Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 06:39 AM EDT

PDB ID	:	5W3X
Title	:	Crystal structure of PopP2 in complex with IP6, AcCoA and the WRKY domain of RRS1-R .
Authors	:	Zhang, Z.M.; Gao, L.; Song, J.
Deposited on	:	2017-06-08
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

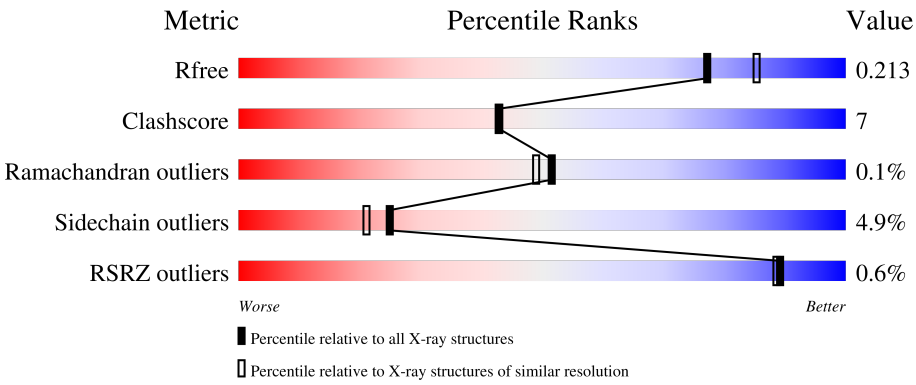
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	84% 10% • 5%
1	C	352	84% 11% • •
2	B	80	4% 70% 12% • 16%
2	D	80	% 75% 14% • 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6934 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
			Total	C	N	O	S			
1	A	335	2569	1585	478	493	13	0	2	0
1	C	342	2608	1608	486	500	14	0	1	0

There are 24 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	THR	-	expression tag	UNP A0A0S4VB05
A	147	ARG	-	expression tag	UNP A0A0S4VB05
A	148	SER	-	expression tag	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	THR	-	expression tag	UNP A0A0S4VB05
C	147	ARG	-	expression tag	UNP A0A0S4VB05
C	148	SER	-	expression tag	UNP A0A0S4VB05

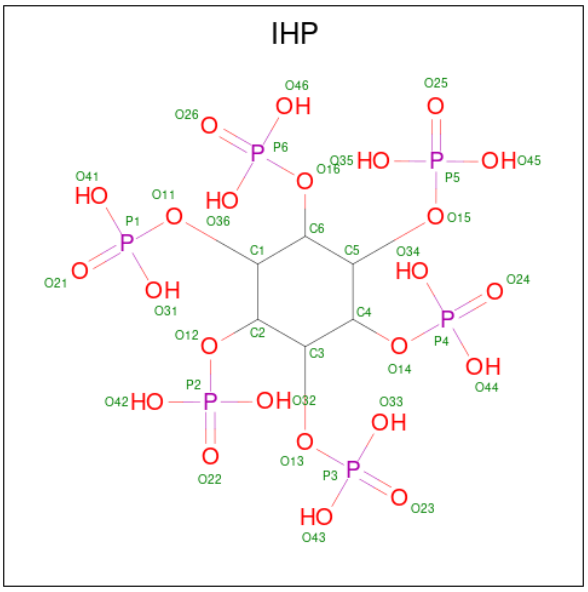
- Molecule 2 is a protein called Disease resistance protein RRS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	67	538	340	99	97	2	0	0	0
			Total	C	N	O	S			
2	D	73	568	359	105	102	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

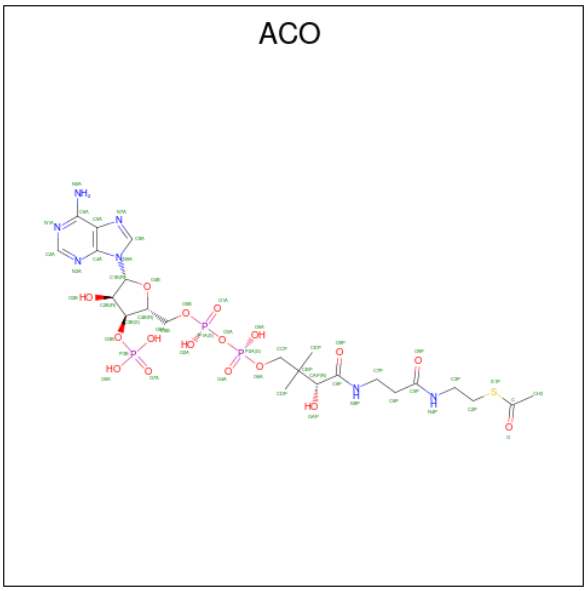
Chain	Residue	Modelled	Actual	Comment	Reference
B	1194	SER	-	expression tag	UNP C4B7M5
D	1194	SER	-	expression tag	UNP C4B7M5

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 4 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

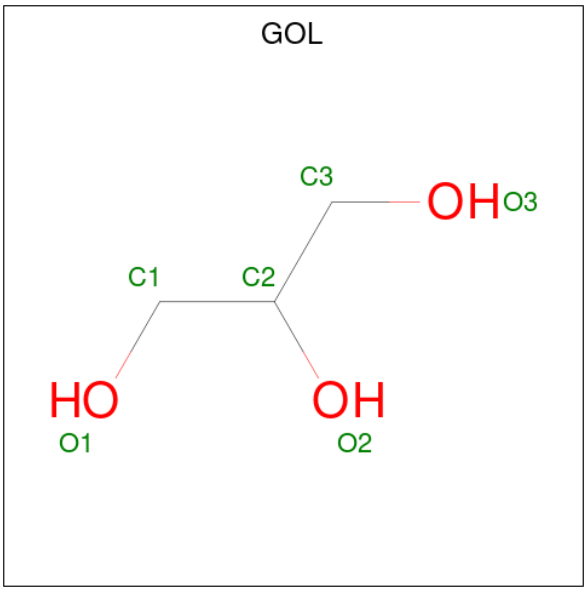


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
4	C	1	31	10	5	13	3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	B	1	1	1	0	0
			Total	Zn		
5	D	1	1	1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

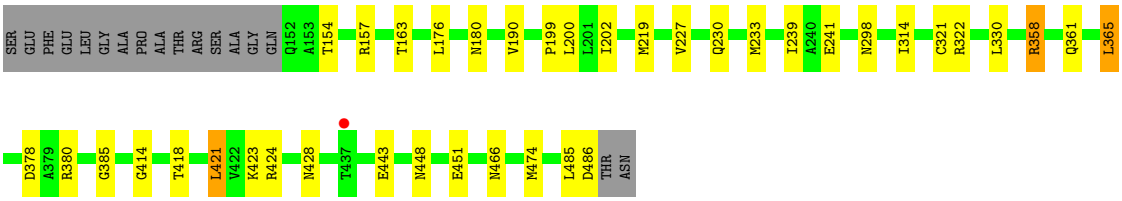
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	227	227	227	0	0
			Total	O		
7	B	23	23	23	0	0
			Total	O		
7	C	231	231	231	0	0
			Total	O		
7	D	28	28	28	0	0

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.

