



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2025 – 12:12 AM JST

PDB ID : 7E1J / pdb_00007e1j
Title : Crystal structure of Pr55Gag-matrix domain in complex with IP6 in space group C121
Authors : DeMirci, H.; Senda, T.; Destan, E.
Deposited on : 2021-02-01
Resolution : 2.72 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

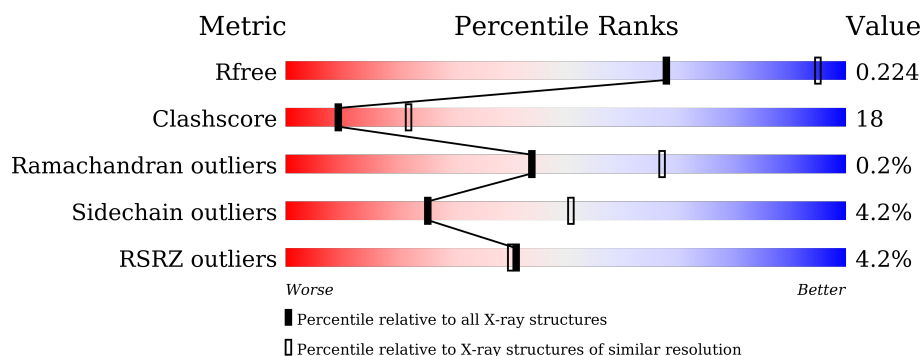
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	117	<div> <div>3%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	B	117	<div> <div>6%</div> <div>64%</div> <div>28%</div> <div>7%</div> </div>
1	C	117	<div> <div>3%</div> <div>65%</div> <div>26%</div> <div>5%</div> </div>
1	D	117	<div> <div>7%</div> <div>62%</div> <div>29%</div> <div>6%</div> </div>
1	E	117	<div> <div>3%</div> <div>57%</div> <div>34%</div> <div>8%</div> </div>
1	F	117	<div> <div>2%</div> <div>66%</div> <div>28%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5742 atoms, of which 36 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.

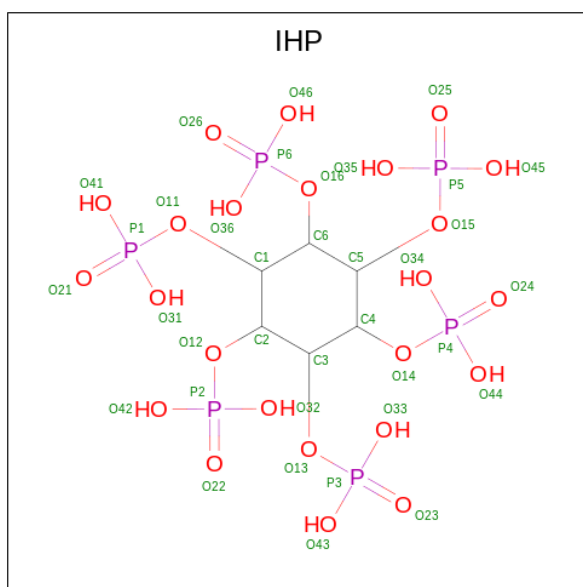
- Molecule 1 is a protein called Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	1	0
			929	579	172	175	3			
1	B	109	Total	C	N	O	S	0	1	0
			875	546	160	166	3			
1	C	111	Total	C	N	O	S	0	0	0
			885	553	161	168	3			
1	D	110	Total	C	N	O	S	0	3	0
			902	562	166	171	3			
1	E	108	Total	C	N	O	S	0	0	1
			861	540	156	163	2			
1	F	111	Total	C	N	O	S	0	1	0
			897	561	166	168	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP T2CJ20
B	-1	SER	-	expression tag	UNP T2CJ20
C	-1	SER	-	expression tag	UNP T2CJ20
D	-1	SER	-	expression tag	UNP T2CJ20
E	-1	SER	-	expression tag	UNP T2CJ20
F	-1	SER	-	expression tag	UNP T2CJ20

- 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 36 6 24 6	0	0
2	B	1	Total C H O P 42 6 6 24 6	0	0
2	C	1	Total C H O P 84 12 12 48 12	0	1
2	D	1	Total C O P 36 6 24 6	0	0
2	E	1	Total C H O P 84 12 12 48 12	0	1
2	F	1	Total C H O P 42 6 6 24 6	0	0

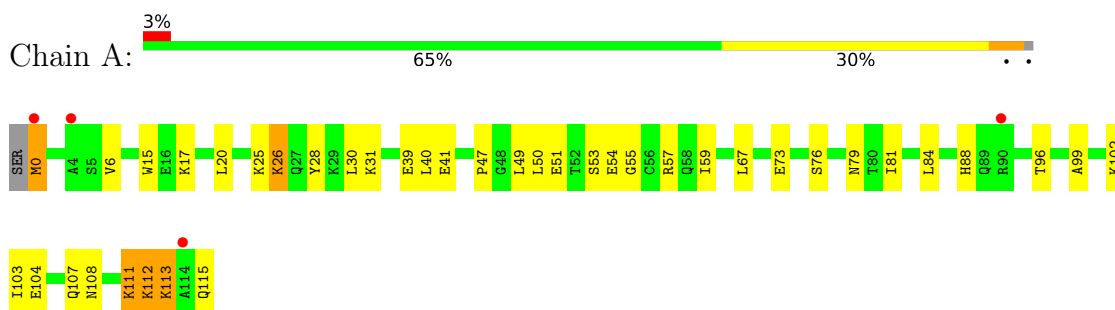
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	10	Total O 10 10	0	0
3	C	13	Total O 13 13	0	0
3	D	13	Total O 13 13	0	0
3	E	9	Total O 9 9	0	0
3	F	11	Total O 11 11	0	0

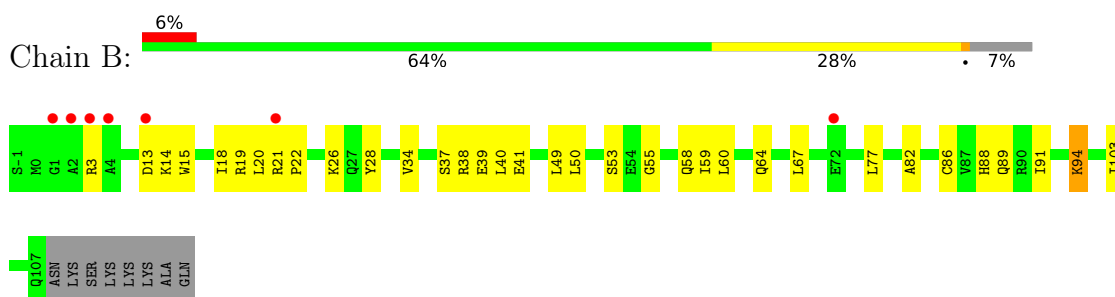
3 Residue-property plots [i](#)

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.

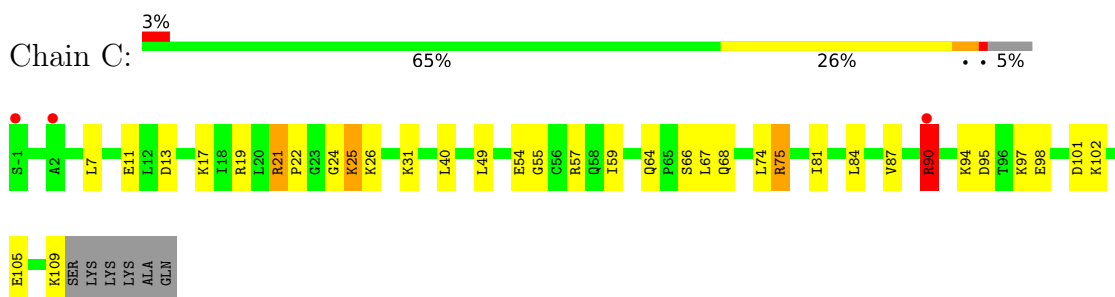
- Molecule 1: Capsid protein p24



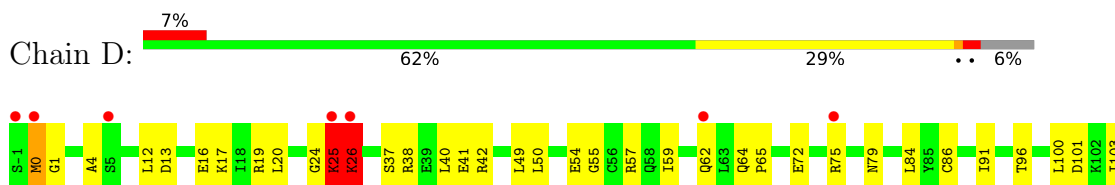
- Molecule 1: Capsid protein p24

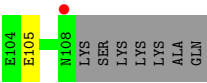


- Molecule 1: Capsid protein p24

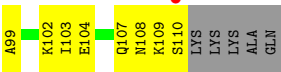
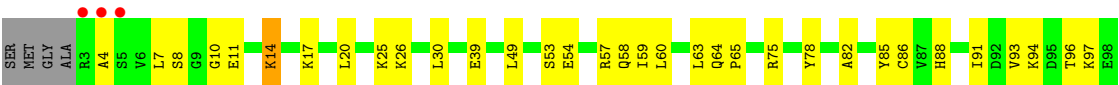


- Molecule 1: Capsid protein p24

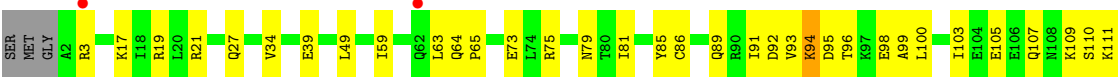




• Molecule 1: Capsid protein p24



• Molecule 1: Capsid protein p24



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	176.18Å 67.41Å 97.50Å 90.00° 123.15° 90.00°	Depositor
Resolution (Å)	44.41 – 2.72 44.41 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.41-2.72) 99.9 (44.41-2.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.73Å)	Xtriage
Refinement program	PHENIX DEV-3318	Depositor
R, R_{free}	0.213 , 0.272 0.225 , 0.224	Depositor DCC
R_{free} test set	1306 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.076 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5742	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: 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	0.36	0/941	0.66	2/1261 (0.2%)
1	B	0.43	1/887 (0.1%)	0.58	2/1192 (0.2%)
1	C	0.55	3/897 (0.3%)	1.10	4/1203 (0.3%)
1	D	0.67	2/917 (0.2%)	0.75	2/1230 (0.2%)
1	E	0.33	0/873	0.46	0/1172
1	F	0.31	0/909	0.47	0/1217
All	All	0.46	6/5424 (0.1%)	0.71	10/7275 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	25	LYS	CD-CE	16.11	1.91	1.51
1	C	90	ARG	CZ-NH2	-8.34	1.22	1.33
1	B	94	LYS	CE-NZ	-7.98	1.29	1.49
1	C	90	ARG	CG-CD	7.31	1.70	1.51
1	C	90	ARG	CB-CG	5.13	1.66	1.52
1	D	26	LYS	CD-CE	5.04	1.63	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ARG	NE-CZ-NH1	30.62	135.61	120.30
1	D	25	LYS	CD-CE-NZ	17.64	152.28	111.70
1	A	0	MET	CG-SD-CE	-13.38	78.79	100.20
1	C	90	ARG	NH1-CZ-NH2	-11.11	107.18	119.40
1	B	94	LYS	CD-CE-NZ	-8.30	92.61	111.70
1	C	90	ARG	CD-NE-CZ	8.08	134.92	123.60
1	B	94	LYS	CB-CG-CD	-6.70	94.17	111.60
1	A	26	LYS	CD-CE-NZ	-6.34	97.12	111.70
1	C	90	ARG	NE-CZ-NH2	-6.20	117.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	LYS	CG-CD-CE	5.73	129.09	111.90

There are no chirality outliers.

There are no planarity outliers.

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	929	0	949	48	0
1	B	875	0	890	32	1
1	C	885	0	907	38	2
1	D	902	0	921	35	0
1	E	861	0	878	28	0
1	F	897	0	923	22	1
2	A	36	0	5	8	0
2	B	36	6	6	0	0
2	C	72	12	8	6	0
2	D	36	0	4	1	0
2	E	72	12	9	5	2
2	F	36	6	6	1	0
3	A	13	0	0	1	0
3	B	10	0	0	2	0
3	C	13	0	0	2	0
3	D	13	0	0	3	0
3	E	9	0	0	0	0
3	F	11	0	0	1	0
All	All	5706	36	5506	197	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 18.

