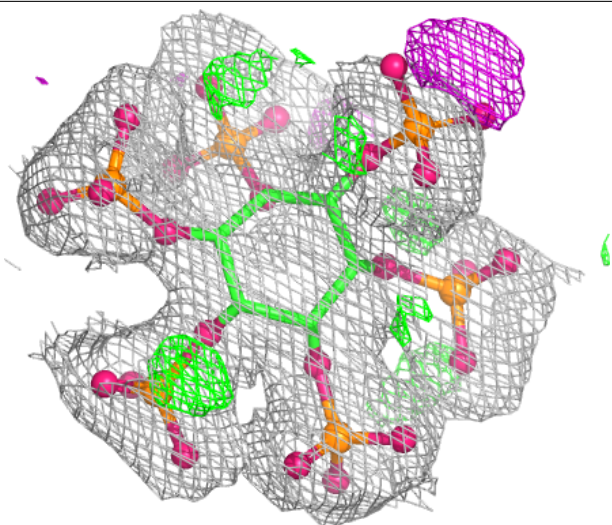
Electron density around IHP C 501:

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



Electron density around IHP D 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.