



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 12:54 PM EDT

PDB ID : 2P1Q
Title : Mechanism of Auxin Perception by the TIR1 ubiquitin ligase
Authors : Tan, X.; Calderon-Villalobos, L.I.A.; Sharon, M.; Robinson, C.V.; Estelle, M.; Zheng, N.
Deposited on : 2007-03-06
Resolution : 1.91 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 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) : 1.13
EDS : 2.14.6
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) : 2.14.6

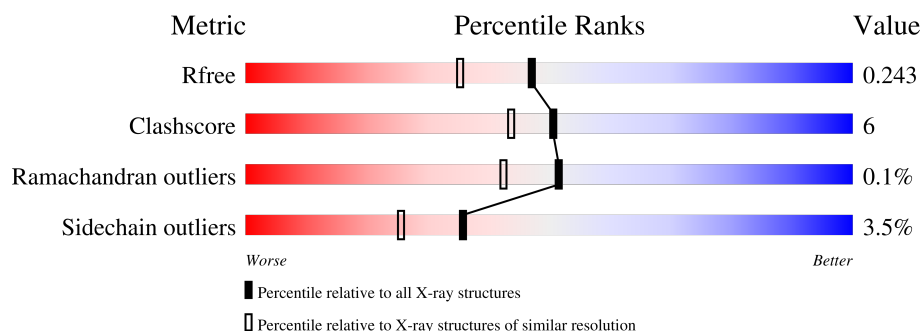
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	160	
2	B	594	
3	C	13	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6401 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			996	631	163	197	5			

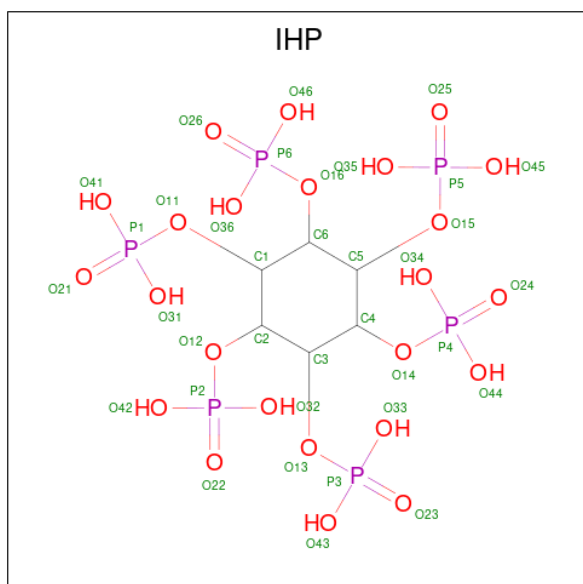
- Molecule 2 is a protein called TRANSPORT INHIBITOR RESPONSE 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	568	Total	C	N	O	S	0	0	0
			4472	2859	755	821	37			

- Molecule 3 is a protein called Auxin-responsive protein IAA7.

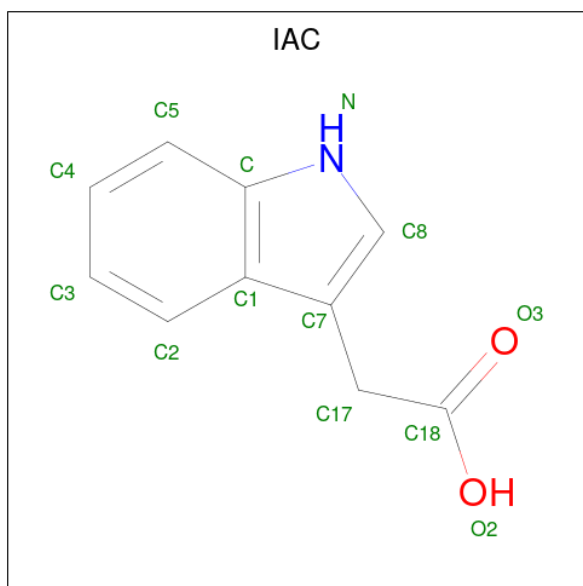
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			114	74	23	17			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 5 is 1H-INDOL-3-YLACETIC ACID (three-letter code: IAC) (formula: $C_{10}H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			13	10	1	2		

