



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:14 AM UTC

PDB ID : 9TFY / pdb_00009tfy
Title : Arabidopsis thaliana Casein Kinase 2 (CK2) alpha1 - beta1 complex bound to inositol hexakisphosphate (InsP6)
Authors : Sturm, K.; Hothorn, M.
Deposited on : 2025-11-27
Resolution : 5.50 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

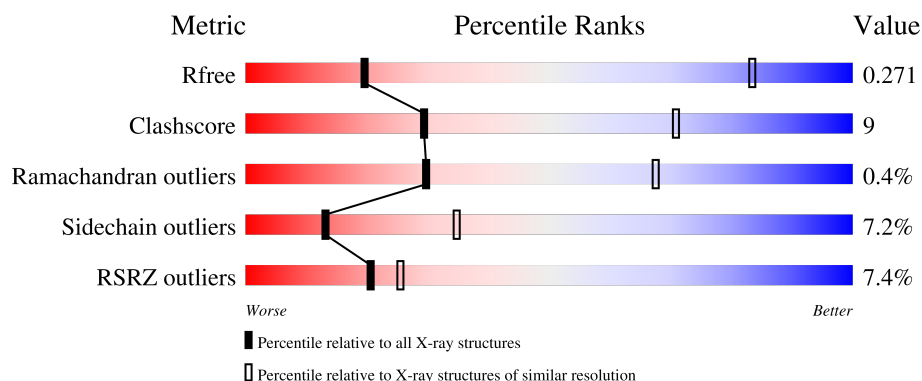
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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 $\leq 5\%$. 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	344	10% 83% 12% ..
1	B	344	8% 83% 12% ..
2	C	194	4% 64% 32% ..
2	D	194	4% 62% 32% 5% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8722 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 Casein kinase II subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2774	1783	478	502	11			
1	B	335	Total	C	N	O	S	0	1	0
			2774	1783	478	502	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	410	ALA	-	expression tag	UNP Q08467
A	411	ALA	-	expression tag	UNP Q08467
A	412	ALA	-	expression tag	UNP Q08467
A	413	LEU	-	expression tag	UNP Q08467
A	414	GLU	-	expression tag	UNP Q08467
A	415	HIS	-	expression tag	UNP Q08467
A	416	HIS	-	expression tag	UNP Q08467
A	417	HIS	-	expression tag	UNP Q08467
A	418	HIS	-	expression tag	UNP Q08467
A	419	HIS	-	expression tag	UNP Q08467
A	420	HIS	-	expression tag	UNP Q08467
B	410	ALA	-	expression tag	UNP Q08467
B	411	ALA	-	expression tag	UNP Q08467
B	412	ALA	-	expression tag	UNP Q08467
B	413	LEU	-	expression tag	UNP Q08467
B	414	GLU	-	expression tag	UNP Q08467
B	415	HIS	-	expression tag	UNP Q08467
B	416	HIS	-	expression tag	UNP Q08467
B	417	HIS	-	expression tag	UNP Q08467
B	418	HIS	-	expression tag	UNP Q08467
B	419	HIS	-	expression tag	UNP Q08467
B	420	HIS	-	expression tag	UNP Q08467

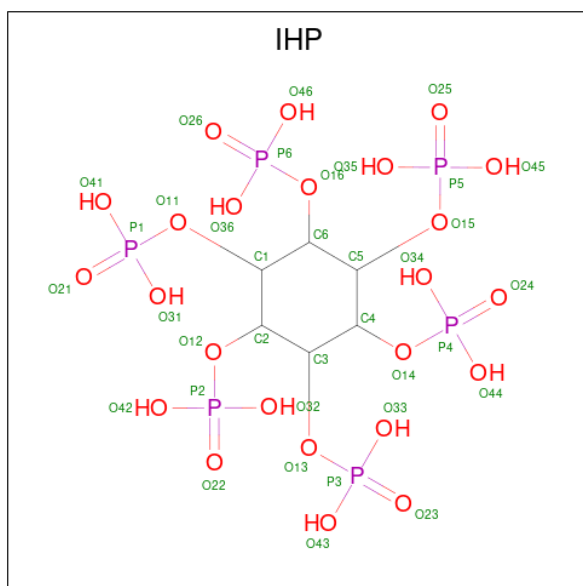
- Molecule 2 is a protein called Casein kinase II subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	191	Total	C	N	O	S	0	0	0
			1550	997	247	293	13			
2	D	191	Total	C	N	O	S	0	0	0
			1550	997	247	293	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	94	MET	-	initiating methionine	UNP P40228
D	94	MET	-	initiating methionine	UNP P40228

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



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

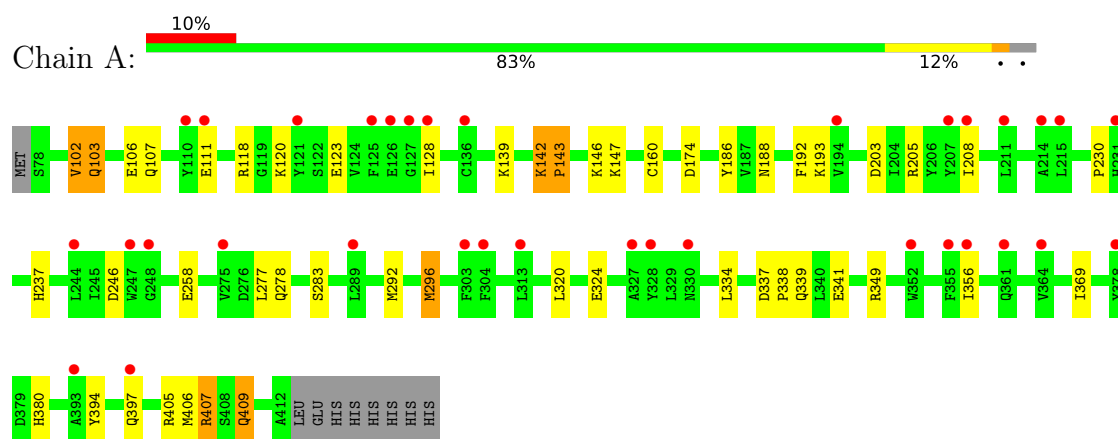
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