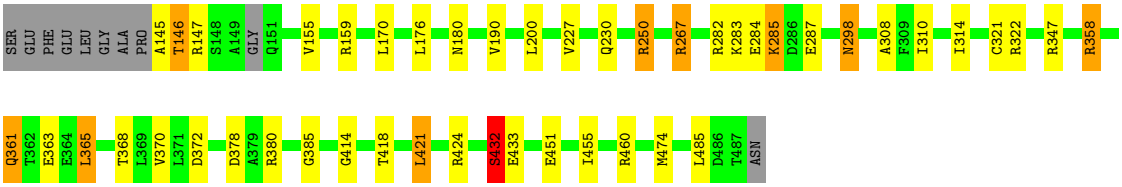
- Molecule 1: PopP2 protein

Chain A:



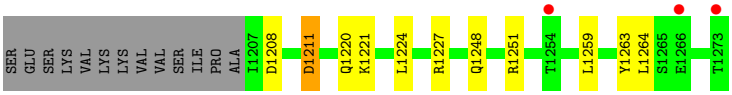
- Molecule 1: PopP2 protein

Chain C:



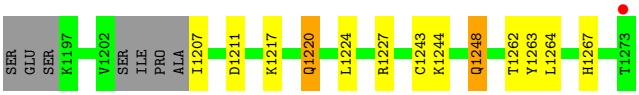
- Molecule 2: Disease resistance protein RRS1

Chain B:



- Molecule 2: Disease resistance protein RRS1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.54Å 87.54Å 87.55Å 71.54° 84.04° 84.00°	Depositor
Resolution (Å)	82.81 – 2.00 82.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (82.81-2.00) 93.8 (82.81-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.212 0.187 , 0.213	Depositor DCC
R_{free} test set	1781 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.477 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ACO, ZN, GOL, 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	0.50	2/2616 (0.1%)	0.65	0/3540
1	C	0.49	0/2651	0.67	2/3586 (0.1%)
2	B	0.31	0/554	0.51	0/749
2	D	0.33	0/583	0.51	0/788
All	All	0.47	2/6404 (0.0%)	0.64	2/8663 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378[A]	ASP	CA-C	5.14	1.66	1.52
1	A	378[B]	ASP	CA-C	5.14	1.66	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	433	GLU	N-CA-CB	-8.53	95.25	110.60
1	C	432	SER	N-CA-C	7.14	130.29	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448[A]	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2569	0	2541	30	0
1	C	2608	0	2580	37	0
2	B	538	0	491	7	0
2	D	568	0	510	9	0
3	A	36	0	6	3	0
3	C	36	0	6	3	0
4	A	31	0	11	1	0
4	C	31	0	11	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	C	6	0	8	2	0
7	A	227	0	0	10	2
7	B	23	0	0	2	0
7	C	231	0	0	10	2
7	D	28	0	0	3	0
All	All	6934	0	6164	85	3

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 (85) 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:284:GLU:HA	1:C:285:LYS:HE3	1.41	0.99
1:A:233:MET:SD	7:A:817:HOH:O	2.24	0.96
1:A:322:ARG:NH1	7:A:601:HOH:O	1.82	0.93
1:C:432:SER:OG	4:C:502:ACO:O6A	1.89	0.90
1:A:321:CYS:SG	7:B:1404:HOH:O	2.31	0.89
1:C:285:LYS:CD	1:C:285:LYS:H	1.87	0.83
1:A:154:THR:HG21	7:A:795:HOH:O	1.81	0.79
1:A:154:THR:HG23	1:A:157:ARG:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:501:IHP:H4	7:C:603:HOH:O	1.85	0.76
1:A:424:ARG:NH2	1:A:451:GLU:OE2	2.20	0.73
1:C:145:ALA:HB2	1:C:159:ARG:HE	1.54	0.72
2:D:1207:ILE:N	7:D:1402:HOH:O	2.23	0.71
1:C:361:GLN:NE2	7:C:606:HOH:O	2.23	0.70
1:A:418:THR:HA	1:A:421:LEU:HD22	1.74	0.68
1:C:285:LYS:H	1:C:285:LYS:HD2	1.55	0.68
4:C:502:ACO:O9A	6:C:503:GOL:H12	1.94	0.68
2:D:1227:ARG:NE	7:D:1401:HOH:O	2.15	0.67
1:C:287:GLU:OE2	7:C:602:HOH:O	2.12	0.67
2:D:1217:LYS:NZ	2:D:1220:GLN:HG3	2.10	0.66
1:C:358:ARG:HG2	1:C:358:ARG:HH21	1.61	0.65
1:A:358:ARG:HG2	1:A:358:ARG:HH21	1.62	0.65
1:C:414:GLY:O	1:C:418:THR:HG23	1.98	0.64
1:C:170:LEU:HD11	1:C:455:ILE:HG23	1.79	0.64
1:C:145:ALA:HB2	1:C:159:ARG:NE	2.13	0.63
1:C:146:THR:OG1	1:C:147:ARG:N	2.33	0.62
1:A:230:GLN:OE1	1:A:322:ARG:NH2	2.33	0.62
1:C:424:ARG:NH2	1:C:451:GLU:OE2	2.28	0.60
3:A:501:IHP:H3	7:A:697:HOH:O	2.01	0.60
6:C:503:GOL:H2	7:C:779:HOH:O	2.02	0.60
1:A:241:GLU:OE1	7:A:602:HOH:O	2.17	0.58
1:A:380:ARG:HD3	7:A:627:HOH:O	2.05	0.57
1:C:418:THR:HA	1:C:421:LEU:HD22	1.87	0.57
1:A:199:PRO:HA	1:A:233:MET:HE3	1.86	0.57
1:C:230:GLN:OE1	1:C:322:ARG:NH2	2.29	0.57
1:A:199:PRO:CA	1:A:233:MET:HE3	2.35	0.56
1:A:414:GLY:O	1:A:418:THR:HG23	2.05	0.55
1:C:250:ARG:HH11	1:C:250:ARG:HG3	1.72	0.55
2:D:1217:LYS:HZ3	2:D:1220:GLN:HG3	1.70	0.55
1:A:163:THR:HG21	1:A:466:ASN:OD1	2.08	0.54
3:C:501:IHP:O34	7:C:603:HOH:O	2.18	0.53
1:C:321:CYS:SG	7:D:1407:HOH:O	2.59	0.53
1:A:180:ASN:OD1	1:A:424:ARG:HD3	2.09	0.53
1:C:460:ARG:NH2	3:C:501:IHP:O31	2.33	0.53
1:C:282:ARG:NH1	1:C:287:GLU:OE2	2.43	0.52
1:C:285:LYS:HD2	1:C:285:LYS:N	2.24	0.52
1:A:423:LYS:NZ	1:A:443:GLU:OE1	2.38	0.52
1:A:298:ASN:HB3	1:A:365:LEU:HD22	1.92	0.52
1:C:285:LYS:H	1:C:285:LYS:CE	2.22	0.51
1:C:145:ALA:N	1:C:159:ARG:HH21	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1211:ASP:OD2	2:D:1263:TYR:OH	2.23	0.51
1:C:298:ASN:HB3	1:C:365:LEU:HD22	1.93	0.50
4:A:502:ACO:P1A	7:A:632:HOH:O	2.69	0.50
1:A:380:ARG:NH2	3:A:501:IHP:O23	2.42	0.49
2:B:1220:GLN:NE2	7:B:1402:HOH:O	2.26	0.49
1:C:227:VAL:HG22	2:D:1264:LEU:HD12	1.95	0.48
1:A:227:VAL:HG22	2:B:1264:LEU:HD12	1.95	0.48
1:C:267:ARG:HD2	1:C:347:ARG:NH2	2.28	0.48
1:C:380:ARG:HG3	7:C:664:HOH:O	2.15	0.47
2:B:1211:ASP:OD1	2:B:1263:TYR:OH	2.26	0.47
1:A:314:ILE:HG23	1:A:385:GLY:HA2	1.97	0.46
2:B:1251:ARG:HA	2:B:1259:LEU:HD23	1.97	0.46
1:C:283:LYS:NZ	7:C:619:HOH:O	2.47	0.45
1:A:322:ARG:NE	7:A:612:HOH:O	2.34	0.45
1:C:310:ILE:HG12	1:C:370:VAL:HB	1.99	0.45
1:C:250:ARG:HG3	1:C:250:ARG:NH1	2.31	0.44
1:C:314:ILE:HG23	1:C:385:GLY:HA2	1.99	0.44
2:D:1264:LEU:HD23	2:D:1264:LEU:HA	1.83	0.44
1:A:202:ILE:HD12	1:A:233:MET:HE1	2.00	0.44
2:D:1248:GLN:HG2	2:D:1262:THR:HB	1.99	0.44
1:A:321:CYS:SG	2:B:1221:LYS:NZ	2.91	0.44
1:A:428:ASN:O	2:B:1227:ARG:HG2	2.18	0.44
1:C:180:ASN:OD1	1:C:424:ARG:HD3	2.17	0.43
1:A:219:MET:HG2	1:A:239:ILE:HD12	1.99	0.43
1:C:145:ALA:N	7:C:626:HOH:O	2.51	0.43
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.91	0.42
1:A:330:LEU:HD13	3:A:501:IHP:O24	2.19	0.42
1:C:363:GLU:OE2	7:C:604:HOH:O	2.21	0.42
1:C:358:ARG:HB2	1:C:372:ASP:HB3	2.02	0.42
1:C:361:GLN:O	7:C:605:HOH:O	2.22	0.42
1:A:486:ASP:O	7:A:604:HOH:O	2.22	0.41
2:B:1264:LEU:HD23	2:B:1264:LEU:HA	1.89	0.41
1:C:145:ALA:HA	1:C:155:VAL:HG12	2.02	0.41
1:A:380:ARG:HG3	7:A:625:HOH:O	2.19	0.41
1:C:308:ALA:HA	1:C:368:THR:O	2.22	0.40
2:D:1243:CYS:SG	2:D:1267:HIS:HA	2.61	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:816:HOH:O	7:C:819:HOH:O[1_455]	2.01	0.19
7:A:717:HOH:O	7:A:775:HOH:O[1_455]	2.14	0.06
7:A:795:HOH:O	7:C:727:HOH:O[1_546]	2.16	0.04