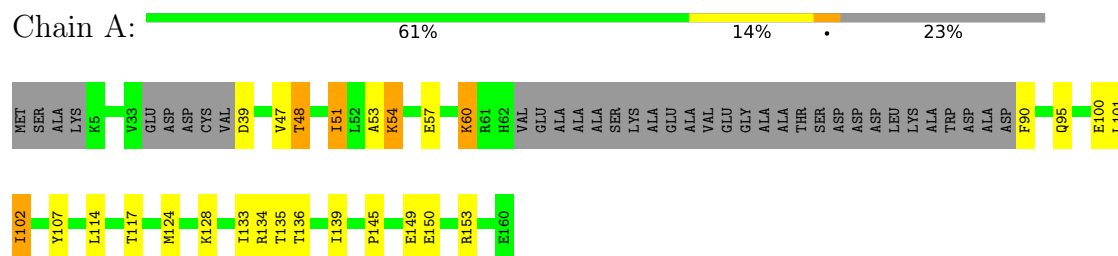
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	87	Total	O	0	0
			87	87		
6	B	666	Total	O	0	0
			666	666		
6	C	17	Total	O	0	0
			17	17		

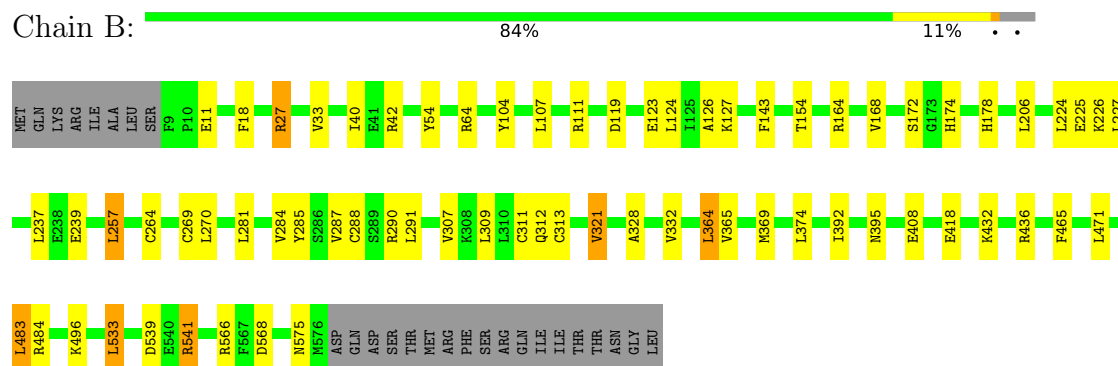
3 Residue-property plots [i](#)

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. 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. 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.

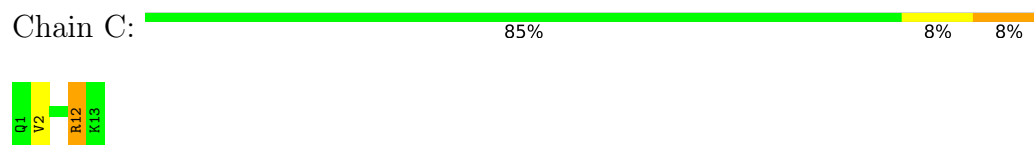
- Molecule 1: SKP1-like protein 1A



- Molecule 2: TRANSPORT INHIBITOR RESPONSE 1 protein



- Molecule 3: Auxin-responsive protein IAA7



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.21Å 82.47Å 125.05Å 90.00° 104.05° 90.00°	Depositor
Resolution (Å)	50.00 – 1.91 49.09 – 1.91	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-1.91) 94.4 (49.09-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.172 , 0.213 0.244 , 0.243	Depositor DCC
R_{free} test set	3723 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6401	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, IAC