All (197) 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:D:25:LYS:CD	1:D:25:LYS:CE	1.91	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:MET:HA	1:D:4:ALA:HB1	1.28	1.15
1:C:25:LYS:HD3	1:C:25:LYS:H	1.25	0.98
1:B:13:ASP:OD1	3:B:301:HOH:O	1.87	0.92
1:A:31:LYS:HD2	1:D:13:ASP:OD1	1.74	0.87
1:D:72:GLU:HG3	1:D:75[A]:ARG:HH21	1.38	0.86
1:F:86:CYS:HB3	1:F:91:ILE:HB	1.57	0.86
1:D:49:LEU:HB2	1:D:59:ILE:HD11	1.58	0.85
1:B:49:LEU:HB2	1:B:59:ILE:HD11	1.61	0.80
1:A:113:LYS:HA	1:A:113:LYS:HE2	1.62	0.80
1:A:0:MET:HA	1:D:4:ALA:CB	2.11	0.78
1:A:108:ASN:O	1:A:111:LYS:HG3	1.84	0.77
1:E:86:CYS:HB3	1:E:91:ILE:HB	1.66	0.77
1:C:19:ARG:NH2	2:C:201[B]:IHP:O33	2.17	0.77
1:E:49:LEU:HB2	1:E:59:ILE:HD11	1.69	0.75
1:E:17:LYS:CE	2:E:201[A]:IHP:O36	2.35	0.75
1:C:64:GLN:HG2	1:C:67:LEU:HD12	1.67	0.75
1:C:75:ARG:HH11	1:C:75:ARG:HB3	1.52	0.73
1:E:8:SER:OG	1:E:11:GLU:HG3	1.90	0.71
1:A:113:LYS:HA	1:A:113:LYS:CE	2.20	0.71
1:F:21:ARG:NH1	3:F:301:HOH:O	2.23	0.69
1:E:17:LYS:HE2	2:E:201[B]:IHP:O41	1.92	0.69
1:A:111:LYS:O	1:A:115:GLN:HG2	1.91	0.69
1:A:31:LYS:HE3	1:D:16:GLU:HB2	1.75	0.69
1:F:107:GLN:O	1:F:110:SER:HB3	1.92	0.69
1:A:49:LEU:O	1:A:55:GLY:HA3	1.93	0.68
1:E:17:LYS:HE2	2:E:201[A]:IHP:O36	1.92	0.68
2:A:201:IHP:H6	2:A:201:IHP:O45	1.92	0.68
1:B:20:LEU:HD12	1:B:26:LYS:HB3	1.76	0.68
1:C:17:LYS:NZ	2:C:201[B]:IHP:O16	2.26	0.67
1:B:82:ALA:HB1	1:B:103:ILE:HD12	1.76	0.67
1:F:49:LEU:HB2	1:F:59:ILE:HD11	1.76	0.66
1:F:93:VAL:HG11	1:F:99:ALA:HA	1.77	0.66
1:E:17:LYS:CE	2:E:201[B]:IHP:O41	2.44	0.66
1:B:21[B]:ARG:HG3	1:B:22:PRO:HD2	1.78	0.65
1:B:89:GLN:HB3	1:B:91:ILE:HD12	1.79	0.65
1:D:19:ARG:HD3	1:D:24:GLY:O	1.97	0.64
1:A:49:LEU:HB2	1:A:59:ILE:HD11	1.78	0.64
1:B:40:LEU:HD11	1:B:50:LEU:HD21	1.78	0.64
1:D:0:MET:HG3	1:D:1:GLY:H	1.61	0.63
1:F:100:LEU:O	1:F:103:ILE:HB	1.97	0.63
1:D:86:CYS:HB3	1:D:91:ILE:HB	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD13	1:B:103:ILE:HD13	1.80	0.63
1:F:85:TYR:CD2	1:F:103:ILE:HD11	2.34	0.62
1:E:54:GLU:O	1:E:58:GLN:HG3	1.99	0.62
1:A:104:GLU:HA	1:A:107:GLN:HB2	1.81	0.62
1:F:92:ASP:OD1	1:F:94:LYS:HE3	2.00	0.62
1:B:89:GLN:HG2	1:B:91:ILE:HD11	1.82	0.62
1:F:59:ILE:HG21	1:F:81:ILE:HD13	1.82	0.61
1:A:31:LYS:NZ	1:D:17:LYS:HG3	2.15	0.61
1:C:101:ASP:O	1:C:105:GLU:HG3	2.01	0.61
1:B:89:GLN:HB3	1:B:91:ILE:CD1	2.31	0.60
1:A:40:LEU:HD11	1:A:50:LEU:HD21	1.83	0.60
1:C:25:LYS:HG2	1:C:26:LYS:HG3	1.83	0.60
1:A:31:LYS:CE	1:D:16:GLU:HB2	2.33	0.59
1:E:64:GLN:N	1:E:65:PRO:HD2	2.17	0.59
1:C:49:LEU:O	1:C:55:GLY:HA3	2.03	0.59
1:A:54:GLU:HA	1:A:57:ARG:HB2	1.86	0.58
1:A:54:GLU:HG3	1:A:57:ARG:HE	1.69	0.58
1:B:20:LEU:CD1	1:B:26:LYS:HB3	2.34	0.57
1:E:82:ALA:HB1	1:E:103:ILE:HD12	1.87	0.57
1:A:113:LYS:O	1:A:113:LYS:HD3	2.04	0.57
1:C:98:GLU:O	1:C:102:LYS:HG2	2.04	0.57
1:C:19:ARG:HD3	1:C:24:GLY:O	2.05	0.57
1:A:0:MET:CA	1:D:4:ALA:HB1	2.19	0.56
1:B:86:CYS:HB3	1:B:91:ILE:HB	1.87	0.56
1:D:38:ARG:O	1:D:42:ARG:HD3	2.06	0.56
1:A:104:GLU:O	1:A:108:ASN:N	2.39	0.55
1:B:82:ALA:CB	1:B:103:ILE:HD12	2.36	0.55
1:D:20:LEU:HD12	1:D:26:LYS:HD3	1.89	0.55
1:A:54:GLU:HG3	1:A:57:ARG:HB3	1.88	0.54
1:D:101:ASP:O	1:D:105:GLU:HG3	2.07	0.54
1:A:31:LYS:HD3	3:D:306:HOH:O	2.07	0.54
1:F:17:LYS:HZ2	2:F:201:IHP:P5	2.32	0.53
1:C:40:LEU:HD11	1:C:59:ILE:HD13	1.90	0.53
1:D:55:GLY:O	1:D:59:ILE:HG13	2.10	0.52
1:E:4:ALA:HB1	1:E:30:LEU:HD21	1.91	0.52
1:F:79:ASN:HB3	1:F:96:THR:HG21	1.90	0.52
1:A:17:LYS:HG2	2:A:201:IHP:P2	2.49	0.52
2:A:201:IHP:O12	2:A:201:IHP:P3	2.67	0.52
1:A:31:LYS:HE2	1:D:13:ASP:HA	1.91	0.51
1:D:79:ASN:HB3	1:D:96:THR:HG21	1.92	0.51
1:A:17:LYS:NZ	2:A:201:IHP:O22	2.34	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HE2	1:A:113:LYS:CA	2.32	0.51
1:F:64:GLN:N	1:F:65:PRO:HD2	2.26	0.51
1:B:38:ARG:HA	1:B:41:GLU:HG2	1.93	0.51
1:C:75:ARG:HB3	1:C:75:ARG:NH1	2.23	0.50
1:B:3:ARG:HH21	1:B:34:VAL:HG21	1.75	0.50
1:F:94:LYS:HD2	1:F:98:GLU:OE1	2.12	0.50
1:A:6:VAL:HG12	1:A:51:GLU:HG3	1.93	0.50
1:C:25:LYS:HD3	1:C:25:LYS:N	2.08	0.50
1:A:26:LYS:HD2	2:D:201:IHP:O21	2.12	0.50
1:C:7:LEU:HD21	1:C:84:LEU:HD22	1.93	0.50
1:A:99:ALA:O	1:A:103:ILE:HG12	2.13	0.49
1:F:3:ARG:HG2	1:F:34:VAL:CG2	2.43	0.49
1:C:11:GLU:HG3	1:C:90:ARG:NH1	2.27	0.49
1:B:19:ARG:HH11	1:B:19:ARG:HG2	1.78	0.49
1:E:97:LYS:HB3	1:E:97:LYS:HE3	1.59	0.49
1:C:17:LYS:NZ	2:C:201[B]:IHP:O34	2.40	0.49
1:E:60:LEU:HD22	1:E:78:TYR:CE2	2.48	0.48
1:B:58:GLN:OE1	1:C:68:GLN:NE2	2.46	0.48
1:E:104:GLU:HA	1:E:107:GLN:HB2	1.96	0.48
1:B:49:LEU:O	1:B:55:GLY:HA3	2.11	0.48
1:E:4:ALA:HB1	1:E:30:LEU:CD2	2.44	0.48
1:C:11:GLU:HG2	1:C:87:VAL:HG12	1.96	0.48
1:D:41:GLU:HG3	1:D:42:ARG:HH11	1.77	0.48
1:D:72:GLU:HG3	1:D:75[A]:ARG:NH2	2.19	0.48
1:A:59:ILE:HG21	1:A:81:ILE:CD1	2.44	0.48
1:C:25:LYS:H	1:C:25:LYS:CD	2.08	0.47
1:D:26:LYS:H	1:D:26:LYS:HG2	1.48	0.47
1:B:49:LEU:CB	1:B:59:ILE:HD11	2.36	0.47
1:A:112:LYS:HG3	1:A:112:LYS:O	2.15	0.47
1:C:25:LYS:HG2	1:C:26:LYS:N	2.28	0.47
1:C:59:ILE:HG21	1:C:81:ILE:HD13	1.96	0.47
1:D:64:GLN:N	1:D:65:PRO:HD2	2.30	0.47
1:F:59:ILE:HG21	1:F:81:ILE:CD1	2.45	0.47
1:D:20:LEU:HD12	1:D:26:LYS:CG	2.45	0.47
1:E:53:SER:OG	1:E:88:HIS:HB3	2.14	0.47
1:E:108:ASN:O	1:E:110:SER:N	2.48	0.47
1:C:54:GLU:HA	1:C:57:ARG:HB3	1.96	0.46
1:D:40:LEU:HD11	1:D:50:LEU:HD21	1.97	0.46
1:E:93:VAL:HG11	1:E:99:ALA:HA	1.96	0.46
1:A:54:GLU:CG	1:A:57:ARG:HE	2.28	0.46
1:C:31:LYS:HB3	3:C:308:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HA	1:A:115:GLN:HE21	1.80	0.46
1:E:20:LEU:O	1:E:96:THR:OG1	2.21	0.46
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.74	0.46
1:A:31:LYS:HZ1	1:D:17:LYS:HG3	1.80	0.46
1:A:73:GLU:HG2	3:A:303:HOH:O	2.16	0.46
1:C:40:LEU:CD1	1:C:59:ILE:HD13	2.46	0.46
1:A:31:LYS:HE2	3:D:306:HOH:O	2.16	0.45
1:A:41:GLU:HB3	1:A:47:PRO:HG3	1.97	0.45
1:B:86:CYS:HA	1:B:91:ILE:HD12	1.97	0.45
1:C:17:LYS:HZ1	2:C:201[B]:IHP:P6	2.39	0.45
1:A:104:GLU:O	1:A:108:ASN:HB2	2.16	0.45
1:B:64:GLN:O	1:B:67:LEU:HB2	2.16	0.45
1:C:22:PRO:CG	1:C:97:LYS:HB2	2.46	0.45
1:A:0:MET:HB2	1:A:0:MET:HE3	1.10	0.45
1:E:63:LEU:C	1:E:65:PRO:HD2	2.38	0.45
1:B:14:LYS:CE	3:B:301:HOH:O	2.62	0.44
1:B:39:GLU:HB3	1:B:77:LEU:HD13	1.98	0.44
1:A:59:ILE:HG21	1:A:81:ILE:HD13	2.00	0.44
2:C:201[B]:IHP:O25	2:C:201[B]:IHP:H4	2.18	0.44
1:A:31:LYS:CE	3:D:306:HOH:O	2.66	0.44
1:D:86:CYS:HA	1:D:91:ILE:HD12	2.00	0.44
1:C:21:ARG:HH21	1:C:25:LYS:NZ	2.16	0.44
1:C:25:LYS:HE2	1:C:26:LYS:HE2	2.00	0.44
1:C:64:GLN:O	1:C:67:LEU:HB2	2.17	0.44
1:A:39:GLU:OE2	1:A:73:GLU:OE1	2.35	0.43
1:D:84:LEU:HA	1:D:84:LEU:HD23	1.75	0.43
1:B:21[B]:ARG:HG3	1:B:22:PRO:CD	2.48	0.43
1:B:89:GLN:CG	1:B:91:ILE:HD11	2.48	0.43
1:C:17:LYS:NZ	2:C:201[B]:IHP:P6	2.91	0.43
1:B:94:LYS:HD3	1:B:94:LYS:HA	1.00	0.43
1:A:30:LEU:CD1	1:D:12:LEU:HD13	2.49	0.43
1:B:15:TRP:CE2	1:B:28:TYR:HB3	2.53	0.42
1:C:66:SER:HB2	1:C:74:LEU:HD21	2.00	0.42
1:A:15:TRP:CZ3	1:A:84:LEU:HG	2.55	0.42
1:A:20:LEU:HD23	1:A:28:TYR:CZ	2.53	0.42
1:C:22:PRO:HG3	1:C:97:LYS:CB	2.49	0.42
1:A:79:ASN:HB3	1:A:96:THR:HG21	2.01	0.42
1:C:19:ARG:O	1:C:95:ASP:HA	2.19	0.42
1:E:17:LYS:CD	2:E:201[A]:IHP:O36	2.67	0.42
1:E:25:LYS:HE2	1:E:25:LYS:HB2	1.55	0.42
1:E:39:GLU:HA	1:E:39:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:LEU:C	1:F:65:PRO:HD2	2.39	0.42
1:B:15:TRP:HA	1:B:18:ILE:HD12	2.01	0.42
1:D:79:ASN:HB3	1:D:96:THR:CG2	2.49	0.42
1:B:53:SER:HB3	1:B:88:HIS:HB3	2.02	0.42
1:D:54:GLU:CD	1:D:57:ARG:HH21	2.22	0.42
1:F:105:GLU:O	1:F:109:LYS:HE2	2.19	0.42
1:A:53:SER:OG	1:A:88:HIS:HB3	2.20	0.42
2:A:201:IHP:P2	2:A:201:IHP:O23	2.78	0.42
1:C:49:LEU:HB2	1:C:59:ILE:HD11	2.01	0.41
1:C:94:LYS:CE	1:C:94:LYS:HA	2.50	0.41
1:D:20:LEU:HD12	1:D:26:LYS:CD	2.50	0.41
1:A:17:LYS:HE3	2:A:201:IHP:O42	2.20	0.41
1:C:94:LYS:HA	1:C:94:LYS:HE2	2.02	0.41
1:E:10:GLY:O	1:E:14:LYS:HD2	2.20	0.41
1:D:100:LEU:O	1:D:103:ILE:HG13	2.21	0.41
1:E:20:LEU:HD12	1:E:26:LYS:HB2	2.03	0.41
2:A:201:IHP:O23	2:A:201:IHP:O32	2.39	0.41
1:F:93:VAL:HG12	1:F:98:GLU:HG2	2.02	0.41
1:B:39:GLU:OE1	1:B:39:GLU:HA	2.21	0.41
1:E:7:LEU:HB3	1:E:11:GLU:HB2	2.03	0.41
1:C:13:ASP:HB3	3:C:310:HOH:O	2.20	0.41
1:C:22:PRO:HG3	1:C:97:LYS:HB2	2.03	0.41
1:E:64:GLN:N	1:E:65:PRO:CD	2.83	0.41
1:E:57:ARG:NH1	1:E:85:TYR:OH	2.54	0.41
1:F:89:GLN:HB2	1:F:91:ILE:HG13	2.03	0.41
1:B:67:LEU:HD12	1:B:67:LEU:HA	1.86	0.40
1:F:39:GLU:OE1	1:F:73:GLU:OE1	2.38	0.40
2:A:201:IHP:O24	1:D:26:LYS:NZ	2.41	0.40
1:B:20:LEU:HD12	1:B:26:LYS:CB	2.46	0.40
1:F:19:ARG:HG2	1:F:27:GLN:HG2	2.04	0.40
1:F:19:ARG:O	1:F:95:ASP:HA	2.22	0.40
1:D:0:MET:HG3	1:D:1:GLY:N	2.33	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)
1:C:26:LYS:NZ	2:E:201[A]:IHP:O32[3_545]	1.22	0.98
1:C:26:LYS:NZ	2:E:201[B]:IHP:O33[3_545]	1.22	0.98
1:B:26:LYS:NZ	1:F:27:GLN:OE1[3_546]	2.08	0.12