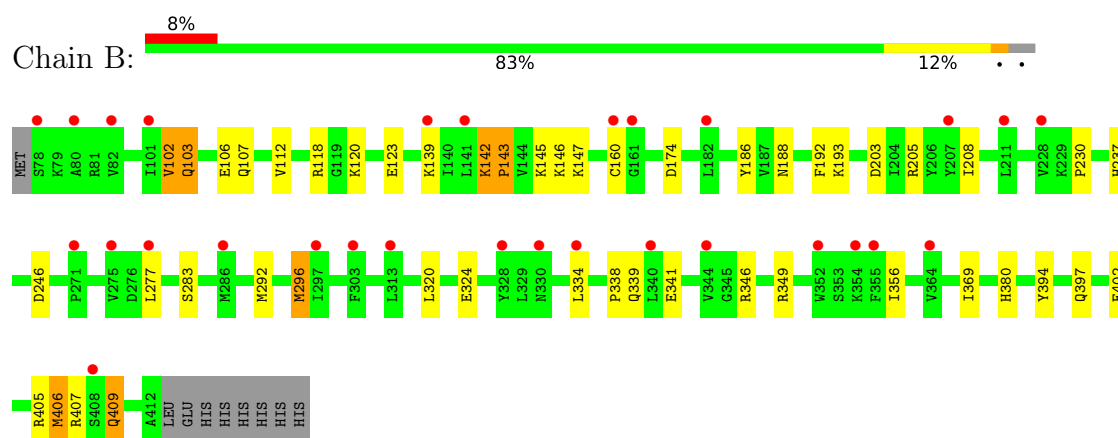
3 Residue-property plots [i](#)

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.

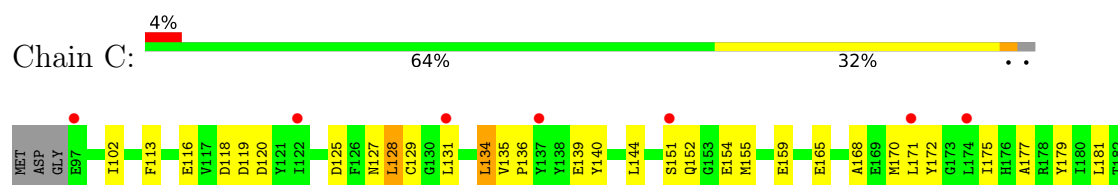
• Molecule 1: Casein kinase II subunit alpha-1



• Molecule 1: Casein kinase II subunit alpha-1

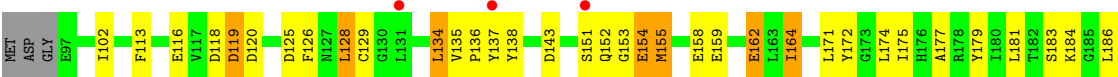


• Molecule 2: Casein kinase II subunit beta-1





● Molecule 2: Casein kinase II subunit beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	210.19Å 210.19Å 272.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.07 – 5.50 40.07 – 5.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.07-5.50) 99.6 (40.07-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 5.37Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.248 , 0.267 0.239 , 0.271	Depositor DCC
R_{free} test set	512 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	306.7	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 324.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	8722	wwPDB-VP
Average B, all atoms (Å ²)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: ZN, 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	0.59	0/2843	0.94	2/3839 (0.1%)
1	B	0.59	0/2843	0.96	0/3839
2	C	0.68	0/1594	1.13	2/2159 (0.1%)
2	D	0.67	0/1594	1.18	6/2159 (0.3%)
All	All	0.62	0/8874	1.03	10/11996 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	153	GLY	CA-C-N	5.56	127.73	120.28
2	D	153	GLY	C-N-CA	5.56	127.73	120.28
2	D	119	ASP	CA-C-N	5.42	129.26	120.60
2	D	119	ASP	C-N-CA	5.42	129.26	120.60
2	C	195	ASN	CA-C-N	5.12	131.31	121.54
2	C	195	ASN	C-N-CA	5.12	131.31	121.54
2	D	195	ASN	CA-C-N	5.11	131.30	121.54
2	D	195	ASN	C-N-CA	5.11	131.30	121.54
1	A	174	ASP	CA-C-N	5.01	128.69	120.63
1	A	174	ASP	C-N-CA	5.01	128.69	120.63