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	335/352 (95%)	328 (98%)	7 (2%)	0	100	100
1	C	339/352 (96%)	332 (98%)	6 (2%)	1 (0%)	41	37
2	B	65/80 (81%)	61 (94%)	4 (6%)	0	100	100
2	D	69/80 (86%)	65 (94%)	4 (6%)	0	100	100
All	All	808/864 (94%)	786 (97%)	21 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	432	SER

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	274/292 (94%)	265 (97%)	9 (3%)	38	37
1	C	277/292 (95%)	262 (95%)	15 (5%)	22	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	52/71 (73%)	48 (92%)	4 (8%)	13	8
2	D	53/71 (75%)	49 (92%)	4 (8%)	13	9
All	All	656/726 (90%)	624 (95%)	32 (5%)	25	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LEU
1	A	190	VAL
1	A	200	LEU
1	A	358	ARG
1	A	361	GLN
1	A	365	LEU
1	A	421	LEU
1	A	474	MET
1	A	485	LEU
2	B	1208	ASP
2	B	1211	ASP
2	B	1224	LEU
2	B	1248	GLN
1	C	146	THR
1	C	176	LEU
1	C	190	VAL
1	C	200	LEU
1	C	250	ARG
1	C	267	ARG
1	C	285	LYS
1	C	298	ASN
1	C	358	ARG
1	C	361	GLN
1	C	365	LEU
1	C	378	ASP
1	C	421	LEU
1	C	474	MET
1	C	485	LEU
2	D	1220	GLN
2	D	1224	LEU
2	D	1244	LYS
2	D	1248	GLN