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	0.98	4/1009 (0.4%)	0.74	2/1359 (0.1%)
2	B	0.77	1/4570 (0.0%)	0.84	10/6195 (0.2%)
3	C	0.98	0/118	0.84	1/159 (0.6%)
All	All	0.81	5/5697 (0.1%)	0.82	13/7713 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	LYS	CE-NZ	18.66	1.95	1.49
1	A	95	GLN	CD-OE1	8.08	1.41	1.24
1	A	95	GLN	CD-NE2	5.29	1.46	1.32
2	B	311	CYS	CB-SG	-5.25	1.73	1.81
1	A	135	THR	CB-OG1	5.18	1.53	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	A	60	LYS	CD-CE-NZ	-8.86	91.32	111.70
2	B	541	ARG	NE-CZ-NH2	-7.95	116.33	120.30
2	B	111	ARG	NE-CZ-NH1	-7.93	116.33	120.30
2	B	321	VAL	CB-CA-C	-6.27	99.50	111.40
2	B	533	LEU	CB-CG-CD1	6.05	121.28	111.00
2	B	321	VAL	CG1-CB-CG2	5.78	120.15	110.90
2	B	436	ARG	NE-CZ-NH1	-5.55	117.53	120.30
2	B	541	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	51	ILE	CG1-CB-CG2	-5.36	99.60	111.40
2	B	483	LEU	CB-CG-CD2	5.35	120.09	111.00
2	B	27	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	C	12	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	996	0	994	17	0
2	B	4472	0	4512	46	0
3	C	114	0	118	3	0
4	B	36	0	6	1	0
5	B	13	0	8	0	0
6	A	87	0	0	3	0
6	B	666	0	0	13	0
6	C	17	0	0	1	0
All	All	6401	0	5638	64	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 6.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:CE	1:A:60:LYS:NZ	1.95	1.27
2:B:11:GLU:OE1	2:B:40:ILE:HD11	1.59	1.03
2:B:369:MET:HG2	2:B:395:ASN:ND2	1.77	1.00
1:A:149:GLU:HB3	6:A:194:HOH:O	1.62	0.98
2:B:288:CYS:O	2:B:312:GLN:O	1.93	0.86
2:B:174:HIS:HD2	6:B:1107:HOH:O	1.58	0.84
2:B:418:GLU:HG2	6:B:1202:HOH:O	1.83	0.77
2:B:285:TYR:HA	2:B:288:CYS:SG	2.31	0.70
2:B:539:ASP:OD2	2:B:541:ARG:HD3	1.91	0.70
1:A:48:THR:HG22	1:A:51:ILE:H	1.56	0.70
2:B:225:GLU:HG2	6:B:1557:HOH:O	1.93	0.69
2:B:496:LYS:HE2	6:B:1158:HOH:O	1.92	0.68
2:B:288:CYS:HB2	2:B:313:CYS:SG	2.33	0.68
1:A:60:LYS:NZ	1:A:60:LYS:CD	2.57	0.68
2:B:178:HIS:NE2	6:B:1107:HOH:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:801:IHP:O44	6:B:1564:HOH:O	2.14	0.66