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	2774	0	2763	40	0
1	B	2774	0	2763	33	0
2	C	1550	0	1468	46	0
2	D	1550	0	1469	50	0
3	A	36	0	6	0	0
3	B	36	0	6	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8722	0	8475	148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (148) 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)
2:C:214:VAL:HB	2:C:256:PRO:HG3	1.41	1.01
1:A:405:ARG:NH1	1:A:409:GLN:HE22	1.76	0.83
2:C:257:HIS:CE1	2:D:277:GLN:HE21	2.00	0.80
1:B:405:ARG:NH1	1:B:409:GLN:HE22	1.81	0.77
1:B:338:PRO:HA	1:B:341:GLU:HG2	1.67	0.77
1:A:338:PRO:HA	1:A:341:GLU:HG2	1.67	0.75
1:B:192:PHE:CD2	1:B:230:PRO:HB3	2.25	0.72
2:C:233:GLU:HG3	2:C:270:LYS:NZ	2.05	0.71
1:A:192:PHE:CD2	1:A:230:PRO:HB3	2.25	0.71
2:D:233:GLU:HG3	2:D:270:LYS:NZ	2.06	0.70
1:A:405:ARG:NH1	1:A:409:GLN:NE2	2.41	0.68
1:B:405:ARG:NH1	1:B:409:GLN:NE2	2.42	0.68
2:C:257:HIS:HE1	2:D:277:GLN:HE21	1.38	0.67
1:B:120:LYS:HZ2	2:D:183:SER:H	1.43	0.67
1:A:120:LYS:HZ2	2:C:183:SER:H	1.41	0.66
2:D:134:LEU:HD12	2:D:135:VAL:HG23	1.77	0.65
2:C:277:GLN:HE21	2:D:257:HIS:CE1	2.14	0.65
1:B:142:LYS:HD3	1:B:143:PRO:HD2	1.79	0.64
2:C:113:PHE:HD1	2:C:198:PHE:HD1	1.46	0.63
2:D:113:PHE:HD1	2:D:198:PHE:HD1	1.46	0.63
1:A:102:VAL:HG21	1:A:146:LYS:NZ	2.13	0.63
2:D:276:VAL:HG11	2:D:278:ARG:HE	1.64	0.62
2:C:275:TYR:OH	2:D:257:HIS:NE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:NZ	2:D:183:SER:H	1.98	0.61
1:A:139:LYS:NZ	1:A:246:ASP:HA	2.14	0.61
1:A:142:LYS:HD3	1:A:143:PRO:HD2	1.81	0.61
2:C:225:VAL:HB	2:C:248:GLY:HA2	1.83	0.61
1:A:102:VAL:HG21	1:A:146:LYS:HZ1	1.66	0.61
1:B:139:LYS:NZ	1:B:246:ASP:HA	2.16	0.60
2:C:118:ASP:HB2	2:C:184:LYS:HZ3	1.67	0.60
1:B:102:VAL:HG21	1:B:146:LYS:NZ	2.16	0.60
1:A:120:LYS:NZ	2:C:183:SER:H	1.99	0.60
1:B:186:TYR:CE2	1:B:188:ASN:HB2	2.36	0.59
2:D:225:VAL:HB	2:D:248:GLY:HA2	1.83	0.59
1:B:174:ASP:HB2	2:C:280:PHE:O	2.03	0.59
2:D:276:VAL:HG11	2:D:278:ARG:NE	2.17	0.58
1:A:103:GLN:H	1:A:103:GLN:CD	2.12	0.58
1:A:208:ILE:HD11	1:A:296:MET:CE	2.34	0.57
1:B:103:GLN:CD	1:B:103:GLN:H	2.14	0.56
2:D:172:TYR:HA	2:D:175:ILE:HD12	1.87	0.55
2:D:214:VAL:HB	2:D:256:PRO:HG3	1.88	0.55
1:B:208:ILE:HD11	1:B:296:MET:CE	2.37	0.55
2:C:172:TYR:HA	2:C:175:ILE:HD12	1.88	0.54
1:A:111:GLU:HB3	2:D:285:HIS:HB2	1.90	0.54
2:D:276:VAL:HG12	2:D:278:ARG:HG3	1.89	0.54
1:B:139:LYS:HZ1	1:B:246:ASP:HA	1.74	0.53
1:B:192:PHE:CZ	1:B:296:MET:SD	3.01	0.53
1:B:324:GLU:OE1	1:B:349:ARG:HB2	2.09	0.53
1:A:192:PHE:HZ	1:A:296:MET:HG3	1.74	0.53
1:A:192:PHE:CZ	1:A:296:MET:SD	3.01	0.53
1:B:320:LEU:O	1:B:324:GLU:OE1	2.27	0.53
2:D:118:ASP:HB2	2:D:184:LYS:HZ3	1.74	0.52
2:C:214:VAL:CB	2:C:256:PRO:HG3	2.27	0.52
1:A:320:LEU:O	1:A:324:GLU:OE1	2.27	0.52
2:D:247:ASP:HB3	2:D:250:TYR:CE2	2.45	0.52
1:A:324:GLU:OE1	1:A:349:ARG:HB2	2.09	0.52
1:A:208:ILE:HD11	1:A:296:MET:HE1	1.92	0.52
1:A:186:TYR:CE2	1:A:188:ASN:HB2	2.44	0.51
1:B:192:PHE:HZ	1:B:296:MET:HG3	1.75	0.51
1:A:337:ASP:OD1	1:A:339:GLN:HG3	2.10	0.51
2:D:118:ASP:HB2	2:D:184:LYS:NZ	2.26	0.50
2:C:118:ASP:HB2	2:C:184:LYS:NZ	2.26	0.50
2:C:144:LEU:HD23	2:C:168:ALA:CB	2.41	0.49
1:B:102:VAL:HG21	1:B:146:LYS:HZ1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:HD11	1:B:296:MET:HE1	1.95	0.49
2:C:265:HIS:CD2	2:C:266:LEU:HD23	2.48	0.49
2:D:198:PHE:HB2	2:D:211:CYS:O	2.13	0.48
2:C:247:ASP:HB3	2:C:250:TYR:CE2	2.47	0.48
2:D:277:GLN:HB2	2:D:284:LEU:HG	1.95	0.48
2:C:198:PHE:HB2	2:C:211:CYS:O	2.13	0.48
2:D:265:HIS:CD2	2:D:266:LEU:HD23	2.49	0.47
2:D:186:LEU:HD11	2:D:258:LEU:HD21	1.95	0.47
2:C:144:LEU:HD23	2:C:168:ALA:HB2	1.96	0.47
2:C:278:ARG:O	2:D:253:THR:O	2.31	0.47