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	333	HIS
2	D	1220	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)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACO	A	502	-	28,33,53	2.97	7 (25%)	35,52,79	1.84	10 (28%)
3	IHP	C	501	-	36,36,36	3.15	15 (41%)	54,60,60	1.91	10 (18%)
3	IHP	A	501	-	36,36,36	3.38	13 (36%)	54,60,60	1.82	9 (16%)
4	ACO	C	502	-	28,33,53	1.79	7 (25%)	35,52,79	1.62	8 (22%)
6	GOL	C	503	-	5,5,5	0.34	0	5,5,5	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACO	A	502	-	-	4/17/37/67	0/3/3/3
3	IHP	C	501	-	-	9/30/54/54	0/1/1/1
3	IHP	A	501	-	-	4/30/54/54	0/1/1/1
4	ACO	C	502	-	-	5/17/37/67	0/3/3/3
6	GOL	C	503	-	-	4/4/4/4	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ACO	P3B-O3B	12.97	1.83	1.59
3	A	501	IHP	P3-O13	9.85	1.77	1.59
3	C	501	IHP	P3-O13	9.07	1.76	1.59
3	C	501	IHP	P1-O11	7.30	1.73	1.59
3	A	501	IHP	P1-O11	6.46	1.71	1.59
3	A	501	IHP	P5-O15	6.05	1.70	1.59
3	A	501	IHP	C5-C4	5.89	1.64	1.52
3	A	501	IHP	P4-O14	5.82	1.70	1.59
3	C	501	IHP	P2-O12	5.54	1.69	1.59
3	C	501	IHP	P5-O15	5.53	1.69	1.59
3	A	501	IHP	P2-O12	5.40	1.69	1.59
3	A	501	IHP	C6-C1	5.35	1.63	1.52
4	A	502	ACO	P2A-O6A	5.32	1.75	1.54
3	C	501	IHP	C5-C4	5.23	1.63	1.52
3	A	501	IHP	C6-C5	4.88	1.62	1.52
3	C	501	IHP	P6-O16	4.84	1.68	1.59
3	A	501	IHP	P6-O16	4.67	1.68	1.59
3	A	501	IHP	C2-C1	4.51	1.61	1.52
3	C	501	IHP	C6-C5	3.95	1.60	1.52
3	C	501	IHP	O15-C5	-3.85	1.30	1.44
4	C	502	ACO	P3B-O8A	-3.80	1.40	1.54
3	A	501	IHP	O15-C5	-3.65	1.30	1.44
3	C	501	IHP	C6-C1	3.60	1.59	1.52
3	C	501	IHP	C2-C1	3.59	1.59	1.52
4	C	502	ACO	P3B-O7A	-3.52	1.39	1.50
3	C	501	IHP	O11-C1	-3.51	1.31	1.44
4	C	502	ACO	P3B-O9A	-3.48	1.41	1.54
4	C	502	ACO	C4A-N3A	-3.41	1.30	1.35
3	C	501	IHP	C4-C3	3.24	1.59	1.52
4	C	502	ACO	C8A-N7A	-3.03	1.29	1.34
4	A	502	ACO	C2B-C1B	2.95	1.58	1.53
3	C	501	IHP	P4-O14	2.88	1.64	1.59
3	A	501	IHP	O11-C1	-2.86	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	IHP	O14-C4	-2.72	1.34	1.44
4	A	502	ACO	O3B-C3B	-2.64	1.34	1.44
4	C	502	ACO	C5A-N7A	-2.39	1.31	1.39
4	A	502	ACO	C2B-C3B	2.30	1.58	1.52
3	A	501	IHP	C4-C3	2.29	1.57	1.52
3	C	501	IHP	O13-C3	-2.09	1.36	1.44
4	A	502	ACO	O2B-C2B	-2.04	1.38	1.43
4	C	502	ACO	O4B-C4B	-2.01	1.40	1.45
4	A	502	ACO	C3B-C4B	2.00	1.58	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	ACO	P1A-O3A-P2A	-6.24	111.41	132.83
3	A	501	IHP	C4-C3-C2	-5.77	97.77	110.41
3	C	501	IHP	O13-C3-C2	5.58	121.83	108.69
3	C	501	IHP	C5-C6-C1	5.39	122.21	110.41
3	A	501	IHP	C5-C6-C1	5.01	121.38	110.41
3	C	501	IHP	C5-C4-C3	4.89	121.12	110.41
3	A	501	IHP	O13-C3-C2	3.96	118.01	108.69
3	C	501	IHP	O11-C1-C2	3.94	117.96	108.69
3	A	501	IHP	O13-C3-C4	3.68	117.36	108.69
3	C	501	IHP	C4-C3-C2	-3.67	102.38	110.41
3	C	501	IHP	O13-C3-C4	3.49	116.90	108.69
4	A	502	ACO	O3B-P3B-O7A	-3.16	97.18	109.39
4	C	502	ACO	O5A-P2A-O3A	3.12	115.11	104.64
4	A	502	ACO	O5A-P2A-O4A	3.11	122.86	110.68
3	C	501	IHP	O12-C2-C1	3.10	116.00	108.69
4	A	502	ACO	O9A-P3B-O8A	3.05	119.31	107.64
3	A	501	IHP	O15-C5-C4	2.94	115.61	108.69
4	C	502	ACO	O4B-C1B-C2B	2.91	111.17	106.93
4	C	502	ACO	P1A-O3A-P2A	-2.89	122.90	132.83
4	A	502	ACO	P1A-O5B-C5B	-2.86	104.90	121.68
3	A	501	IHP	O14-C4-C5	2.85	115.42	108.69
3	C	501	IHP	O45-P5-O15	2.82	118.63	105.99
4	C	502	ACO	O5B-P1A-O1A	2.68	119.53	109.07
3	A	501	IHP	O11-C1-C2	2.56	114.72	108.69
4	C	502	ACO	N3A-C2A-N1A	-2.51	124.76	128.68
4	C	502	ACO	O2B-C2B-C3B	2.45	118.11	111.17
4	C	502	ACO	N6A-C6A-N1A	2.44	123.64	118.57
3	C	501	IHP	O15-C5-C4	2.35	114.23	108.69
4	C	502	ACO	O4B-C4B-C3B	2.27	109.73	104.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	IHP	O12-C2-C3	2.23	113.95	108.69
4	A	502	ACO	O6A-P2A-O4A	-2.16	102.22	110.68
4	A	502	ACO	O6A-P2A-O5A	-2.11	99.58	107.64
3	A	501	IHP	O45-P5-O15	2.08	115.31	105.99
3	C	501	IHP	O41-P1-O11	2.06	115.24	105.99
4	A	502	ACO	O8A-P3B-O7A	2.05	118.69	110.68
4	A	502	ACO	O4B-C4B-C3B	2.04	109.24	104.87
4	A	502	ACO	C2A-N1A-C6A	-2.03	115.29	118.75

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	IHP	C3-C4-O14-P4
3	A	501	IHP	C4-O14-P4-O34
3	C	501	IHP	C1-C2-O12-P2
4	A	502	ACO	C5B-O5B-P1A-O2A
4	A	502	ACO	C5B-O5B-P1A-O3A
4	C	502	ACO	C5B-O5B-P1A-O2A
4	C	502	ACO	C5B-O5B-P1A-O3A
4	C	502	ACO	P1A-O3A-P2A-O5A
6	C	503	GOL	O1-C1-C2-C3
6	C	503	GOL	C1-C2-C3-O3
6	C	503	GOL	O2-C2-C3-O3
3	A	501	IHP	C4-O14-P4-O24
3	C	501	IHP	C4-O14-P4-O24
3	C	501	IHP	C5-O15-P5-O25
3	C	501	IHP	C4-O14-P4-O34
4	C	502	ACO	C3B-O3B-P3B-O9A
4	A	502	ACO	C5B-O5B-P1A-O1A
4	C	502	ACO	C5B-O5B-P1A-O1A
6	C	503	GOL	O1-C1-C2-O2
3	C	501	IHP	C2-O12-P2-O22
3	C	501	IHP	C3-O13-P3-O23
3	C	501	IHP	C6-O16-P6-O26
3	A	501	IHP	C5-O15-P5-O45
3	C	501	IHP	C1-O11-P1-O31
3	C	501	IHP	C2-O12-P2-O42
4	A	502	ACO	P2A-O3A-P1A-O2A