1:A:48:THR:HG21	6:A:181:HOH:O	1.96	0.65
1:A:102:ILE:HD13	1:A:117:THR:HB	1.80	0.63
2:B:369:MET:HG2	2:B:395:ASN:HD21	1.63	0.62
2:B:465:PHE:HZ	3:C:2:VAL:HG11	1.64	0.62
2:B:566:ARG:HG2	2:B:568:ASP:OD1	2.02	0.60
2:B:432:LYS:HG2	6:B:1414:HOH:O	2.02	0.60
2:B:364:LEU:HD13	2:B:392:ILE:HD13	1.83	0.59
2:B:539:ASP:OD2	2:B:541:ARG:CD	2.51	0.58
2:B:496:LYS:CE	6:B:1158:HOH:O	2.50	0.58
2:B:18:PHE:O	2:B:27:ARG:NH2	2.38	0.56
2:B:365:VAL:O	2:B:369:MET:HG3	2.07	0.55
2:B:281:LEU:O	2:B:284:VAL:HG22	2.08	0.54
2:B:224:LEU:HD11	2:B:257:LEU:HD11	1.88	0.54
1:A:47:VAL:HG23	1:A:107:TYR:CE2	2.44	0.53
1:A:51:ILE:HG12	1:A:100:GLU:HB3	1.89	0.53
2:B:369:MET:HG2	2:B:395:ASN:HD22	1.70	0.53
2:B:42:ARG:HB2	2:B:64:ARG:O	2.09	0.52
1:A:54:LYS:HE2	1:A:90:PHE:CE1	2.45	0.52
1:A:124:MET:O	1:A:128:LYS:HE2	2.10	0.52
1:A:48:THR:CG2	1:A:51:ILE:H	2.22	0.51
2:B:11:GLU:OE1	2:B:40:ILE:CD1	2.47	0.51
1:A:53:ALA:O	1:A:57:GLU:HG3	2.12	0.50
1:A:134:ARG:HB2	1:A:139:ILE:O	2.12	0.49
2:B:285:TYR:CD2	2:B:312:GLN:NE2	2.80	0.48
2:B:119:ASP:O	2:B:123:GLU:HG3	2.13	0.48
2:B:11:GLU:HG2	6:B:1259:HOH:O	2.13	0.48
2:B:284:VAL:O	2:B:287:VAL:HB	2.14	0.47
2:B:408:GLU:HG2	6:B:1127:HOH:O	2.14	0.47
2:B:328:ALA:HB3	6:B:1262:HOH:O	2.14	0.47
1:A:145:PRO:O	1:A:149:GLU:HG3	2.14	0.47
2:B:54:TYR:CZ	2:B:566:ARG:HD2	2.51	0.45
2:B:239:GLU:HG2	2:B:269:CYS:HB3	1.99	0.45
2:B:566:ARG:CG	2:B:568:ASP:OD1	2.65	0.44
2:B:307:VAL:HG13	2:B:332:VAL:HG11	2.00	0.44
2:B:484:ARG:HG2	6:B:1479:HOH:O	2.17	0.44
1:A:133:ILE:HG21	2:B:33:VAL:HG11	2.00	0.43
2:B:465:PHE:CZ	3:C:2:VAL:HG11	2.48	0.43
2:B:143:PHE:CZ	2:B:168:VAL:HG22	2.54	0.42
2:B:264:CYS:O	2:B:290:ARG:NH2	2.51	0.42
2:B:226:LYS:NZ	6:B:1032:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ALA:HB1	2:B:154:THR:HB	2.02	0.42
1:A:153:ARG:NH1	6:A:194:HOH:O	2.53	0.42
2:B:104:TYR:O	2:B:107:LEU:HB2	2.19	0.41
2:B:270:LEU:HD12	2:B:291:LEU:HD11	2.02	0.41
2:B:123:GLU:O	2:B:127:LYS:HG2	2.21	0.41
1:A:47:VAL:HG23	1:A:107:TYR:CD2	2.56	0.41
2:B:127:LYS:HB2	2:B:127:LYS:HE2	1.88	0.41
3:C:12:ARG:HD3	6:C:510:HOH:O	2.21	0.41