2:C:186:LEU:HD11	2:C:258:LEU:HD21	1.96	0.47
1:A:142:LYS:HZ1	2:C:127:ASN:HB3	1.79	0.47
1:A:139:LYS:HZ3	1:A:246:ASP:HA	1.79	0.47
2:D:228:TYR:HE1	2:D:260:LEU:HD21	1.80	0.46
1:A:277:LEU:HD12	1:A:334:LEU:HD11	1.96	0.46
2:C:265:HIS:CD2	2:C:266:LEU:CD2	2.99	0.46
1:A:258:GLU:CD	1:A:278:GLN:HB2	2.40	0.46
2:C:134:LEU:HD12	2:C:135:VAL:HG23	1.98	0.46
2:D:206:CYS:SG	2:D:232:CYS:HB3	2.56	0.46
1:B:277:LEU:HD12	1:B:334:LEU:HD11	1.98	0.46
1:A:139:LYS:HZ1	1:A:246:ASP:HA	1.81	0.46
1:A:292:MET:O	1:A:296:MET:SD	2.74	0.46
1:B:292:MET:O	1:B:296:MET:SD	2.74	0.45
2:D:265:HIS:CD2	2:D:266:LEU:CD2	2.99	0.45
2:C:277:GLN:HE22	2:D:260:LEU:HD11	1.81	0.45
2:C:125:ASP:HA	2:C:128:LEU:HG	1.98	0.45
2:D:238:PRO:HG2	2:D:244:GLY:HA2	1.99	0.45
1:B:112:VAL:O	2:C:285:HIS:HB2	2.16	0.45
1:B:192:PHE:HZ	1:B:296:MET:CG	2.29	0.45
1:B:192:PHE:HZ	1:B:296:MET:SD	2.40	0.45
1:A:128:ILE:CD1	2:D:285:HIS:CD2	2.99	0.45
2:C:238:PRO:HG2	2:C:244:GLY:HA2	1.98	0.45
1:A:128:ILE:HD13	2:D:285:HIS:CD2	2.52	0.45
2:D:118:ASP:CB	2:D:184:LYS:HZ1	2.30	0.45
1:A:192:PHE:HZ	1:A:296:MET:CG	2.29	0.44
1:A:192:PHE:HZ	1:A:296:MET:SD	2.40	0.44
1:B:145:LYS:HD3	3:B:501:IHP:O42	2.16	0.44
2:C:279:VAL:HG12	2:D:254:THR:HG23	1.99	0.44
2:C:170:MET:SD	2:C:221:ARG:NH2	2.90	0.44
2:C:233:GLU:HG3	2:C:270:LYS:HZ1	1.80	0.44
2:D:233:GLU:HG3	2:D:270:LYS:HZ1	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:HD11	1:B:369:ILE:HD11	2.00	0.44
2:C:118:ASP:CB	2:C:184:LYS:NZ	2.81	0.44
2:D:125:ASP:HA	2:D:128:LEU:HG	1.99	0.43
2:D:118:ASP:CB	2:D:184:LYS:NZ	2.81	0.43
2:D:158:GLU:O	2:D:162:GLU:HG3	2.19	0.43
1:B:405:ARG:HH12	1:B:409:GLN:HE22	1.59	0.43
2:D:152:GLN:HG2	2:D:155:MET:HB2	2.00	0.43
1:A:407:ARG:HA	1:A:407:ARG:HE	1.82	0.43
2:C:257:HIS:CE1	2:D:277:GLN:NE2	2.80	0.43
2:D:226:LYS:HZ3	2:D:226:LYS:HG2	1.68	0.43
2:C:179:TYR:HE2	2:C:184:LYS:HD3	1.84	0.43
2:C:171:LEU:O	2:C:175:ILE:HG13	2.19	0.43
1:A:356:ILE:HD11	1:A:369:ILE:HD11	2.01	0.43
1:B:118:ARG:HA	1:B:123:GLU:OE2	2.19	0.42
1:A:143:PRO:O	2:C:129:CYS:SG	2.77	0.42
2:D:137:TYR:HD1	2:D:164:ILE:HG23	1.85	0.42
2:D:171:LEU:O	2:D:175:ILE:HG13	2.19	0.42
2:C:135:VAL:HA	2:C:136:PRO:HD2	1.85	0.42
2:C:179:TYR:O	2:C:185:GLY:HA3	2.20	0.42
2:D:179:TYR:HE2	2:D:184:LYS:HD3	1.84	0.42
2:D:215:GLY:HA3	2:D:248:GLY:C	2.44	0.42
1:A:118:ARG:HA	1:A:123:GLU:OE2	2.19	0.42
2:C:228:TYR:HE1	2:C:260:LEU:HD21	1.84	0.42
1:B:205:ARG:HG2	1:B:394:TYR:CZ	2.55	0.42
2:C:177:ALA:O	2:C:181:LEU:HG	2.19	0.42
2:C:215:GLY:HA3	2:C:248:GLY:C	2.45	0.42
1:B:283:SER:OG	1:B:380:HIS:HB2	2.20	0.41
2:D:177:ALA:O	2:D:181:LEU:HG	2.19	0.41
1:A:205:ARG:HG2	1:A:394:TYR:CZ	2.56	0.41
2:D:136:PRO:O	2:D:137:TYR:HB2	2.20	0.41
1:B:402:GLU:O	1:B:406:MET:HG2	2.21	0.41
1:A:283:SER:OG	1:A:380:HIS:HB2	2.20	0.41
1:A:203:ASP:OD2	1:A:237:HIS:HE1	2.04	0.41
2:D:171:LEU:HG	2:D:175:ILE:HD11	2.02	0.40
1:A:142:LYS:NZ	2:C:127:ASN:HB3	2.37	0.40
2:D:154:GLU:H	2:D:154:GLU:HG3	1.63	0.40
2:D:126:PHE:O	2:D:129:CYS:SG	2.73	0.40
1:A:338:PRO:HA	1:A:341:GLU:CG	2.47	0.40
1:B:203:ASP:OD2	1:B:237:HIS:HE1	2.04	0.40
2:C:128:LEU:HA	2:C:131:LEU:HD12	2.02	0.40
2:C:277:GLN:HE21	2:D:257:HIS:HE1	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:HD3	1:A:120:LYS:HA	1.95	0.40
2:C:140:TYR:OH	2:C:152:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/344 (97%)	320 (96%)	13 (4%)	1 (0%)	36	72
1	B	334/344 (97%)	321 (96%)	12 (4%)	1 (0%)	36	72
2	C	189/194 (97%)	166 (88%)	23 (12%)	0	100	100
2	D	189/194 (97%)	166 (88%)	21 (11%)	2 (1%)	11	45
All	All	1046/1076 (97%)	973 (93%)	69 (7%)	4 (0%)	30	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	138	TYR
1	A	143	PRO
2	D	207	CYS
1	B	143	PRO