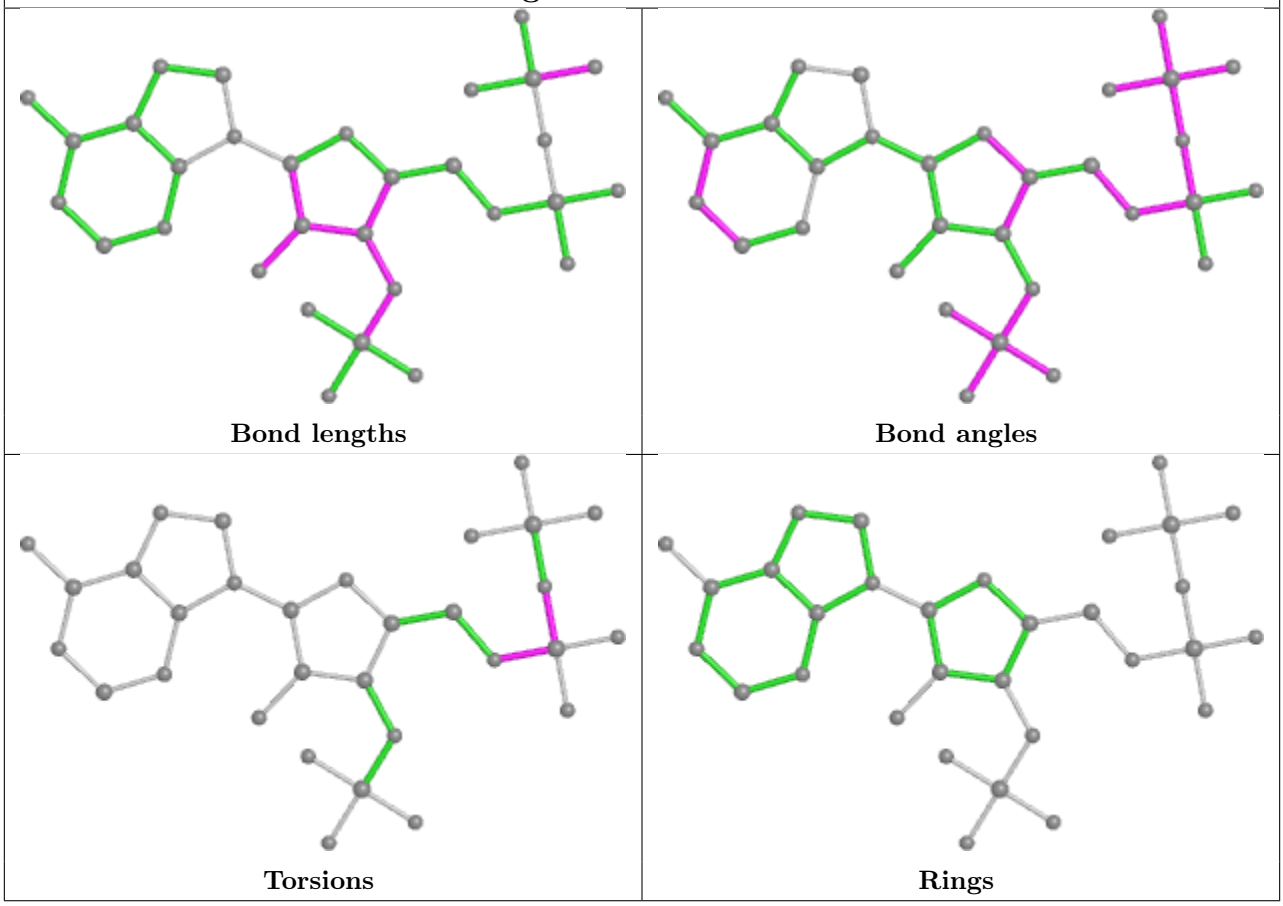
There are no ring outliers.

5 monomers are involved in 10 short contacts:

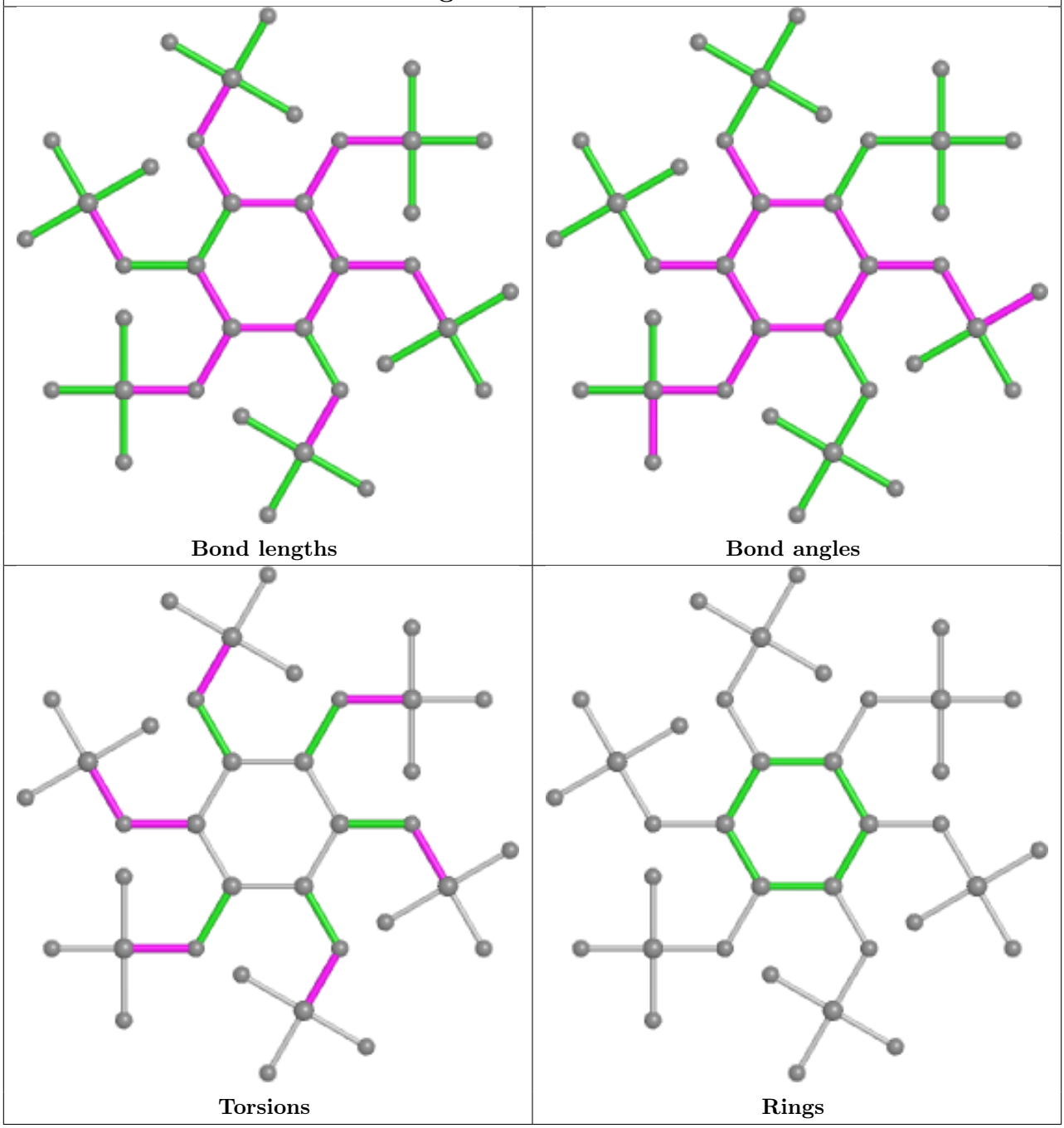
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	ACO	1	0
3	C	501	IHP	3	0
3	A	501	IHP	3	0
4	C	502	ACO	2	0
6	C	503	GOL	2	0

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 then 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.