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	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	B	108/117 (92%)	108 (100%)	0	0	100	100
1	C	109/117 (93%)	105 (96%)	4 (4%)	0	100	100
1	D	111/117 (95%)	110 (99%)	1 (1%)	0	100	100
1	E	106/117 (91%)	99 (93%)	6 (6%)	1 (1%)	14	34
1	F	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
All	All	659/702 (94%)	643 (98%)	15 (2%)	1 (0%)	44	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	109	LYS

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	99/101 (98%)	93 (94%)	6 (6%)	15	35
1	B	94/101 (93%)	93 (99%)	1 (1%)	70	87
1	C	96/101 (95%)	91 (95%)	5 (5%)	19	42
1	D	98/101 (97%)	92 (94%)	6 (6%)	15	35
1	E	93/101 (92%)	89 (96%)	4 (4%)	25	50
1	F	97/101 (96%)	94 (97%)	3 (3%)	35	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	577/606 (95%)	552 (96%)	25 (4%)	25	50

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	76	SER
1	A	102	LYS
1	A	111	LYS
1	A	112	LYS
1	A	113	LYS
1	B	37	SER
1	C	21	ARG
1	C	25	LYS
1	C	75	ARG
1	C	90	ARG
1	C	109	LYS
1	D	0	MET
1	D	25	LYS
1	D	26	LYS
1	D	37	SER
1	D	62[A]	GLN
1	D	62[B]	GLN
1	E	14	LYS
1	E	75	ARG
1	E	94	LYS
1	E	102	LYS
1	F	75	ARG
1	F	94	LYS
1	F	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	B	62	GLN
1	C	68	GLN
1	C	108	ASN
1	E	68	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	E	201[B]	-	36,36,36	2.59	8 (22%)	54,60,60	3.26	13 (24%)
2	IHP	F	201	-	36,36,36	1.95	9 (25%)	54,60,60	1.44	9 (16%)
2	IHP	E	201[A]	-	36,36,36	2.13	7 (19%)	54,60,60	2.10	9 (16%)
2	IHP	D	201	-	36,36,36	1.67	8 (22%)	54,60,60	2.63	16 (29%)
2	IHP	B	201	-	36,36,36	1.77	7 (19%)	54,60,60	2.09	13 (24%)
2	IHP	A	201	-	36,36,36	3.19	11 (30%)	54,60,60	3.10	12 (22%)
2	IHP	C	201[B]	-	36,36,36	2.17	9 (25%)	54,60,60	3.43	13 (24%)
2	IHP	C	201[A]	-	36,36,36	2.20	10 (27%)	54,60,60	2.23	9 (16%)

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	E	201[B]	-	-	5/30/54/54	0/1/1/1
2	IHP	F	201	-	-	4/30/54/54	0/1/1/1
2	IHP	E	201[A]	-	-	7/30/54/54	0/1/1/1
2	IHP	D	201	-	-	8/30/54/54	0/1/1/1
2	IHP	B	201	-	-	5/30/54/54	0/1/1/1
2	IHP	A	201	-	-	9/30/54/54	0/1/1/1
2	IHP	C	201[B]	-	-	6/30/54/54	0/1/1/1
2	IHP	C	201[A]	-	-	6/30/54/54	0/1/1/1

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	IHP	P4-O14	12.19	1.82	1.59
2	E	201[B]	IHP	P1-O11	9.03	1.76	1.59
2	E	201[A]	IHP	P6-O16	7.68	1.73	1.59
2	A	201	IHP	P5-O15	6.60	1.71	1.59
2	E	201[B]	IHP	P2-O12	6.35	1.71	1.59
2	C	201[A]	IHP	P1-O11	5.87	1.70	1.59
2	C	201[A]	IHP	P2-O12	5.80	1.70	1.59
2	C	201[B]	IHP	P6-O16	5.74	1.70	1.59
2	A	201	IHP	C5-C4	5.45	1.63	1.52
2	E	201[B]	IHP	P3-O13	5.29	1.69	1.59
2	C	201[B]	IHP	C2-C1	5.02	1.62	1.52
2	C	201[A]	IHP	P3-O13	4.83	1.68	1.59
2	A	201	IHP	P4-O44	-4.83	1.36	1.54
2	E	201[B]	IHP	P6-O16	4.72	1.68	1.59
2	A	201	IHP	C6-C5	4.68	1.62	1.52
2	E	201[A]	IHP	P4-O14	4.53	1.67	1.59
2	C	201[B]	IHP	C4-C3	4.45	1.61	1.52
2	B	201	IHP	P4-O14	4.40	1.67	1.59
2	A	201	IHP	P6-O16	4.40	1.67	1.59
2	D	201	IHP	P6-O16	4.38	1.67	1.59
2	C	201[B]	IHP	C6-C1	4.37	1.61	1.52
2	B	201	IHP	P6-O16	4.22	1.67	1.59
2	A	201	IHP	C3-C2	4.18	1.60	1.52
2	E	201[A]	IHP	P2-O12	4.14	1.67	1.59
2	F	201	IHP	P2-O12	4.12	1.67	1.59
2	A	201	IHP	P4-O24	4.12	1.63	1.50
2	F	201	IHP	P3-O13	4.06	1.67	1.59
2	C	201[B]	IHP	P5-O15	3.98	1.66	1.59
2	E	201[B]	IHP	P4-O14	3.96	1.66	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201[A]	IHP	P5-O15	3.96	1.66	1.59
2	E	201[B]	IHP	C6-C1	3.87	1.60	1.52
2	F	201	IHP	P5-O15	3.84	1.66	1.59
2	C	201[A]	IHP	P4-O14	3.83	1.66	1.59
2	F	201	IHP	P4-O14	3.75	1.66	1.59
2	F	201	IHP	P1-O11	3.72	1.66	1.59
2	F	201	IHP	P6-O16	3.71	1.66	1.59
2	D	201	IHP	P4-O14	3.65	1.66	1.59
2	C	201[B]	IHP	C3-C2	3.63	1.59	1.52
2	D	201	IHP	P2-O12	3.56	1.66	1.59
2	C	201[B]	IHP	P1-O11	3.56	1.66	1.59
2	E	201[B]	IHP	P5-O15	3.48	1.65	1.59
2	C	201[A]	IHP	P6-O16	3.44	1.65	1.59
2	B	201	IHP	P1-O11	3.44	1.65	1.59
2	B	201	IHP	C2-C1	3.30	1.59	1.52
2	E	201[A]	IHP	P3-O13	3.16	1.65	1.59
2	B	201	IHP	P2-O12	3.13	1.65	1.59
2	C	201[B]	IHP	P3-O13	3.06	1.65	1.59
2	A	201	IHP	P2-O12	3.03	1.65	1.59
2	C	201[A]	IHP	C6-C1	3.02	1.58	1.52
2	E	201[A]	IHP	C2-C1	2.95	1.58	1.52
2	A	201	IHP	P1-O11	2.92	1.64	1.59
2	F	201	IHP	C3-C2	2.91	1.58	1.52
2	F	201	IHP	C6-C5	2.86	1.58	1.52
2	E	201[A]	IHP	P1-O11	2.79	1.64	1.59
2	D	201	IHP	P1-O11	2.78	1.64	1.59
2	D	201	IHP	P3-O13	2.76	1.64	1.59
2	B	201	IHP	P3-O13	2.60	1.64	1.59
2	E	201[B]	IHP	C4-C3	2.48	1.57	1.52
2	C	201[A]	IHP	C5-C4	2.46	1.57	1.52
2	E	201[A]	IHP	P5-O15	2.42	1.63	1.59
2	A	201	IHP	P3-O13	2.38	1.63	1.59
2	D	201	IHP	C2-C1	2.32	1.57	1.52
2	C	201[A]	IHP	C6-C5	2.22	1.56	1.52
2	C	201[A]	IHP	C4-C3	2.19	1.56	1.52
2	D	201	IHP	P5-O15	2.19	1.63	1.59
2	D	201	IHP	C3-C2	2.14	1.56	1.52
2	C	201[B]	IHP	P2-O12	2.07	1.63	1.59
2	F	201	IHP	C6-C1	2.06	1.56	1.52
2	B	201	IHP	P5-O15	2.05	1.63	1.59