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	300/309 (97%)	287 (96%)	13 (4%)	26	47
1	B	300/309 (97%)	285 (95%)	15 (5%)	22	43
2	C	169/171 (99%)	151 (89%)	18 (11%)	6	21
2	D	169/171 (99%)	148 (88%)	21 (12%)	4	17
All	All	938/960 (98%)	871 (93%)	67 (7%)	13	35

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	A	103	GLN
1	A	106	GLU
1	A	107	GLN
1	A	142	LYS
1	A	147	LYS
1	A	160	CYS
1	A	193	LYS
1	A	296	MET
1	A	397	GLN
1	A	406	MET
1	A	407	ARG
1	A	409	GLN
1	B	102	VAL
1	B	103	GLN
1	B	106	GLU
1	B	107	GLN
1	B	142	LYS
1	B	147	LYS
1	B	160	CYS
1	B	193	LYS
1	B	296	MET
1	B	339	GLN
1	B	346	ARG
1	B	397	GLN
1	B	406	MET
1	B	407	ARG
1	B	409	GLN
2	C	102	ILE
2	C	116	GLU
2	C	119	ASP
2	C	120	ASP
2	C	128	LEU

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Mol	Chain	Res	Type
2	C	134	LEU
2	C	139	GLU
2	C	151	SER
2	C	154	GLU
2	C	155	MET
2	C	159	GLU
2	C	165	GLU
2	C	214	VAL
2	C	217	SER
2	C	224	THR
2	C	261	MET
2	C	279	VAL
2	C	284	LEU
2	D	102	ILE
2	D	116	GLU
2	D	119	ASP
2	D	120	ASP
2	D	128	LEU
2	D	134	LEU
2	D	143	ASP
2	D	151	SER
2	D	154	GLU
2	D	155	MET
2	D	159	GLU
2	D	162	GLU
2	D	164	ILE
2	D	174	LEU
2	D	214	VAL
2	D	217	SER
2	D	224	THR
2	D	273	GLN
2	D	274	ASN
2	D	279	VAL
2	D	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	131	ASN
1	A	188	ASN
1	A	254	HIS

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Mol	Chain	Res	Type
1	A	409	GLN
1	B	87	ASN
1	B	188	ASN
1	B	254	HIS
1	B	310	GLN
1	B	409	GLN
2	C	152	GLN
2	C	160	GLN
2	C	277	GLN
2	D	152	GLN
2	D	277	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	IHP	B	501	-	36,36,36	1.15	4 (11%)	60,60,60	0.88	2 (3%)
3	IHP	A	501	-	36,36,36	1.13	4 (11%)	60,60,60	1.13	6 (10%)

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
3	IHP	B	501	-	-	10/30/54/54	0/1/1/1
3	IHP	A	501	-	-	8/30/54/54	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	IHP	P2-O12	3.15	1.65	1.59
3	A	501	IHP	P5-O15	2.93	1.64	1.59
3	B	501	IHP	P4-O14	2.89	1.64	1.59
3	B	501	IHP	P6-O16	2.65	1.64	1.59
3	A	501	IHP	P2-O12	2.61	1.64	1.59
3	A	501	IHP	P1-O11	2.32	1.63	1.59
3	A	501	IHP	P3-O13	2.16	1.63	1.59
3	B	501	IHP	P3-O13	2.12	1.63	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	IHP	O14-P4-O24	-3.48	96.91	109.33
3	A	501	IHP	P6-O16-C6	2.51	130.12	123.43
3	A	501	IHP	C6-C5-C4	2.44	115.79	110.43
3	B	501	IHP	C5-C6-C1	2.37	115.64	110.43
3	B	501	IHP	P2-O12-C2	2.28	129.52	123.43
3	A	501	IHP	C3-C2-C1	2.23	115.32	110.43
3	A	501	IHP	O44-P4-O14	2.23	114.54	105.85
3	A	501	IHP	C4-C3-C2	2.21	115.29	110.43

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	IHP	C3-C4-O14-P4
3	A	501	IHP	C5-C4-O14-P4
3	B	501	IHP	C2-C1-O11-P1
3	B	501	IHP	C6-C1-O11-P1
3	B	501	IHP	C1-C2-O12-P2
3	B	501	IHP	C3-C2-O12-P2

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Mol	Chain	Res	Type	Atoms
3	B	501	IHP	C1-C6-O16-P6
3	B	501	IHP	C4-C5-O15-P5
3	A	501	IHP	C4-C3-O13-P3
3	B	501	IHP	C6-C5-O15-P5
3	A	501	IHP	C1-O11-P1-O21
3	A	501	IHP	C2-O12-P2-O32
3	B	501	IHP	C6-O16-P6-O36
3	B	501	IHP	C5-C6-O16-P6
3	A	501	IHP	C4-C5-O15-P5
3	A	501	IHP	C2-O12-P2-O42
3	A	501	IHP	C6-O16-P6-O36
3	B	501	IHP	C2-O12-P2-O42

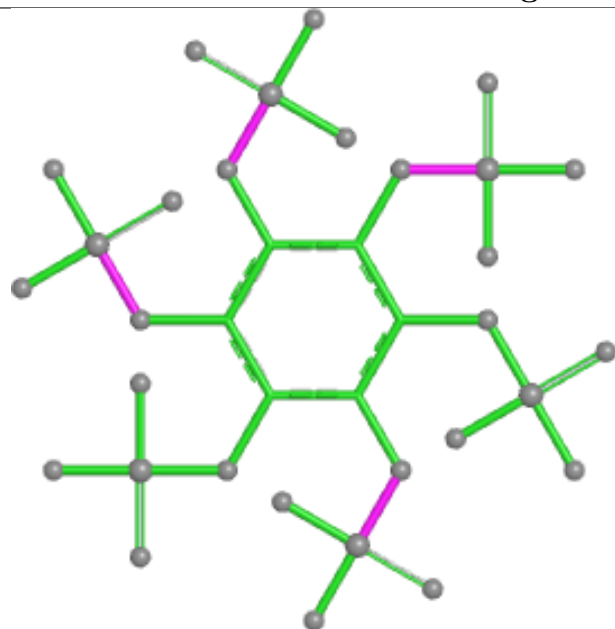
There are no ring outliers.