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	118/160 (74%)	117 (99%)	1 (1%)	0	100	100
2	B	566/594 (95%)	555 (98%)	10 (2%)	1 (0%)	47	38
3	C	11/13 (85%)	11 (100%)	0	0	100	100
All	All	695/767 (91%)	683 (98%)	11 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	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	112/137 (82%)	104 (93%)	8 (7%)	14	6
2	B	501/525 (95%)	487 (97%)	14 (3%)	43	34
3	C	12/12 (100%)	12 (100%)	0	100	100
All	All	625/674 (93%)	603 (96%)	22 (4%)	36	25

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	48	THR
1	A	54	LYS
1	A	101	LEU
1	A	102	ILE
1	A	114	LEU
1	A	136	THR
1	A	150	GLU
2	B	124	LEU
2	B	164	ARG
2	B	206	LEU
2	B	227	LEU
2	B	237	LEU
2	B	257	LEU
2	B	309	LEU
2	B	321	VAL
2	B	364	LEU
2	B	374	LEU
2	B	471	LEU
2	B	483	LEU
2	B	533	LEU
2	B	575	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
2	B	174	HIS
2	B	312	GLN
2	B	317	GLN
2	B	383	GLN

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Mol	Chain	Res	Type
2	B	395	ASN
2	B	501	ASN
2	B	575	ASN
3	C	1	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	IHP	B	801	-	36,36,36	1.46	6 (16%)	54,60,60	0.99	2 (3%)
5	IAC	B	901	-	10,14,14	1.22	2 (20%)	11,19,19	1.36	1 (9%)

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	IHP	B	801	-	-	3/30/54/54	0/1/1/1
5	IAC	B	901	-	-	0/2/4/4	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	IHP	P2-O12	4.31	1.67	1.59
4	B	801	IHP	P5-O15	3.81	1.66	1.59
4	B	801	IHP	P3-O13	2.75	1.64	1.59
4	B	801	IHP	P2-O32	2.73	1.65	1.54
4	B	801	IHP	P3-O43	2.23	1.63	1.54
5	B	901	IAC	C3-C2	2.12	1.41	1.36
5	B	901	IAC	C4-C5	2.08	1.41	1.36
4	B	801	IHP	P3-O33	2.03	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	IAC	C2-C1-C	2.91	122.03	118.17
4	B	801	IHP	O41-P1-O21	2.30	119.70	110.68
4	B	801	IHP	O13-P3-O23	2.10	117.49	109.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	IHP	C1-O11-P1-O21
4	B	801	IHP	C1-O11-P1-O41
4	B	801	IHP	C4-O14-P4-O44

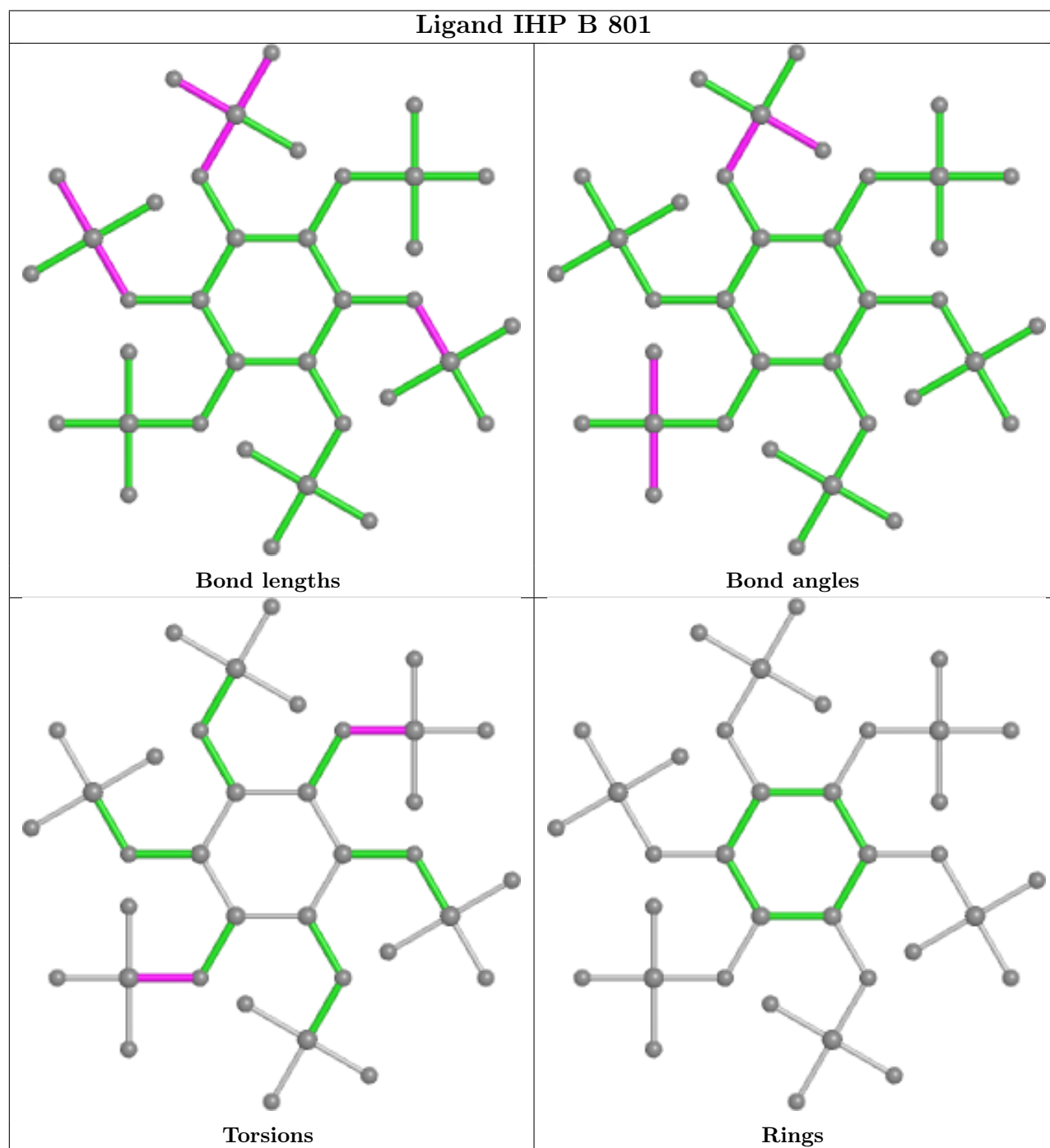
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	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.