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201[B]	IHP	C6-C5-C4	13.57	140.11	110.41
2	E	201[B]	IHP	C3-C2-C1	13.13	139.17	110.41
2	C	201[B]	IHP	O14-C4-C5	11.63	136.11	108.69
2	E	201[B]	IHP	O16-C6-C5	11.35	135.44	108.69
2	D	201	IHP	C5-C6-C1	-9.80	88.96	110.41
2	C	201[B]	IHP	O16-C6-C1	9.31	130.64	108.69
2	C	201[A]	IHP	C3-C2-C1	9.29	130.76	110.41
2	C	201[A]	IHP	O11-C1-C2	9.28	130.56	108.69
2	A	201	IHP	O15-C5-C4	9.13	130.20	108.69
2	E	201[A]	IHP	O16-C6-C1	9.07	130.06	108.69
2	A	201	IHP	O14-C4-C5	8.75	129.31	108.69
2	A	201	IHP	C4-C3-C2	8.51	129.04	110.41
2	E	201[B]	IHP	C6-C5-C4	8.50	129.02	110.41
2	A	201	IHP	O14-P4-O24	7.76	139.34	109.39
2	E	201[A]	IHP	C6-C1-C2	7.41	126.63	110.41
2	A	201	IHP	C6-C5-C4	7.16	126.09	110.41
2	E	201[B]	IHP	O13-C3-C2	7.02	125.23	108.69
2	C	201[B]	IHP	O12-C2-C3	7.01	125.20	108.69
2	B	201	IHP	O16-C6-C1	6.95	125.07	108.69
2	D	201	IHP	O16-C6-C5	6.42	123.82	108.69
2	C	201[B]	IHP	C5-C6-C1	-5.92	97.44	110.41
2	C	201[B]	IHP	C6-C1-C2	5.89	123.32	110.41
2	A	201	IHP	C3-C2-C1	5.78	123.07	110.41
2	B	201	IHP	O14-C4-C3	5.43	121.48	108.69
2	D	201	IHP	C6-C1-C2	5.35	122.13	110.41
2	E	201[B]	IHP	O16-C6-C1	-5.23	96.36	108.69
2	D	201	IHP	C6-C5-C4	5.18	121.76	110.41
2	D	201	IHP	O15-C5-C6	5.17	120.88	108.69
2	E	201[B]	IHP	O11-C1-C2	5.12	120.75	108.69
2	E	201[A]	IHP	C5-C6-C1	-5.01	99.45	110.41
2	F	201	IHP	O12-C2-C1	4.97	120.39	108.69
2	C	201[B]	IHP	O11-C1-C2	4.95	120.36	108.69
2	A	201	IHP	O15-C5-C6	-4.90	97.13	108.69
2	A	201	IHP	C5-C4-C3	-4.87	99.76	110.41
2	B	201	IHP	O12-C2-C3	4.64	119.63	108.69
2	D	201	IHP	O12-C2-C3	4.54	119.38	108.69
2	E	201[B]	IHP	O14-C4-C3	4.49	119.27	108.69
2	B	201	IHP	C6-C1-C2	4.45	120.16	110.41
2	A	201	IHP	O13-C3-C4	-4.42	98.26	108.69
2	D	201	IHP	C5-C4-C3	-4.34	100.90	110.41
2	D	201	IHP	C3-C2-C1	4.19	119.58	110.41
2	A	201	IHP	O44-P4-O24	-4.16	94.39	110.68
2	C	201[B]	IHP	C4-C3-C2	4.13	119.46	110.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201[A]	IHP	C6-C5-C4	4.03	119.24	110.41
2	B	201	IHP	C5-C6-C1	-4.02	101.62	110.41
2	D	201	IHP	O11-C1-C6	3.99	118.09	108.69
2	D	201	IHP	O14-C4-C5	3.93	117.95	108.69
2	C	201[A]	IHP	O13-C3-C2	3.89	117.85	108.69
2	E	201[B]	IHP	O41-P1-O11	3.64	122.30	105.99
2	F	201	IHP	O15-C5-C4	3.60	117.17	108.69
2	B	201	IHP	C3-C2-C1	3.57	118.24	110.41
2	B	201	IHP	C4-C3-C2	3.57	118.22	110.41
2	D	201	IHP	O16-C6-C1	3.54	117.03	108.69
2	E	201[A]	IHP	O36-P6-O16	3.51	121.70	105.99
2	B	201	IHP	O36-P6-O16	3.46	121.49	105.99
2	C	201[A]	IHP	O13-C3-C4	3.35	116.58	108.69
2	B	201	IHP	O14-C4-C5	3.28	116.42	108.69
2	A	201	IHP	O44-P4-O34	-3.26	95.17	107.64
2	B	201	IHP	O12-C2-C1	-3.22	101.09	108.69
2	D	201	IHP	O13-C3-C2	3.20	116.23	108.69
2	B	201	IHP	C5-C4-C3	-3.18	103.45	110.41
2	F	201	IHP	O11-C1-C6	3.17	116.15	108.69
2	E	201[A]	IHP	O14-C4-C5	3.17	116.15	108.69
2	C	201[B]	IHP	C3-C2-C1	3.16	117.33	110.41
2	C	201[B]	IHP	C5-C4-C3	-3.13	103.57	110.41
2	C	201[B]	IHP	O11-C1-C6	-3.12	101.34	108.69
2	E	201[A]	IHP	C6-C5-C4	3.12	117.23	110.41
2	D	201	IHP	C4-C3-C2	2.80	116.53	110.41
2	D	201	IHP	O14-C4-C3	2.76	115.20	108.69
2	F	201	IHP	O14-C4-C3	2.74	115.14	108.69
2	B	201	IHP	O13-C3-C4	2.74	115.14	108.69
2	F	201	IHP	O16-C6-C5	2.72	115.09	108.69
2	C	201[A]	IHP	O16-C6-C1	2.70	115.06	108.69
2	E	201[B]	IHP	O11-C1-C6	2.67	114.98	108.69
2	C	201[B]	IHP	O16-C6-C5	2.66	114.96	108.69
2	B	201	IHP	C6-C5-C4	2.62	116.14	110.41
2	E	201[B]	IHP	O14-C4-C5	-2.60	102.56	108.69
2	C	201[A]	IHP	O14-C4-C5	2.58	114.77	108.69
2	A	201	IHP	O13-C3-C2	-2.50	102.81	108.69
2	F	201	IHP	O13-C3-C2	2.45	114.45	108.69
2	F	201	IHP	C5-C4-C3	-2.44	105.08	110.41
2	F	201	IHP	O11-C1-C2	2.41	114.36	108.69
2	E	201[A]	IHP	C4-C3-C2	2.36	115.58	110.41
2	F	201	IHP	O14-C4-C5	2.35	114.23	108.69
2	C	201[A]	IHP	O15-C5-C6	2.29	114.08	108.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	IHP	O12-C2-C1	2.25	114.00	108.69
2	C	201[B]	IHP	O16-P6-O26	2.21	117.92	109.39
2	E	201[B]	IHP	O41-P1-O21	-2.20	102.05	110.68
2	E	201[A]	IHP	C3-C2-C1	2.18	115.19	110.41
2	E	201[B]	IHP	O44-P4-O14	2.18	115.74	105.99
2	D	201	IHP	O13-C3-C4	2.14	113.74	108.69
2	C	201[A]	IHP	O12-C2-C3	2.12	113.68	108.69
2	E	201[A]	IHP	O11-C1-C2	-2.05	103.86	108.69
2	E	201[B]	IHP	O12-P2-O22	2.02	117.21	109.39

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	IHP	C6-C5-O15-P5
2	A	201	IHP	C1-O11-P1-O21
2	A	201	IHP	C2-O12-P2-O22
2	B	201	IHP	C3-C2-O12-P2
2	B	201	IHP	C5-O15-P5-O25
2	C	201[A]	IHP	C5-O15-P5-O25
2	C	201[B]	IHP	C3-C2-O12-P2
2	C	201[B]	IHP	C5-C4-O14-P4
2	C	201[B]	IHP	C4-C5-O15-P5
2	D	201	IHP	C3-C2-O12-P2
2	D	201	IHP	C6-C5-O15-P5
2	D	201	IHP	C3-O13-P3-O23
2	D	201	IHP	C5-O15-P5-O25
2	E	201[A]	IHP	C1-O11-P1-O21
2	E	201[B]	IHP	C5-C6-O16-P6
2	E	201[B]	IHP	C2-O12-P2-O32
2	F	201	IHP	C2-O12-P2-O42
2	F	201	IHP	C3-O13-P3-O23
2	F	201	IHP	C4-O14-P4-O24
2	C	201[A]	IHP	C1-C2-O12-P2
2	E	201[B]	IHP	C4-C5-O15-P5
2	A	201	IHP	C4-O14-P4-O24
2	B	201	IHP	C4-O14-P4-O24
2	E	201[A]	IHP	C4-O14-P4-O24
2	A	201	IHP	C1-O11-P1-O41
2	B	201	IHP	C3-O13-P3-O43
2	C	201[A]	IHP	C4-O14-P4-O34
2	D	201	IHP	C1-O11-P1-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	201	IHP	C5-O15-P5-O45
2	E	201[B]	IHP	C3-C4-O14-P4
2	E	201[A]	IHP	C6-C1-O11-P1
2	A	201	IHP	C1-C6-O16-P6
2	E	201[A]	IHP	C6-C5-O15-P5
2	A	201	IHP	C5-O15-P5-O25
2	B	201	IHP	C2-O12-P2-O22
2	D	201	IHP	C2-O12-P2-O22
2	E	201[A]	IHP	C6-O16-P6-O26
2	F	201	IHP	C6-O16-P6-O26
2	A	201	IHP	C2-O12-P2-O32
2	A	201	IHP	C5-O15-P5-O35
2	C	201[A]	IHP	C4-C5-O15-P5
2	C	201[A]	IHP	C2-O12-P2-O42
2	C	201[A]	IHP	C5-O15-P5-O45
2	C	201[B]	IHP	C1-O11-P1-O41
2	C	201[B]	IHP	C2-O12-P2-O42
2	C	201[B]	IHP	C4-O14-P4-O44
2	D	201	IHP	C2-O12-P2-O42
2	E	201[A]	IHP	C3-C2-O12-P2
2	E	201[A]	IHP	C1-O11-P1-O31
2	E	201[B]	IHP	C6-O16-P6-O36

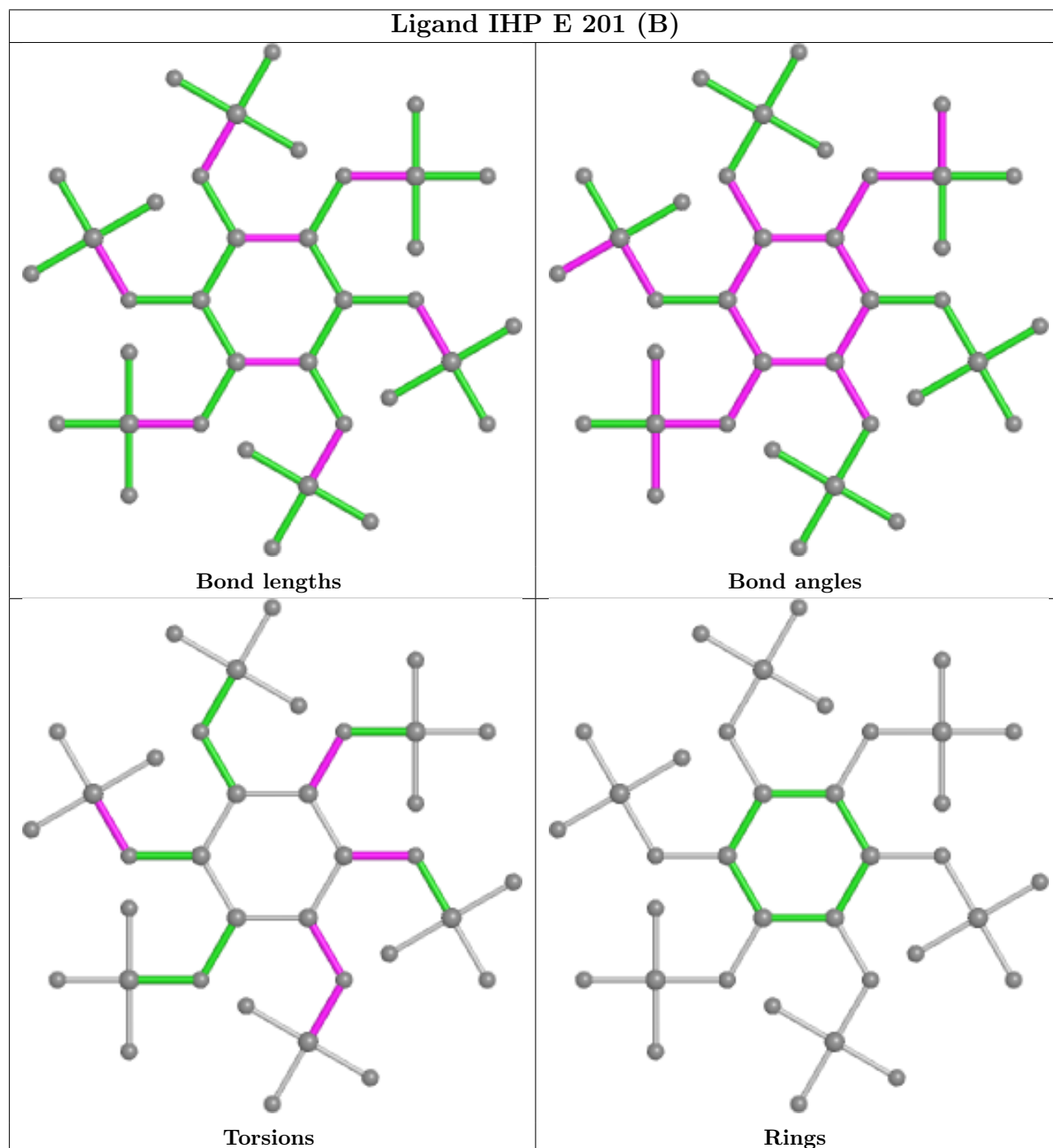
There are no ring outliers.

6 monomers are involved in 23 short contacts:

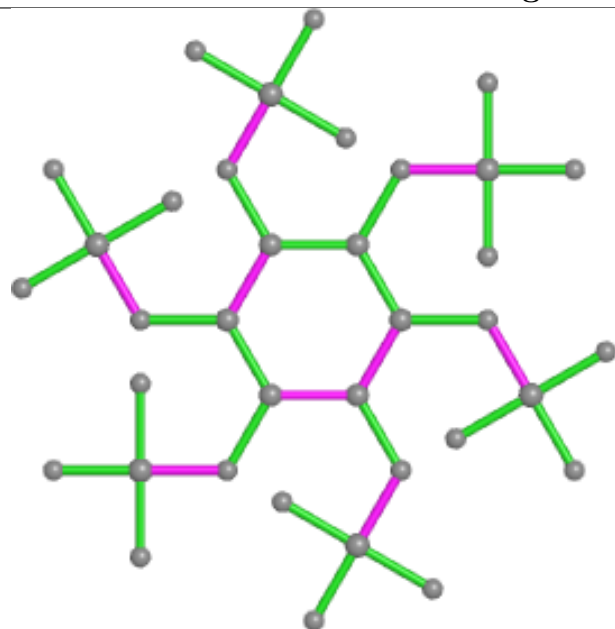
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201[B]	IHP	2	1
2	F	201	IHP	1	0
2	E	201[A]	IHP	3	1
2	D	201	IHP	1	0
2	A	201	IHP	8	0
2	C	201[B]	IHP	6	0

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

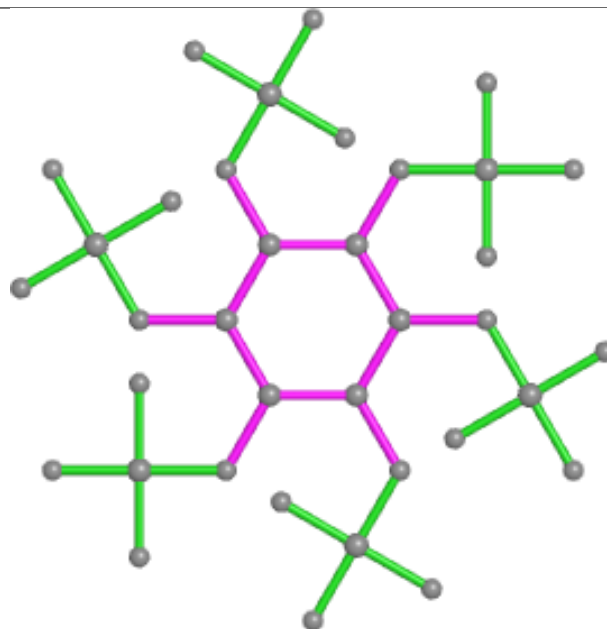
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