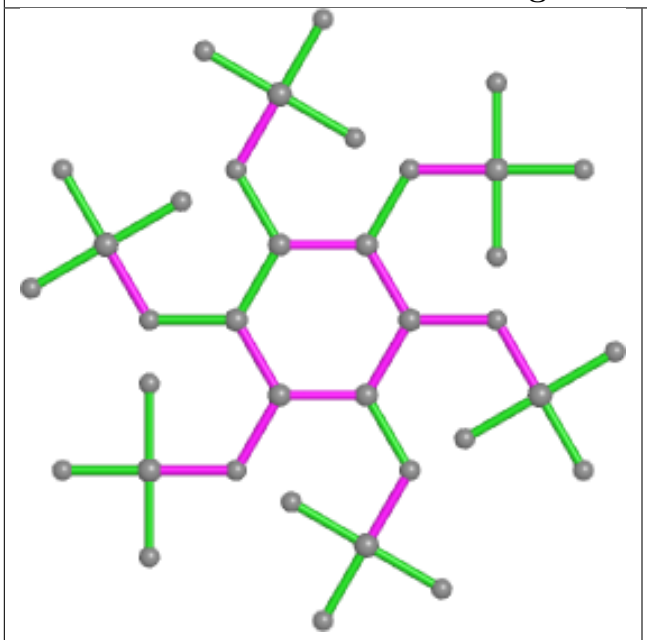
Ligand ACO A 502



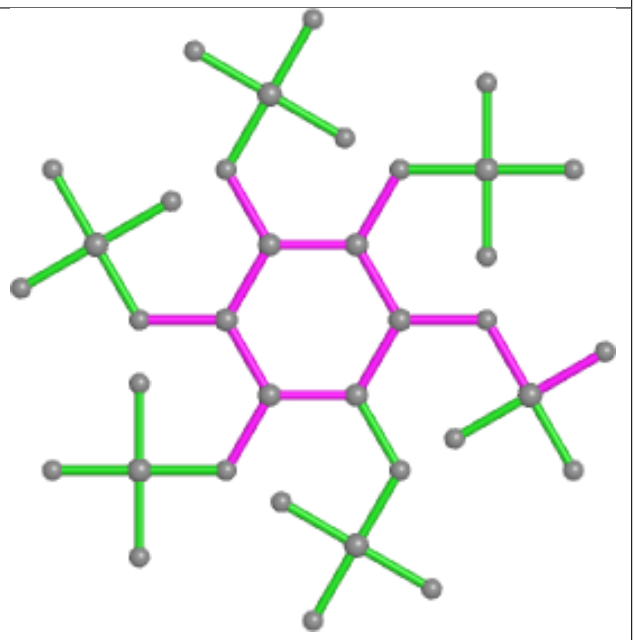
Ligand IHP C 501



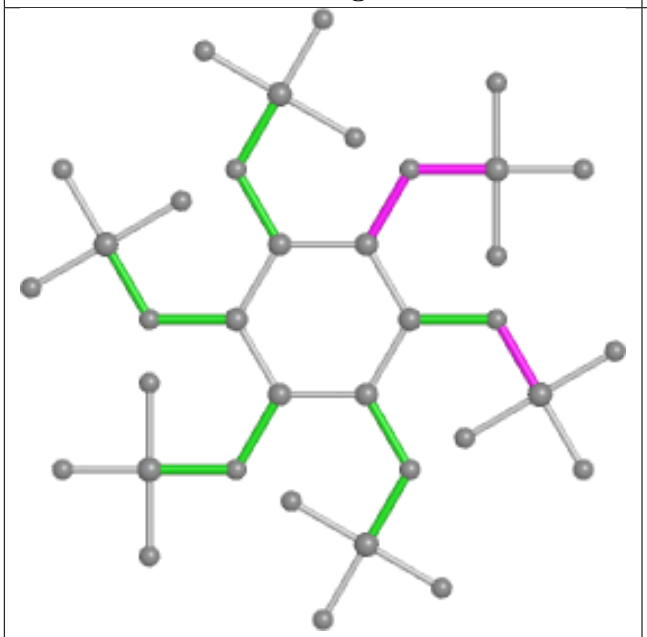
Ligand IHP A 501



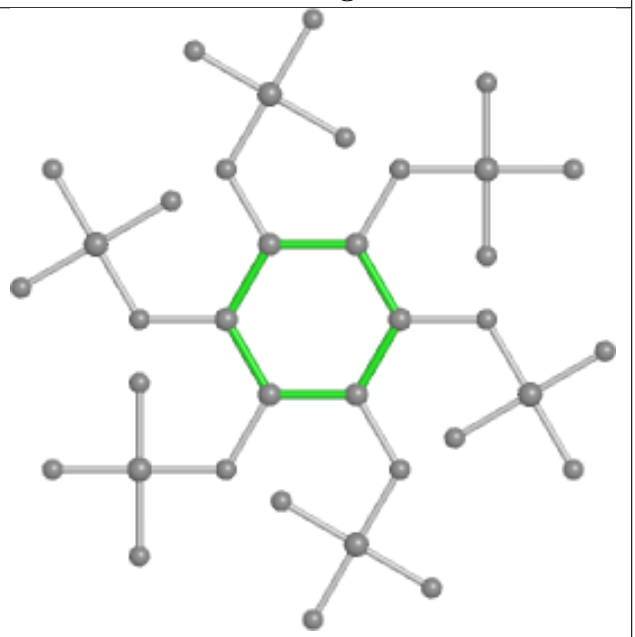
Bond lengths



Bond angles

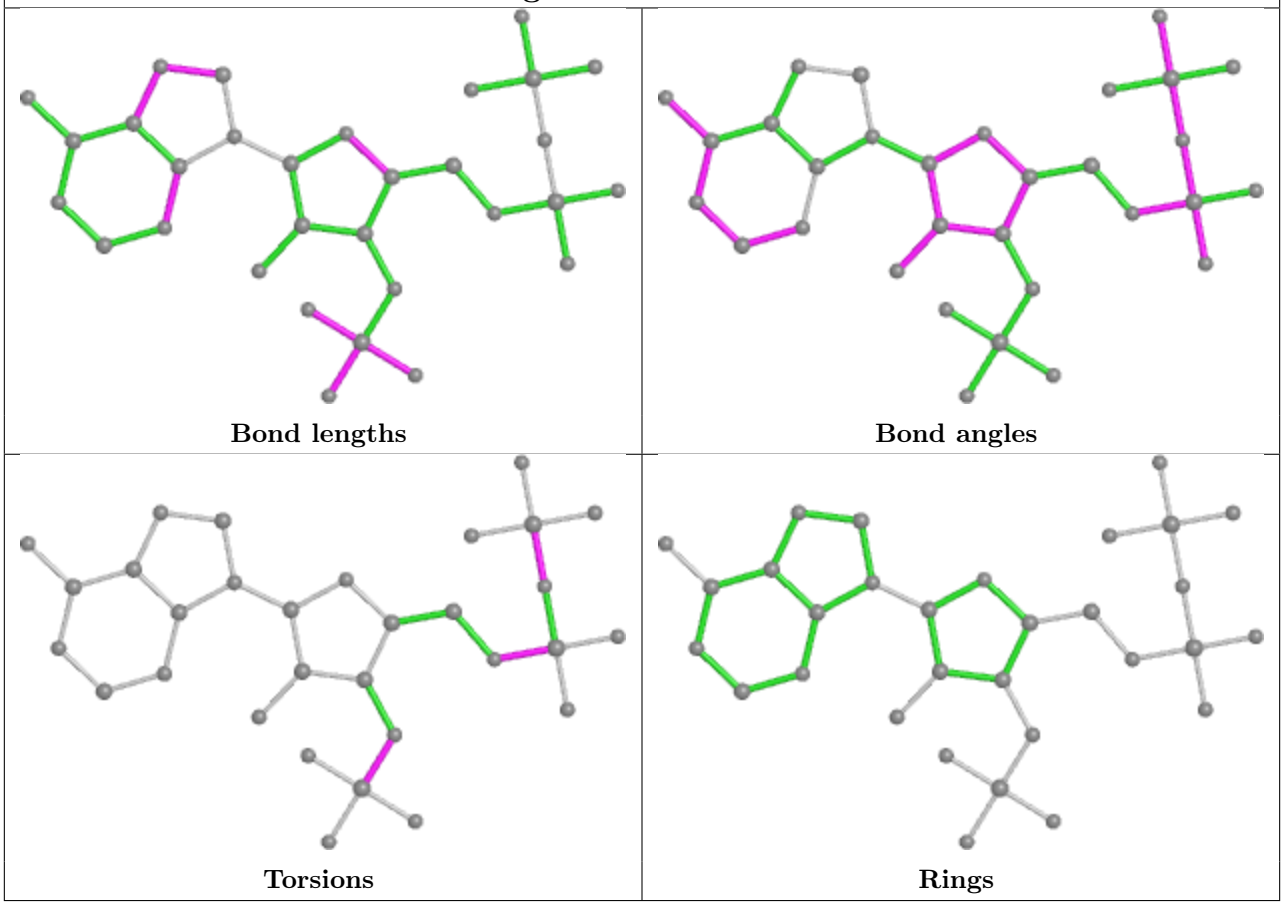


Torsions



Rings

Ligand ACO C 502



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, 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	335/352 (95%)	-0.52	1 (0%)	94	93	24, 35, 62, 99	0
1	C	342/352 (97%)	-0.53	0	100	100	24, 35, 67, 92	0
2	B	67/80 (83%)	0.04	3 (4%)	33	32	32, 53, 96, 114	0
2	D	73/80 (91%)	-0.13	1 (1%)	75	74	30, 54, 94, 111	0
All	All	817/864 (94%)	-0.44	5 (0%)	89	88	24, 38, 80, 114	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1273	THR	5.9