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

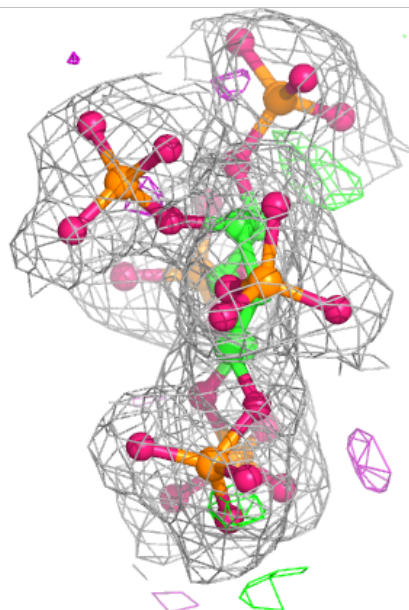
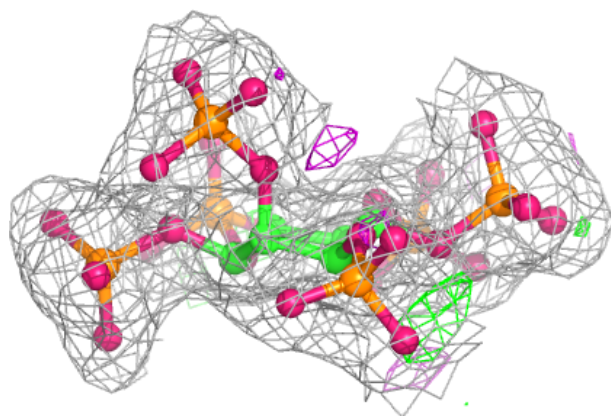
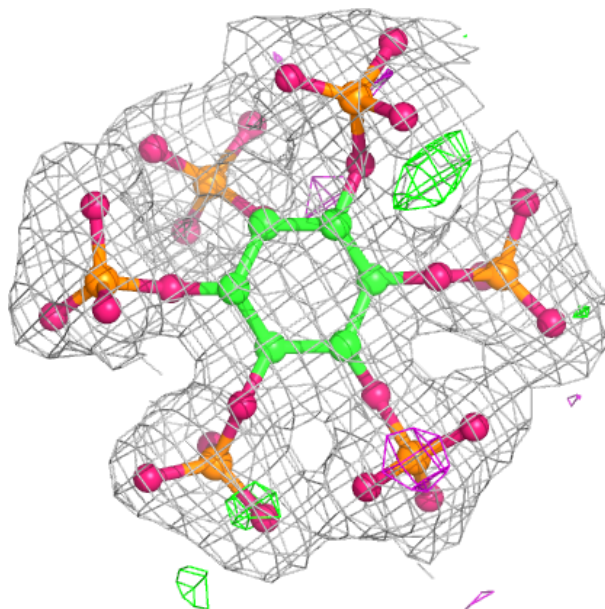
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 801:

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



6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.