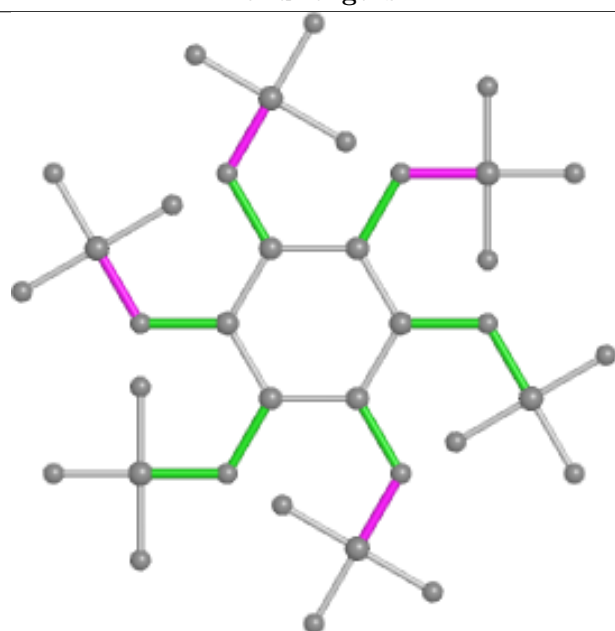
Ligand IHP F 201



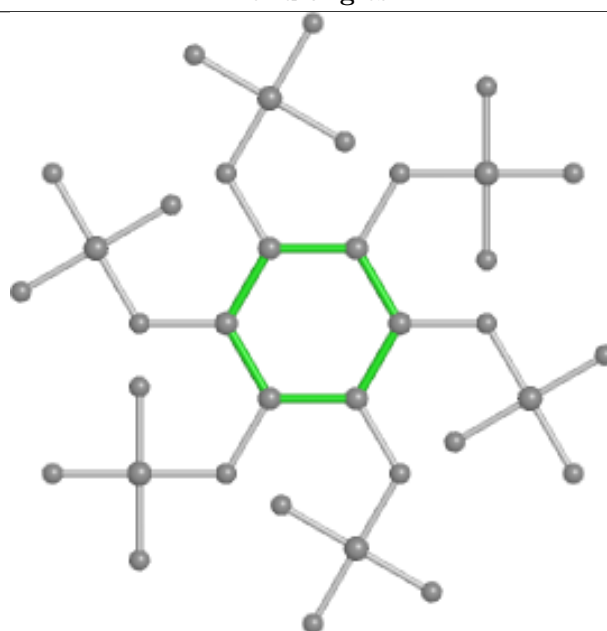
Bond lengths



Bond angles

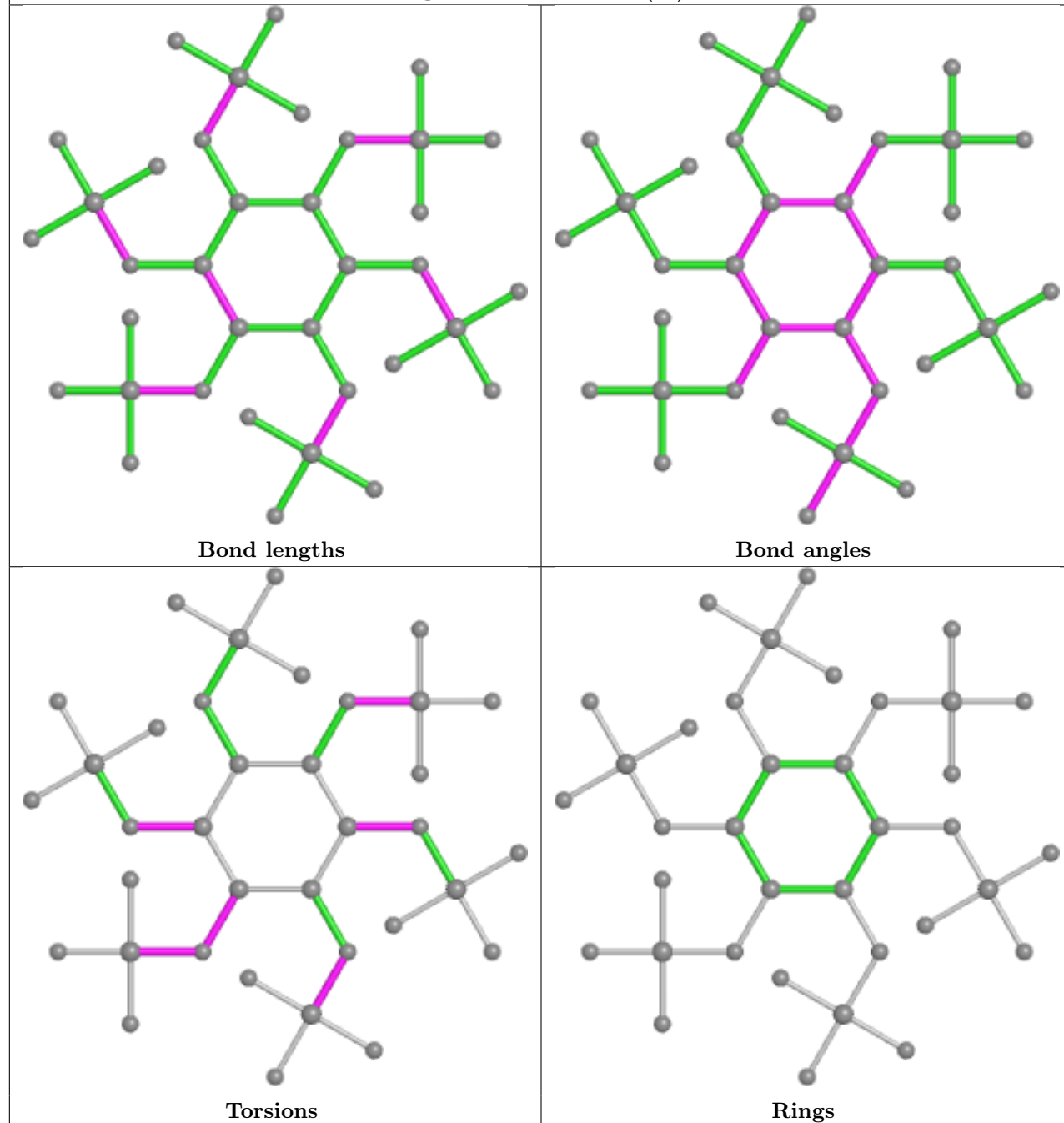


Torsions

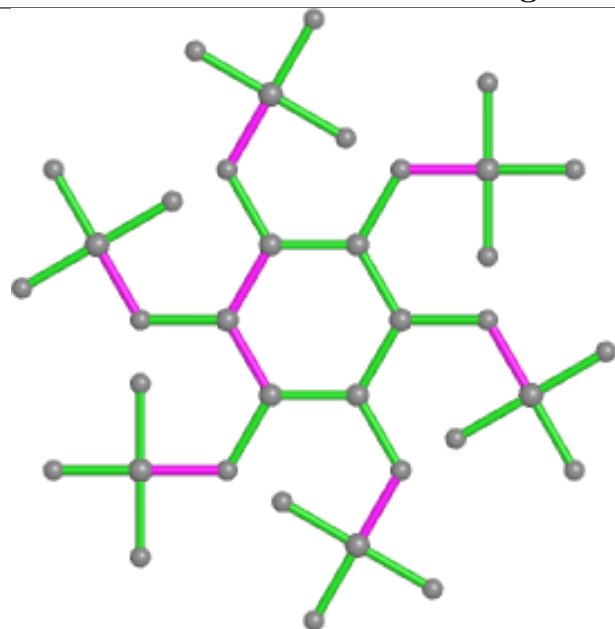


Rings

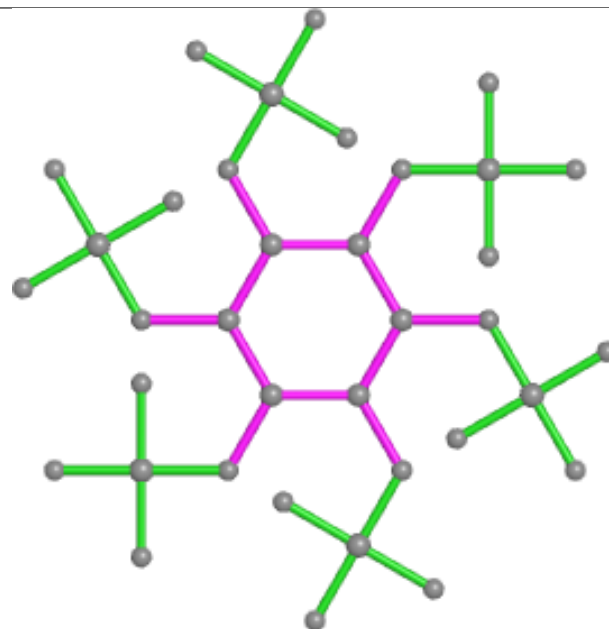
Ligand IHP E 201 (A)