2	D	1273	THR	4.2
2	B	1266	GLU	2.9
2	B	1254	THR	2.3
1	A	437	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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,

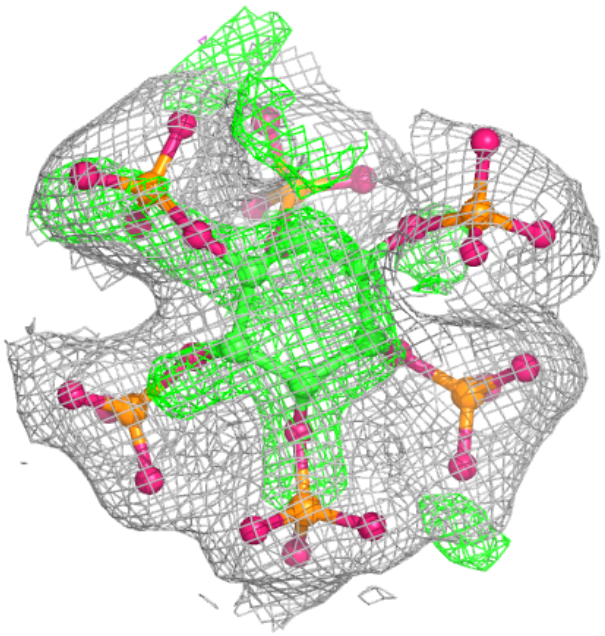
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

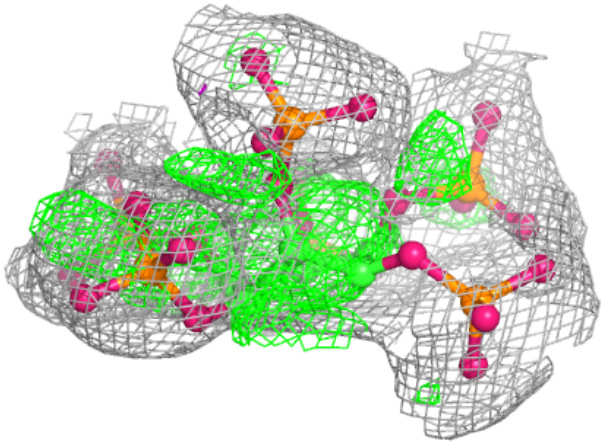
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	C	503	6/6	0.91	0.17	20,20,20,20	0
3	IHP	A	501	36/36	0.95	0.14	33,57,91,95	0
4	ACO	C	502	31/51	0.96	0.09	27,34,119,150	0
3	IHP	C	501	36/36	0.96	0.12	34,54,111,116	0
4	ACO	A	502	31/51	0.97	0.08	26,35,106,133	0
5	ZN	D	1301	1/1	0.98	0.12	56,56,56,56	0
5	ZN	B	1301	1/1	0.98	0.12	54,54,54,54	0

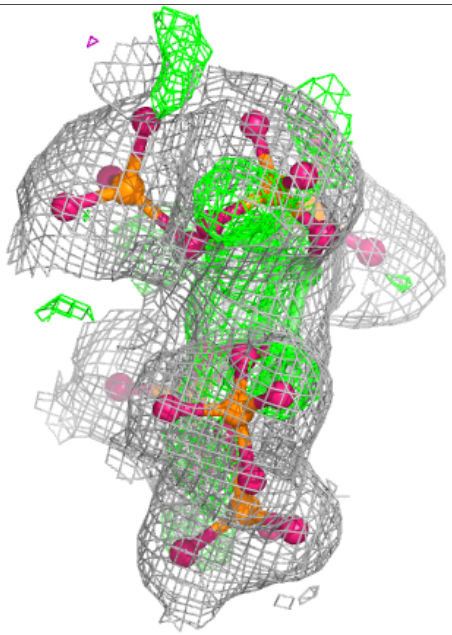
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