1 monomer is involved in 1 short contact:

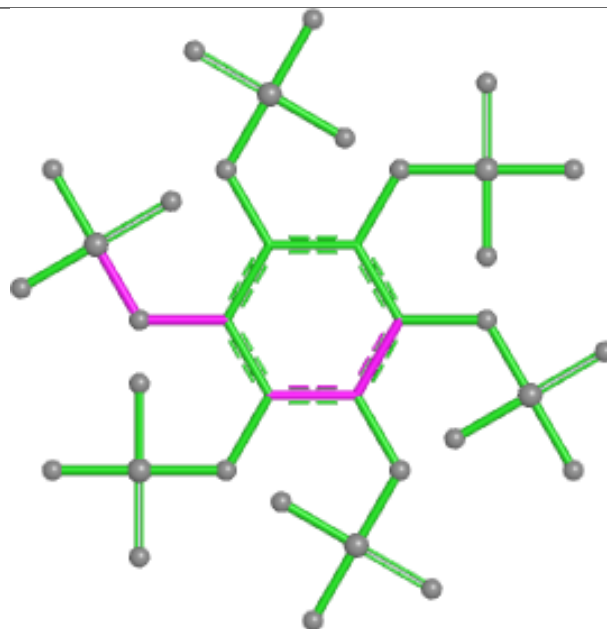
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	IHP	1	0

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.