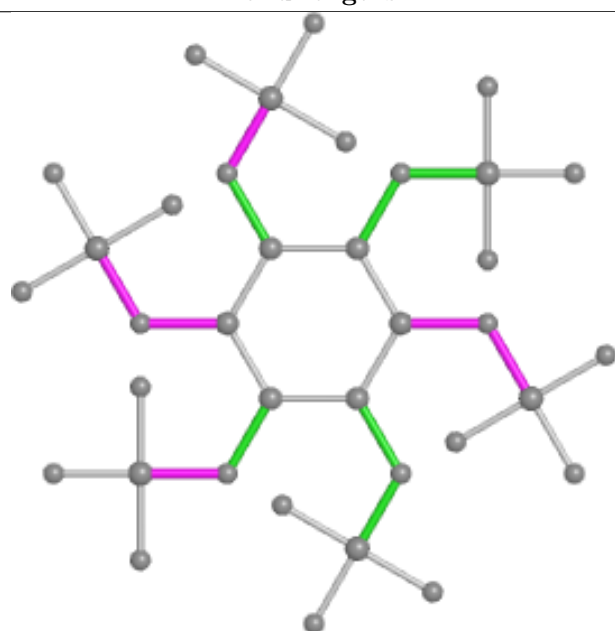
Ligand IHP D 201



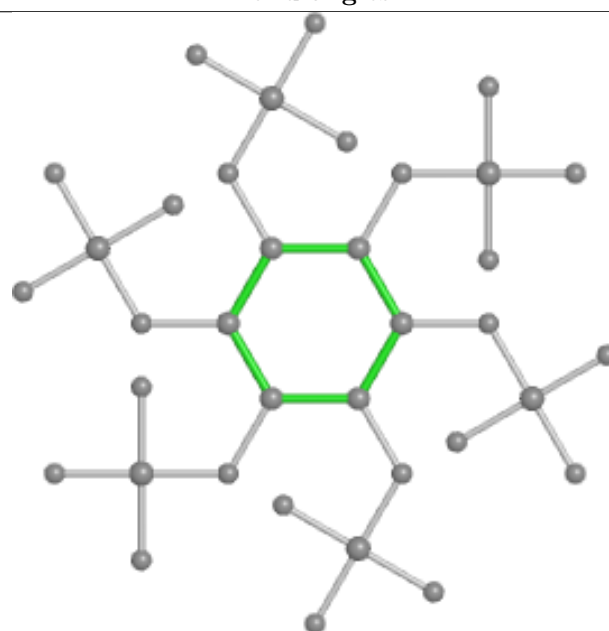
Bond lengths



Bond angles

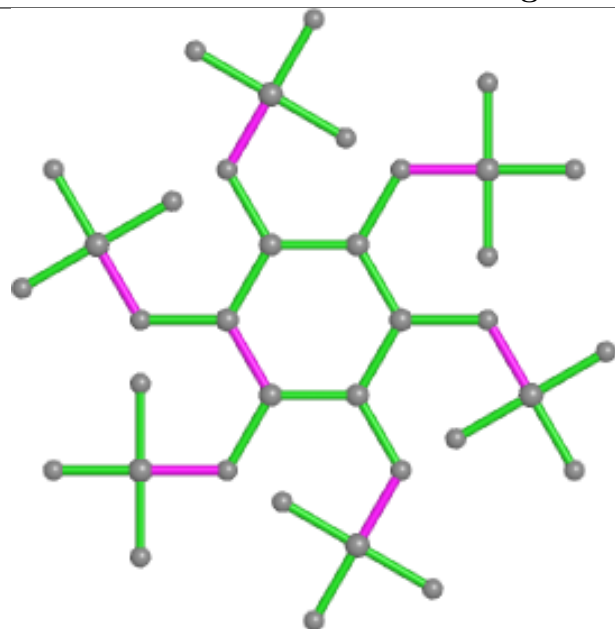


Torsions

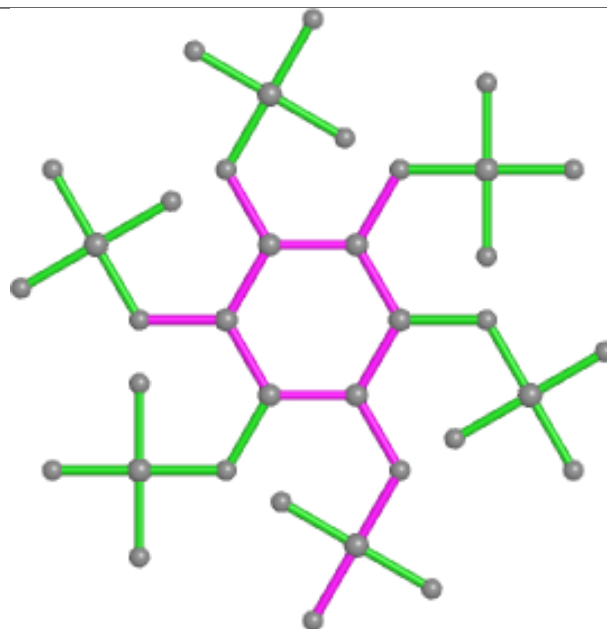


Rings

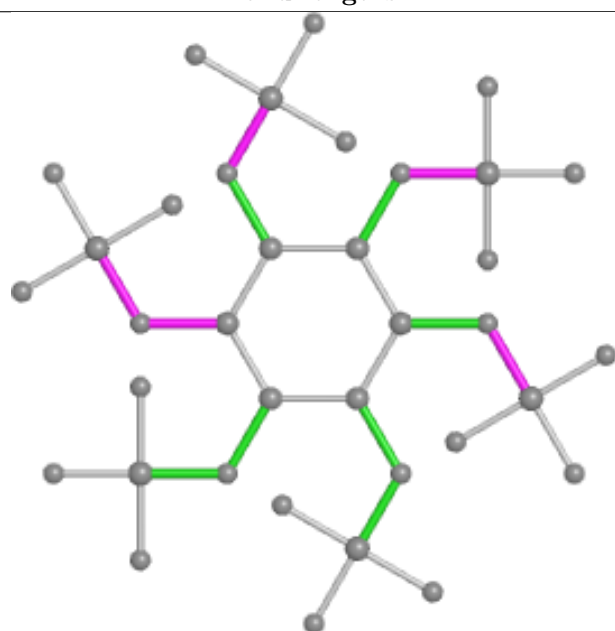
Ligand IHP B 201



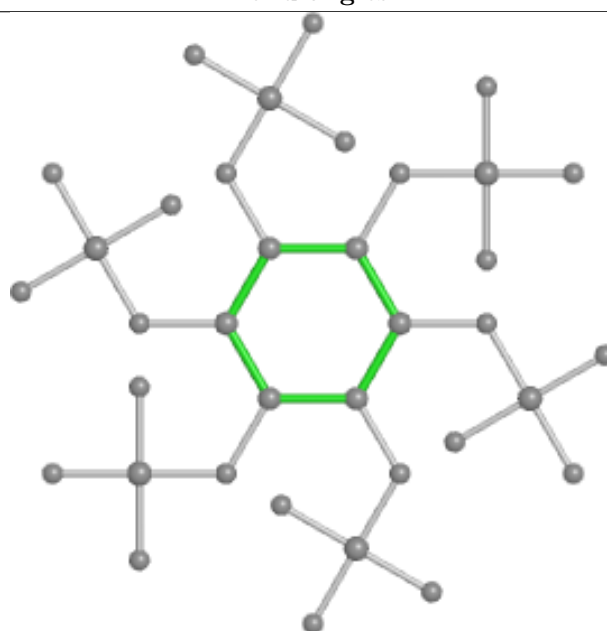
Bond lengths



Bond angles

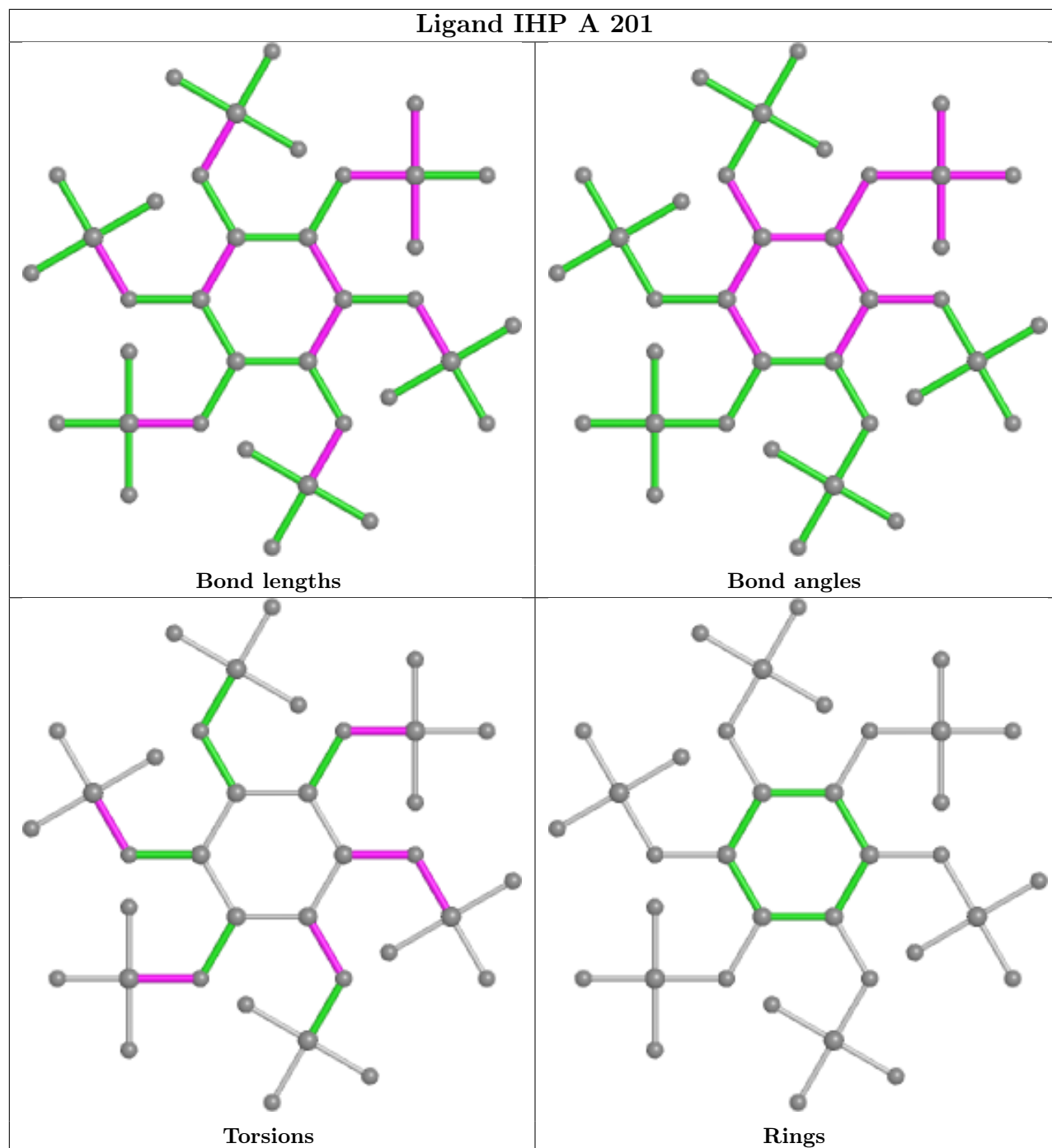


Torsions

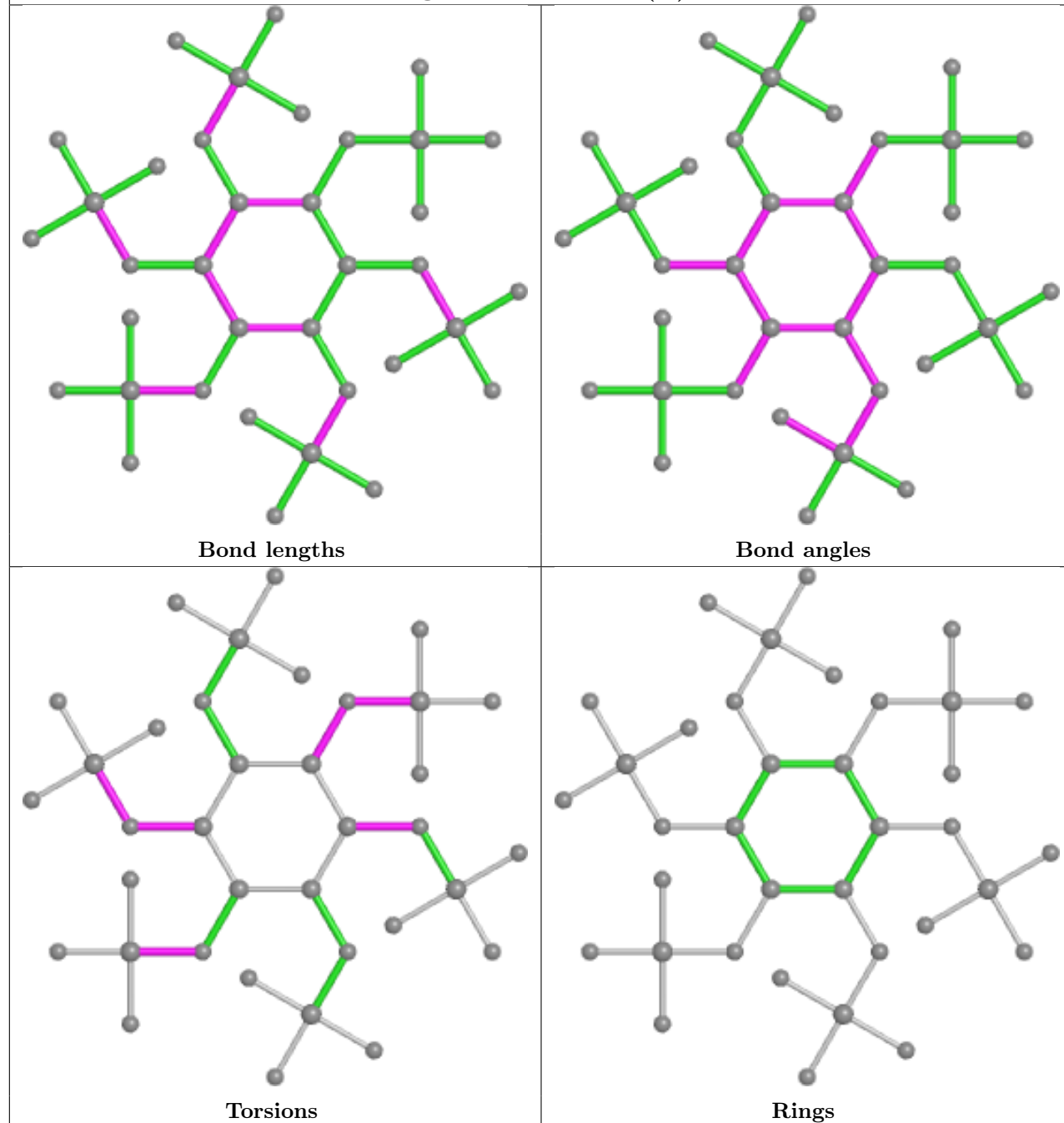


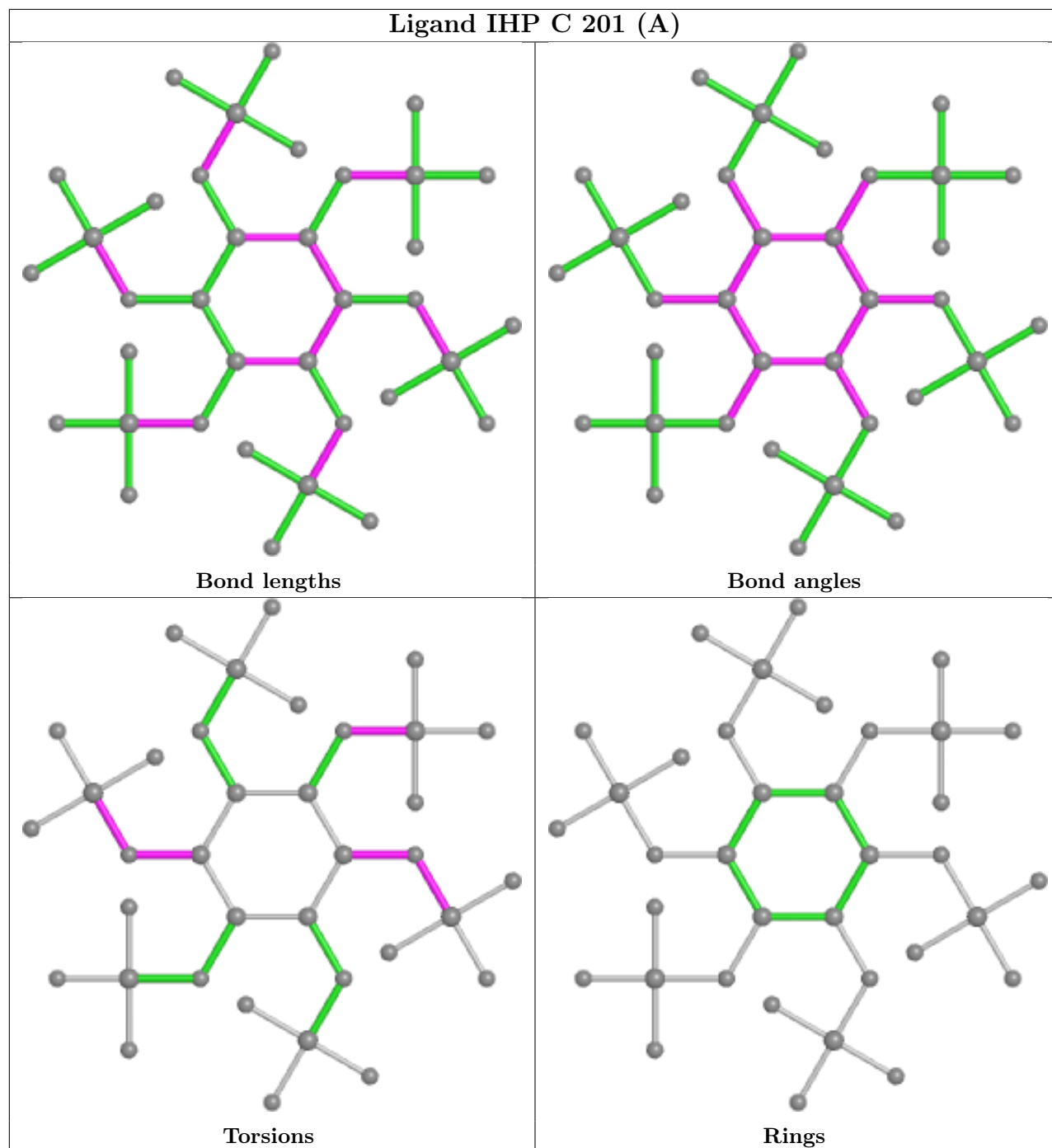
Rings

Ligand IHP A 201



Ligand IHP C 201 (B)