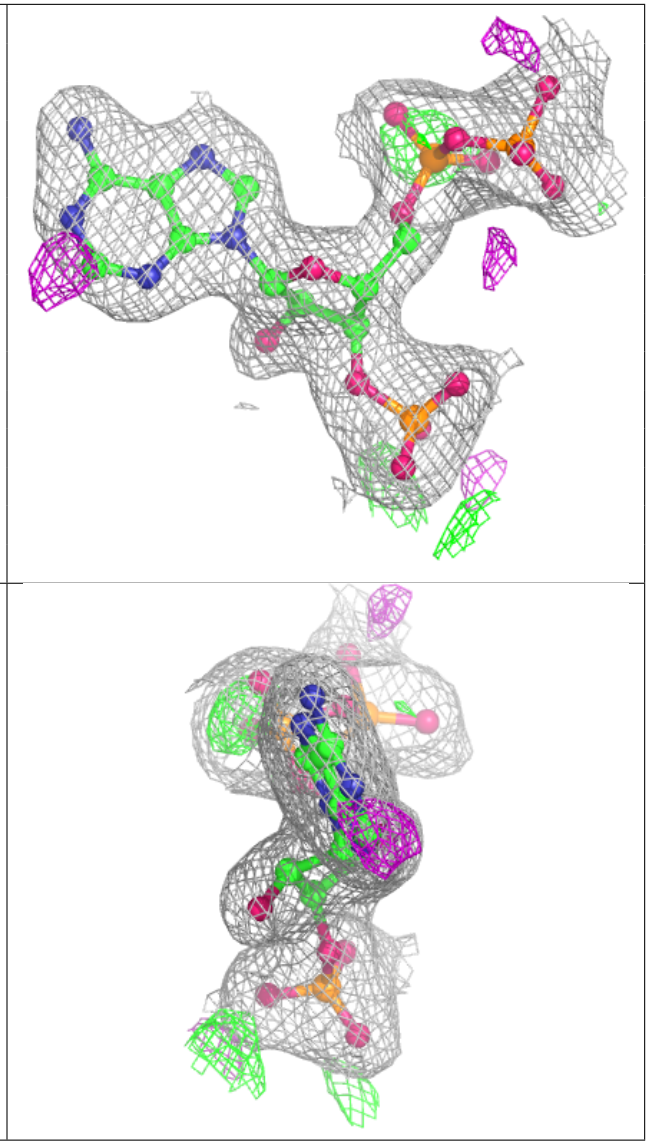






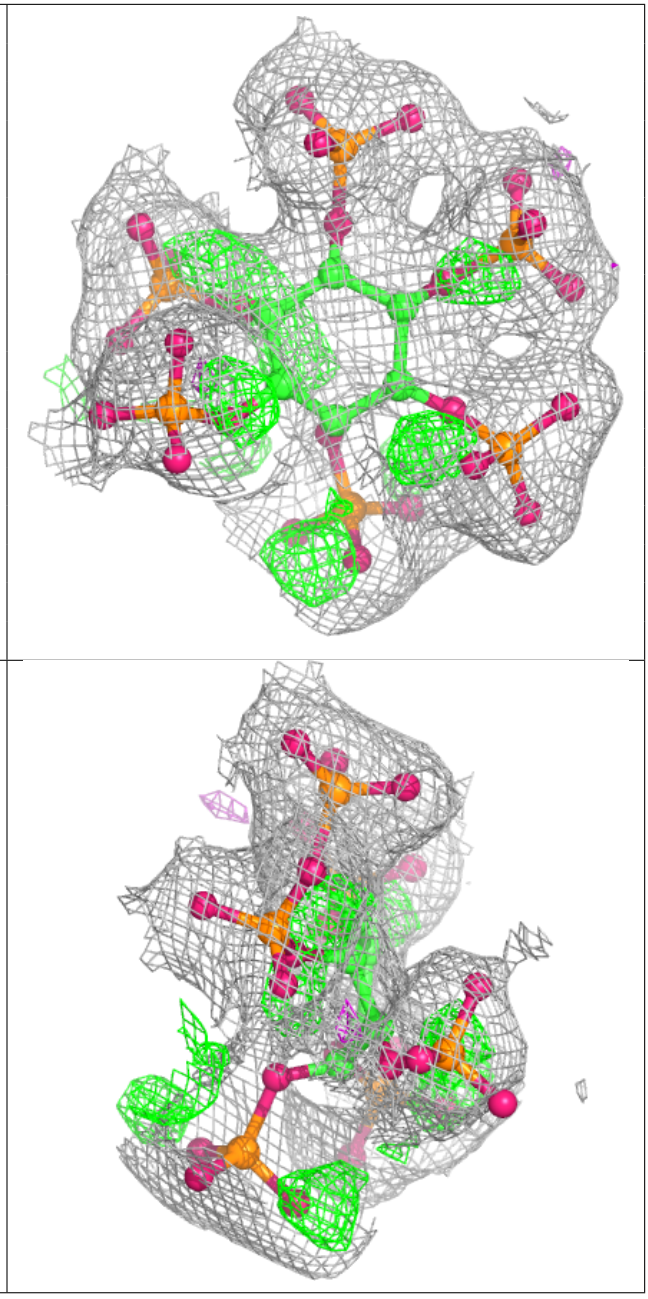
Electron density around ACO C 502:

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



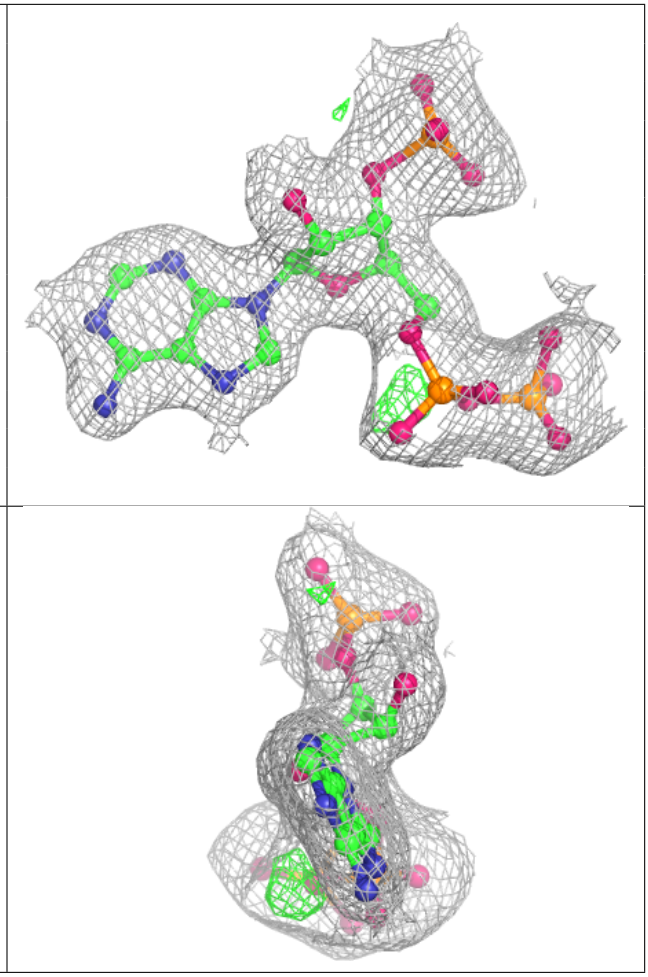
Electron density around IHP C 501:

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



Electron density around 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)



6.5 Other polymers (i)

There are no such residues in this entry.