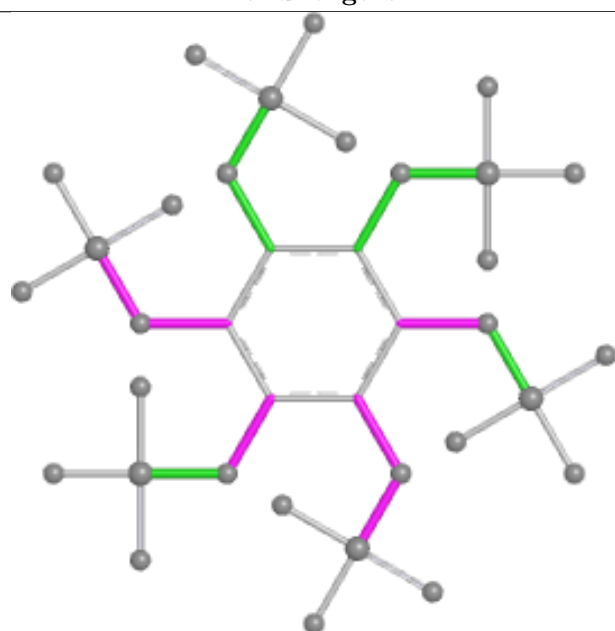
Ligand IHP B 501



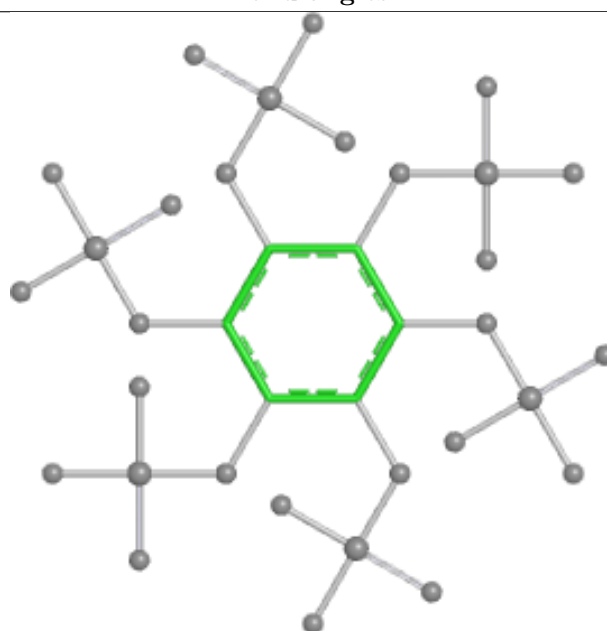
Bond lengths



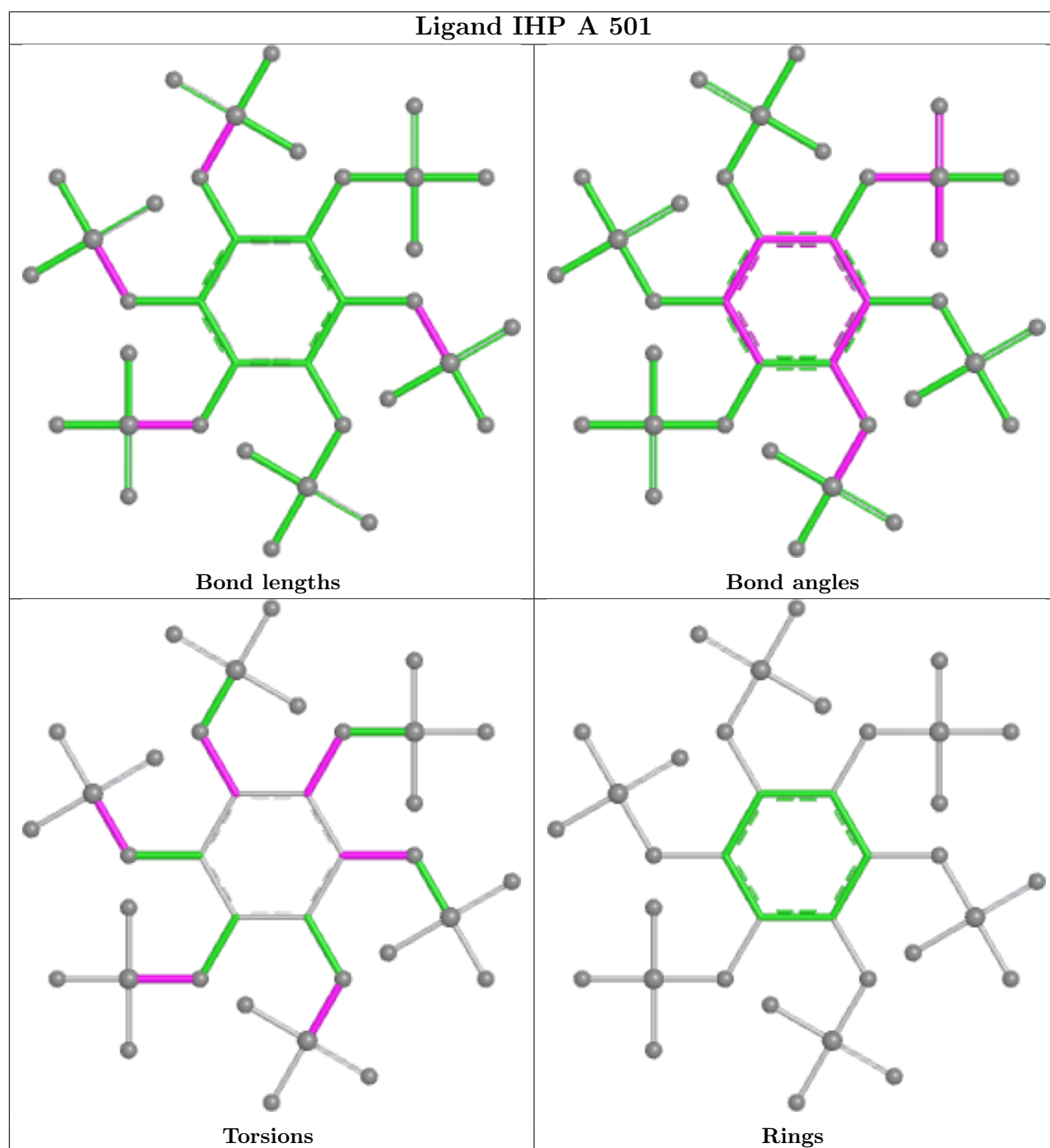
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	335/344 (97%)	0.68	34 (10%)	12 19	200, 300, 300, 300	2 (0%)
1	B	335/344 (97%)	0.53	29 (8%)	16 21	200, 300, 300, 300	2 (0%)
2	C	191/194 (98%)	0.30	8 (4%)	40 38	300, 300, 300, 300	0
2	D	191/194 (98%)	0.37	7 (3%)	45 41	300, 300, 300, 300	0
All	All	1052/1076 (97%)	0.50	78 (7%)	20 25	200, 300, 300, 300	4 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	ILE	5.1
2	D	222	SER	4.7
2	C	122	ILE	4.3
2	C	222	SER	4.3
1	B	101	ILE	4.2
1	B	330	ASN	4.2
1	A	361	GLN	3.9
1	A	355	PHE	3.8
1	A	211	LEU	3.7
1	A	330	ASN	3.5
1	B	328	TYR	3.4
2	D	213	PRO	3.2
2	C	151	SER	3.2
2	C	131	LEU	3.1
2	D	151	SER	3.1
1	A	356	ILE	3.1
1	B	352	TRP	3.0
1	B	313	LEU	3.0
1	A	111	GLU	3.0
1	A	247	TRP	3.0
1	A	194	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	80	ALA	2.9
2	C	137	TYR	2.9
1	A	208	ILE	2.9
2	D	131	LEU	2.9
1	A	136	CYS	2.8
1	A	127	GLY	2.8
1	A	275	VAL	2.7
1	A	248	GLY	2.7
1	B	228	VAL	2.7
1	A	215	LEU	2.7
1	B	277	LEU	2.7
1	A	393	ALA	2.7
1	A	352	TRP	2.7
1	B	182	LEU	2.6
1	A	397	GLN	2.6
1	B	207	TYR	2.6
1	A	303	PHE	2.6
1	B	141	LEU	2.5
1	A	110	TYR	2.5
1	A	125	PHE	2.5
1	B	297	ILE	2.5
1	A	231	HIS	2.5
1	A	289	LEU	2.4
1	A	214	ALA	2.4
1	A	327	ALA	2.4
2	D	253	THR	2.4
1	B	275	VAL	2.4
1	B	334	LEU	2.4
1	B	160	CYS	2.4
1	B	271	PRO	2.4
1	A	126	GLU	2.4
1	B	161	GLY	2.3
2	C	171	LEU	2.3
1	B	286	MET	2.3
1	A	244	LEU	2.3
1	B	355	PHE	2.3
1	B	354	LYS	2.2
2	C	174	LEU	2.2
1	A	207	TYR	2.2
1	A	328	TYR	2.2
1	B	344	VAL	2.2
2	D	251	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	303	PHE	2.2
1	A	364	VAL	2.2
1	A	378	TYR	2.2
1	A	121	TYR	2.1
1	B	139	LYS	2.1
1	B	408	SER	2.1
1	B	340	LEU	2.1
2	C	97	GLU	2.1
1	B	82	VAL	2.1
2	D	137	TYR	2.0
1	B	364	VAL	2.0
1	B	211	LEU	2.0
1	A	304	PHE	2.0
1	A	313	LEU	2.0
1	B	78	SER	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](#)