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	116/117 (99%)	0.27	4 (3%)	48	47	31, 59, 113, 167	1 (0%)
1	B	109/117 (93%)	0.27	7 (6%)	27	25	30, 60, 117, 131	1 (0%)
1	C	111/117 (94%)	0.11	3 (2%)	56	55	43, 60, 106, 136	0
1	D	110/117 (94%)	0.04	8 (7%)	22	21	31, 51, 89, 109	3 (2%)
1	E	108/117 (92%)	0.27	4 (3%)	45	44	39, 62, 110, 138	0
1	F	111/117 (94%)	0.14	2 (1%)	67	67	29, 61, 105, 141	1 (0%)
All	All	665/702 (94%)	0.18	28 (4%)	41	40	29, 59, 111, 167	6 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	110	SER	6.8
1	E	4	ALA	4.8
1	D	-1	SER	4.6
1	B	2	ALA	4.3
1	A	0	MET	3.4
1	C	2	ALA	3.3
1	B	4	ALA	3.2
1	B	21[A]	ARG	3.2
1	F	3	ARG	3.1
1	D	0	MET	3.1
1	D	26	LYS	3.0
1	D	108	ASN	2.9
1	B	3	ARG	2.8
1	E	5	SER	2.7
1	D	62[A]	GLN	2.7
1	C	-1	SER	2.5
1	D	75[A]	ARG	2.5
1	A	4	ALA	2.4
1	F	62	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1	GLY	2.4
1	A	90[A]	ARG	2.3
1	C	90	ARG	2.3
1	E	3	ARG	2.3
1	B	72	GLU	2.2
1	D	5	SER	2.2
1	D	25	LYS	2.2
1	A	114	ALA	2.0
1	B	13	ASP	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](#)

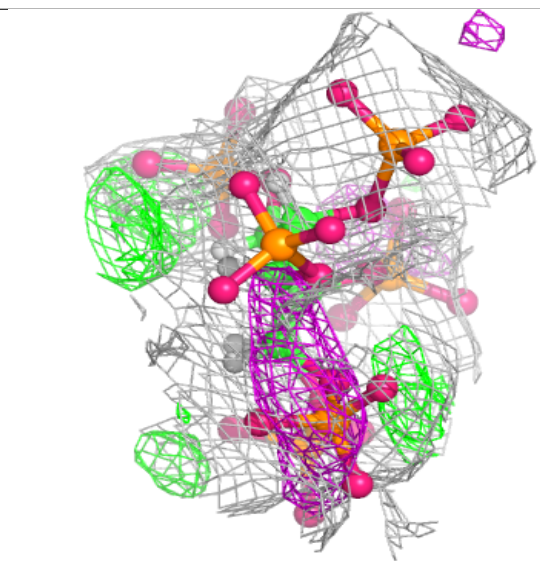
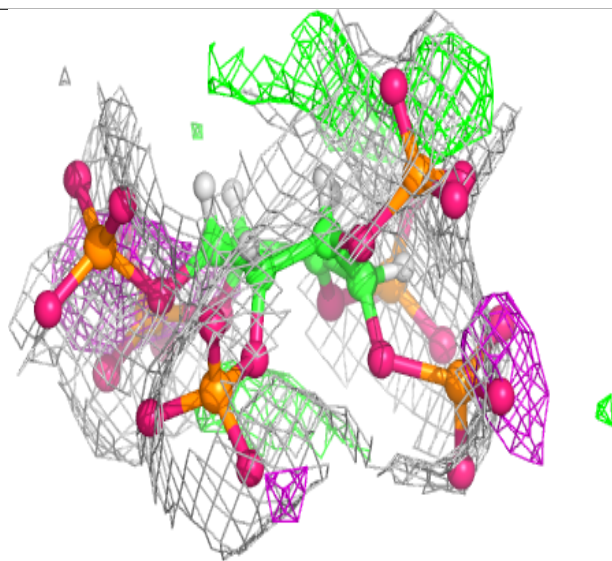
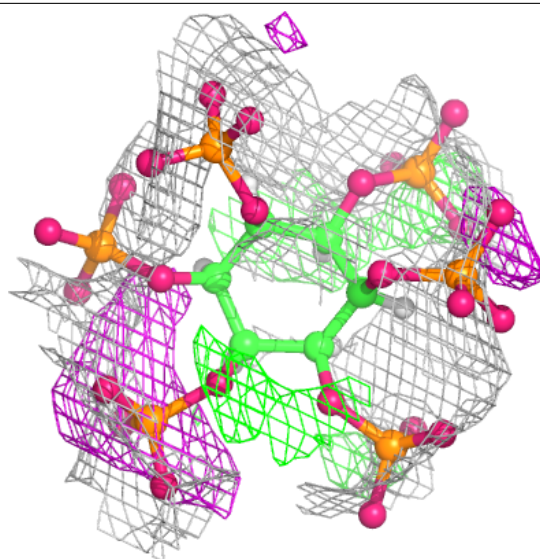
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IHP	E	201[A]	36/36	0.14	0.18	119,126,152,153	42
2	IHP	E	201[B]	36/36	0.14	0.18	118,126,151,153	42
2	IHP	A	201	36/36	0.58	0.17	177,182,189,191	0
2	IHP	D	201	36/36	0.68	0.14	137,162,170,170	0
2	IHP	F	201	36/36	0.73	0.17	106,115,138,140	42
2	IHP	B	201	36/36	0.76	0.14	105,118,140,142	0
2	IHP	C	201[A]	36/36	0.78	0.14	135,140,167,169	42
2	IHP	C	201[B]	36/36	0.78	0.14	134,140,167,169	42

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.

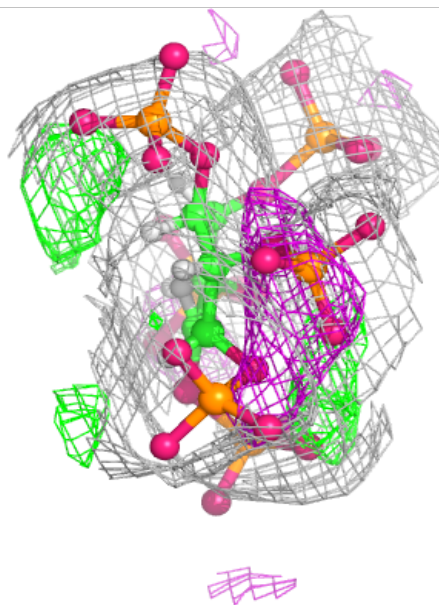
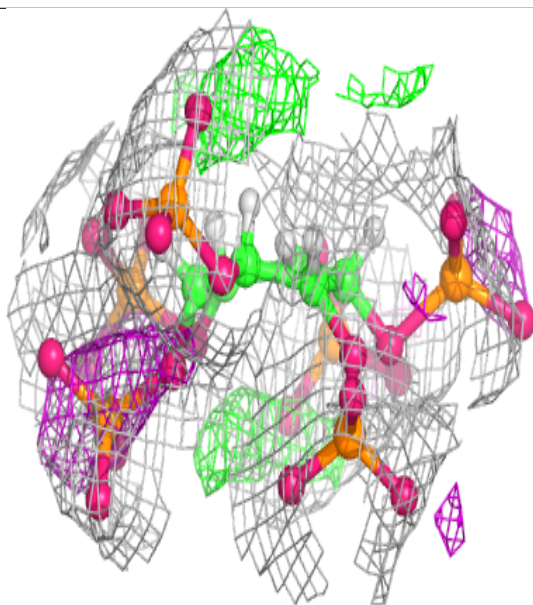
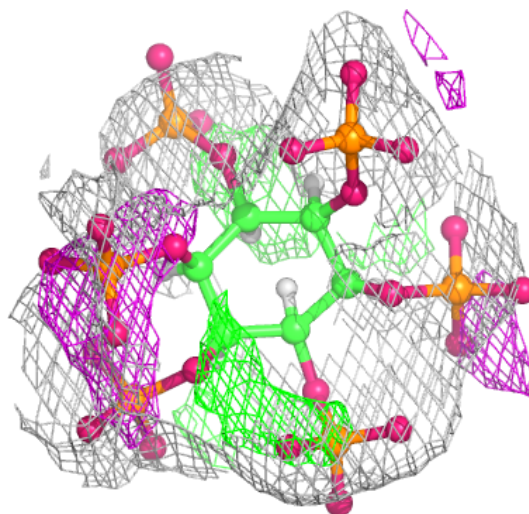
Electron density around IHP E 201 (A):

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



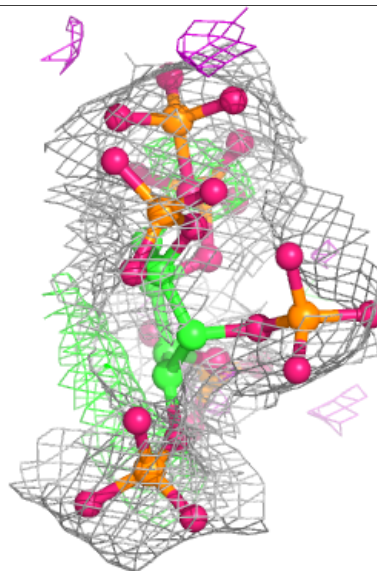
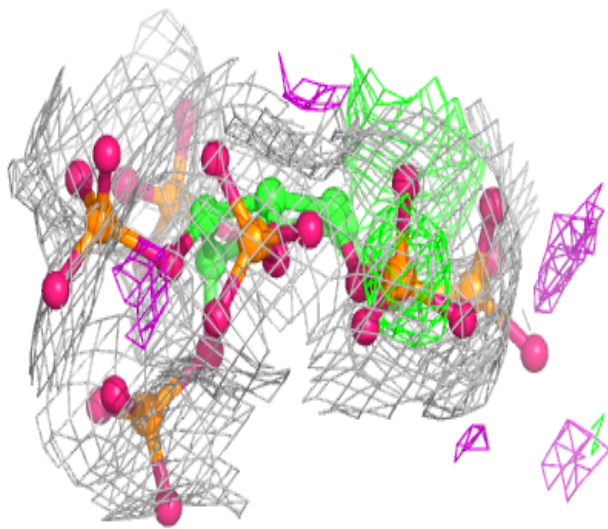
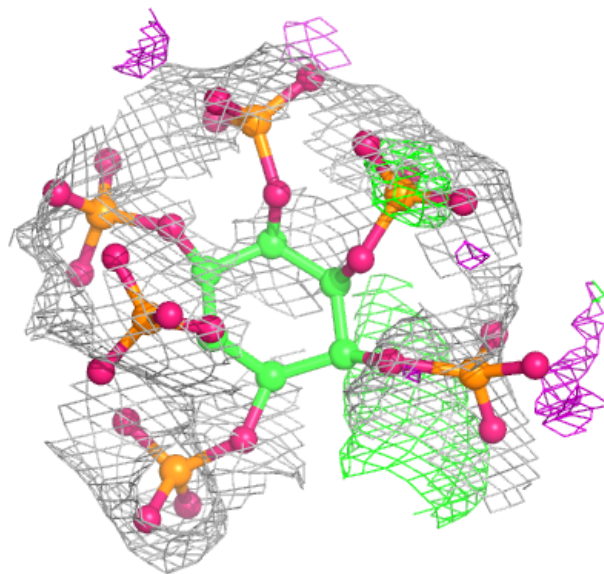
Electron density around IHP E 201 (B):

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



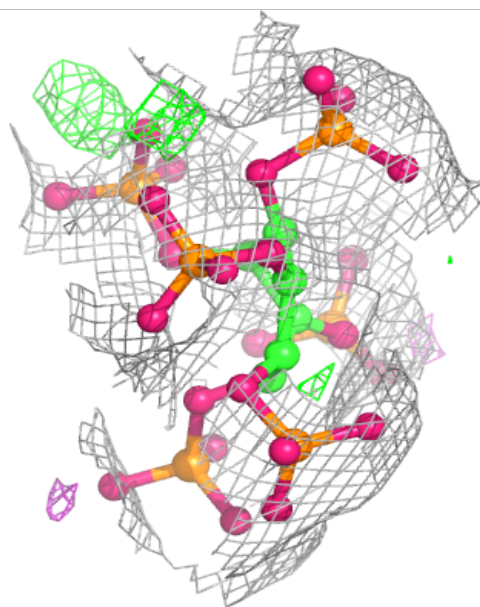
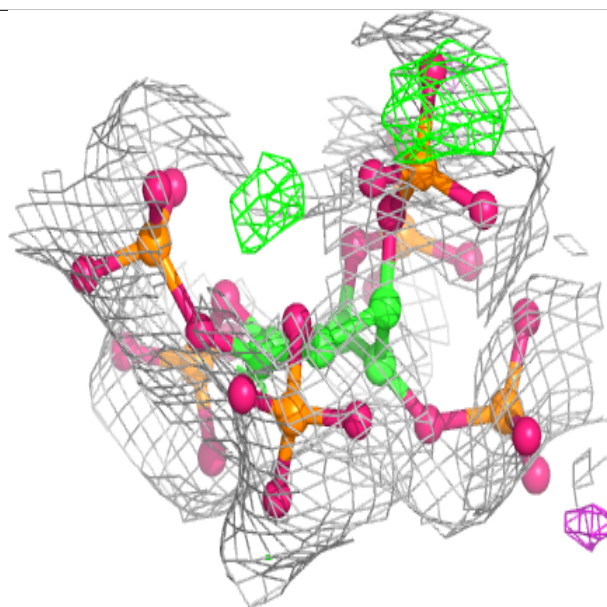
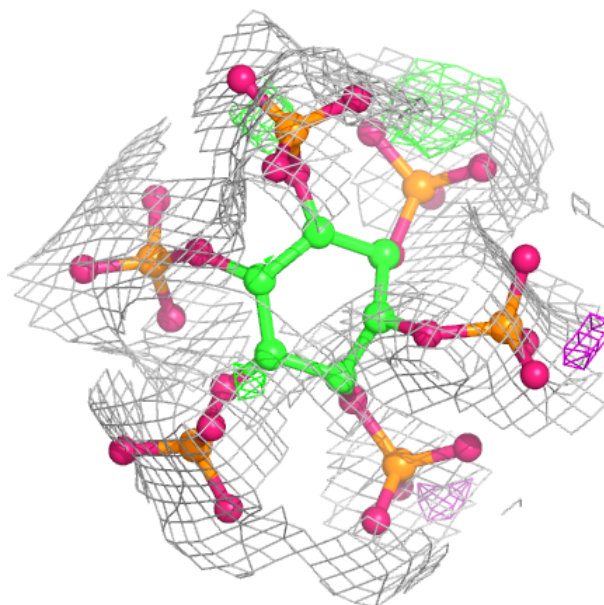
Electron density around IHP A 201:

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



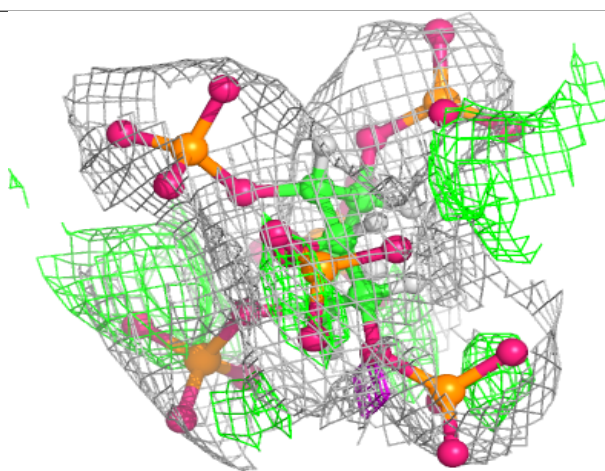
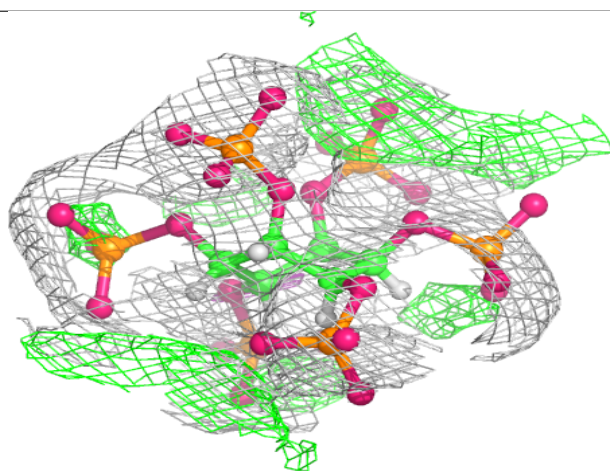
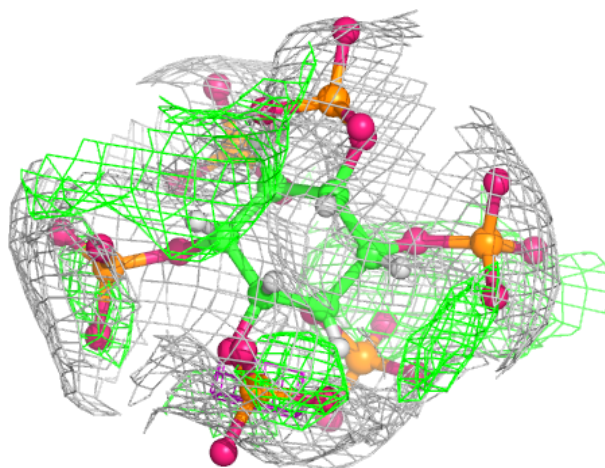
Electron density around IHP D 201:

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



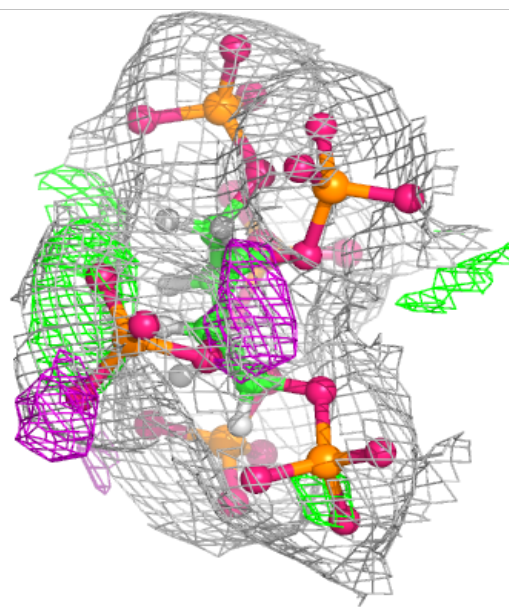
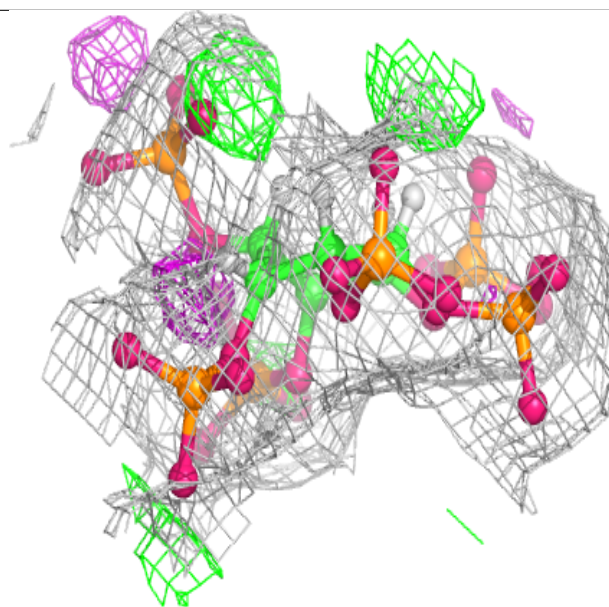
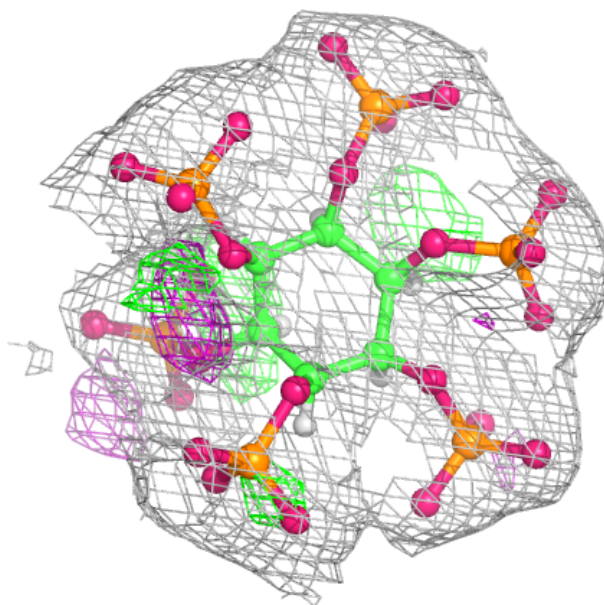
Electron density around IHP F 201:

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



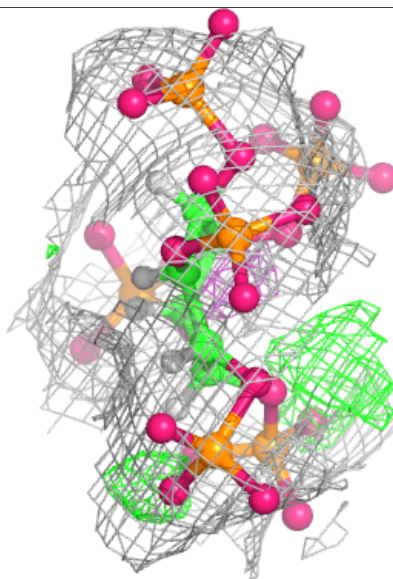
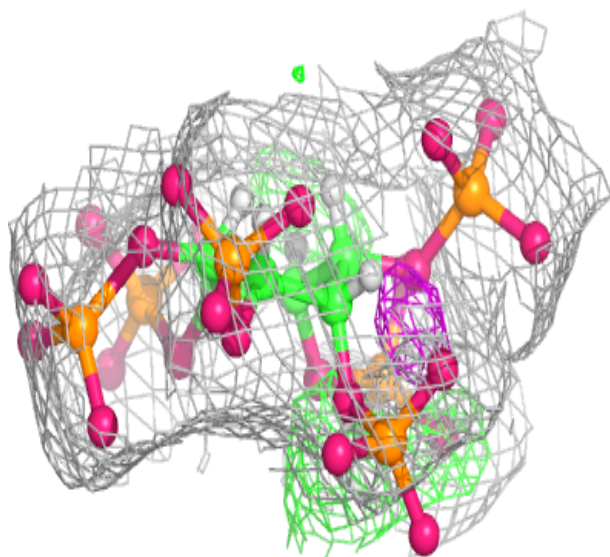
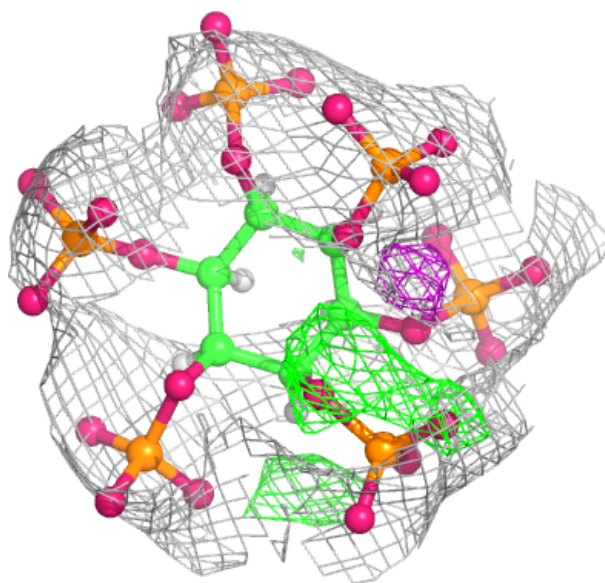
Electron density around IHP B 201:

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



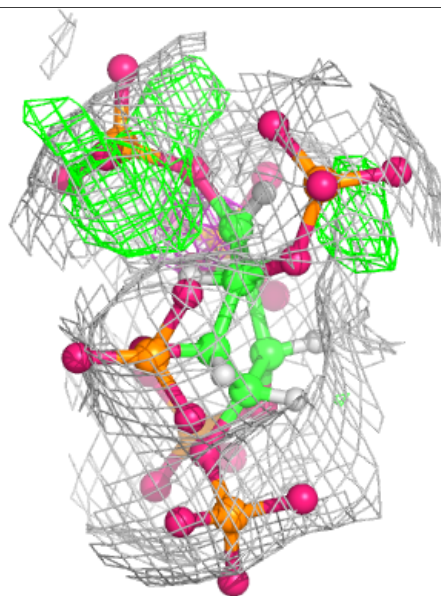
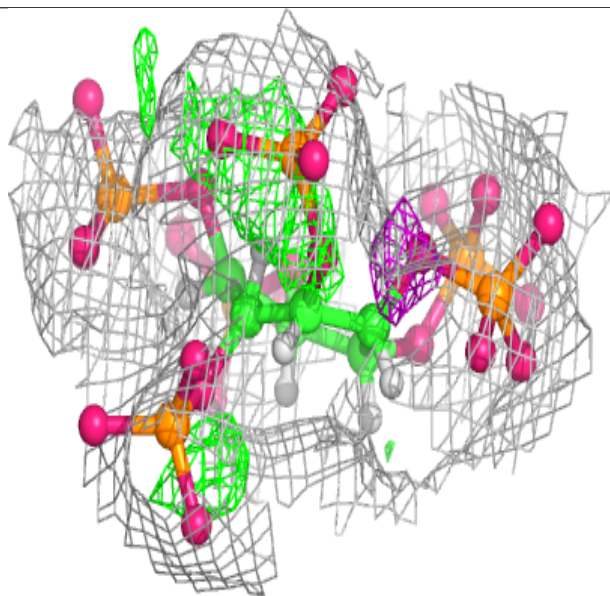
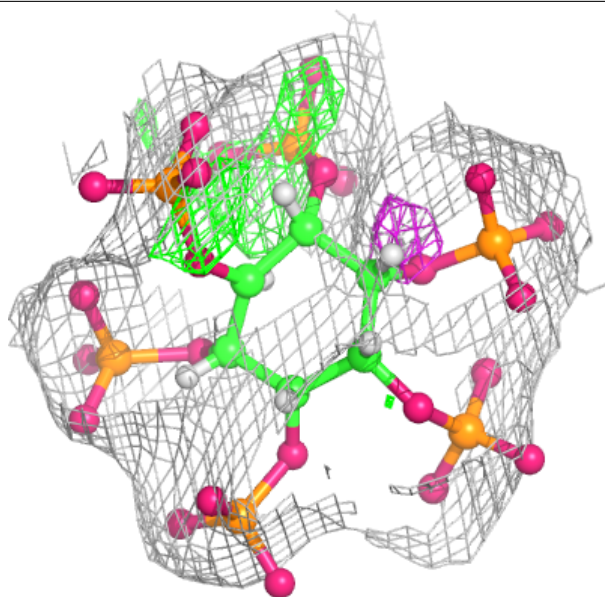
Electron density around IHP C 201 (A):

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



Electron density around IHP C 201 (B):

$2mF_o-DF_c$ (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.