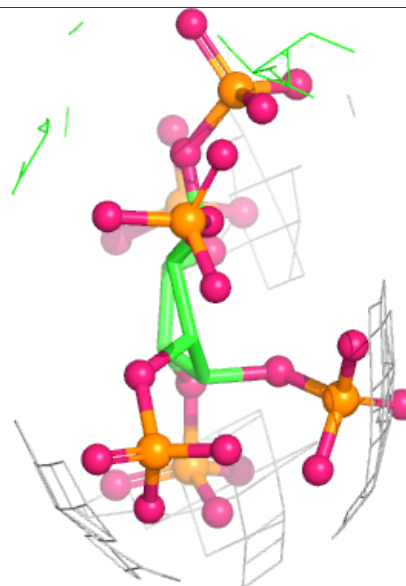
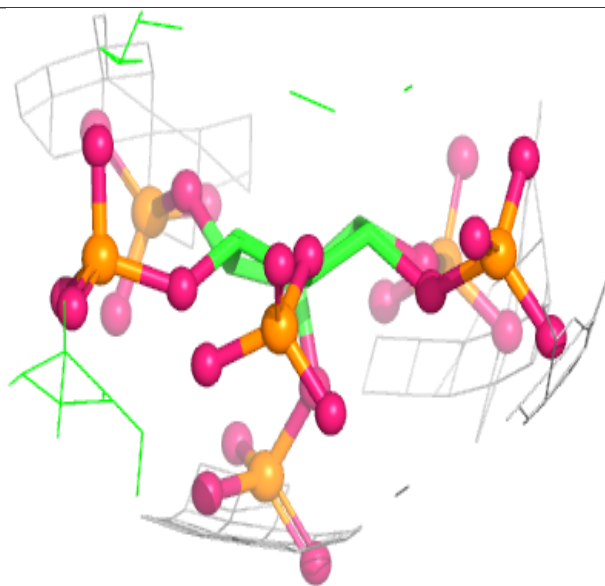
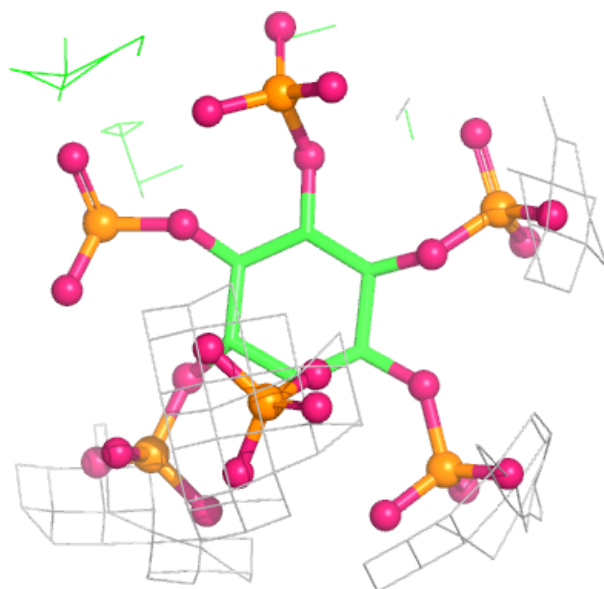
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IHP	B	501	36/36	0.68	0.14	300,300,300,300	0
3	IHP	A	501	36/36	0.78	0.10	300,300,300,300	0
4	ZN	D	301	1/1	0.99	0.07	300,300,300,300	0
4	ZN	C	301	1/1	1.00	0.12	300,300,300,300	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.

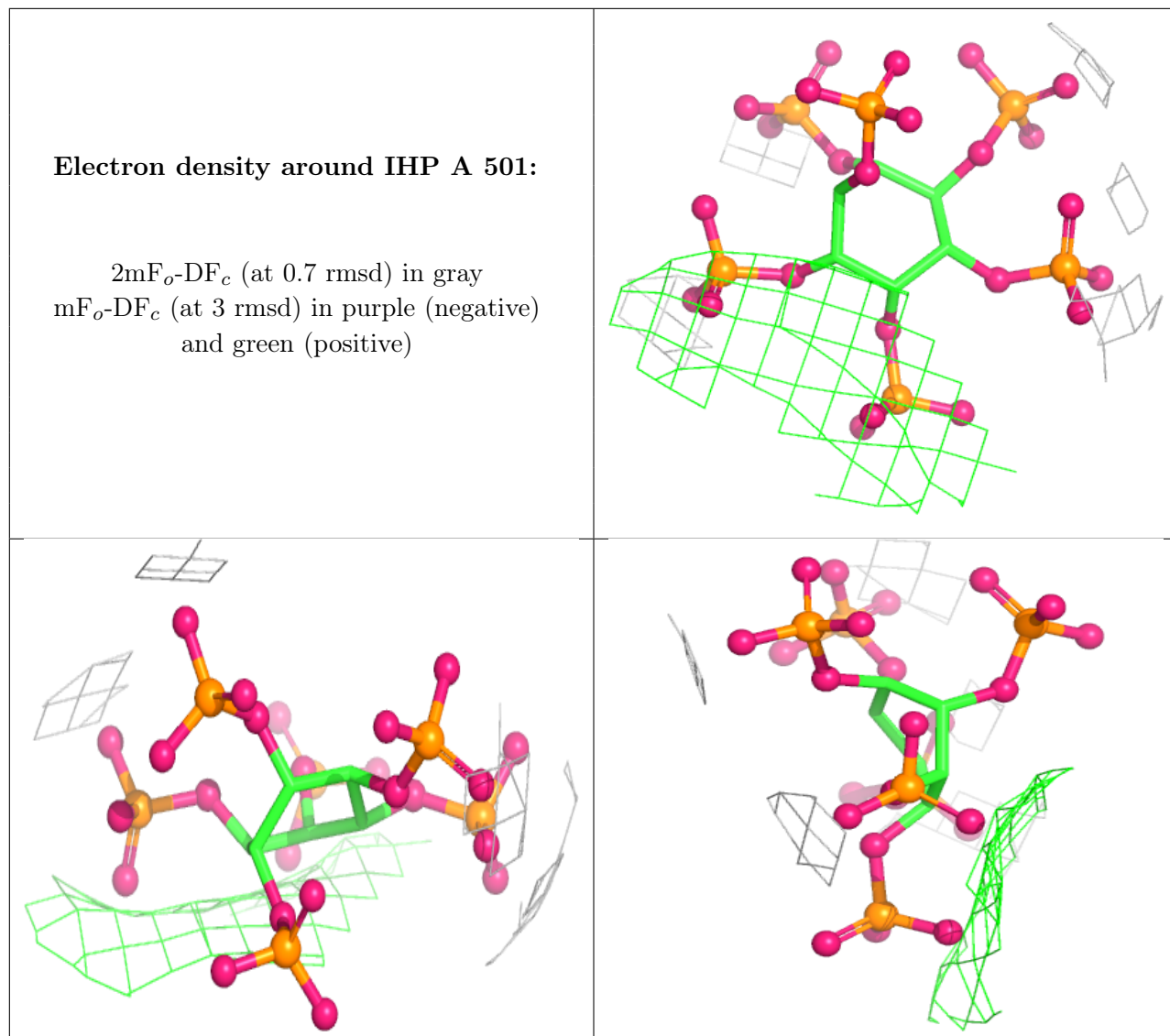
Electron density around IHP B 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.