



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:59 AM UTC

PDB ID : 4WPC / pdb_00004wpc
Title : Crystal structure of Rgd1p F-BAR domain in complex with inositol phosphate
Authors : Moravcevic, K.; Lemmon, M.A.
Deposited on : 2014-10-17
Resolution : 3.34 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)
Xtrriage (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

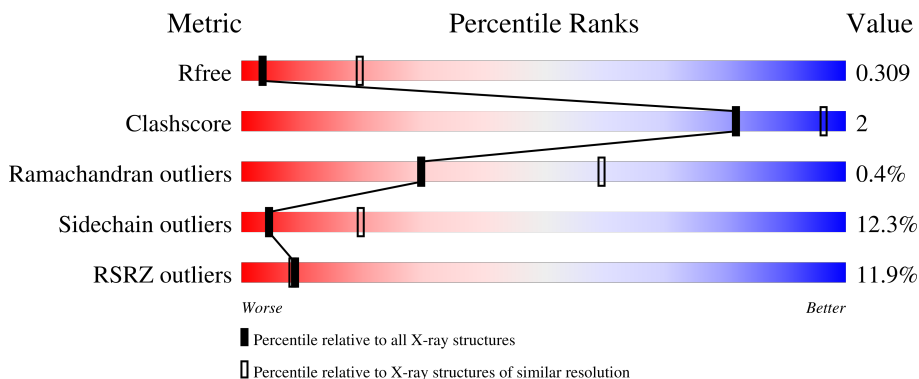
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	317	 9% 76% 11% 11%
1	B	317	 13% 78% 13% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8441 atoms, of which 4055 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.

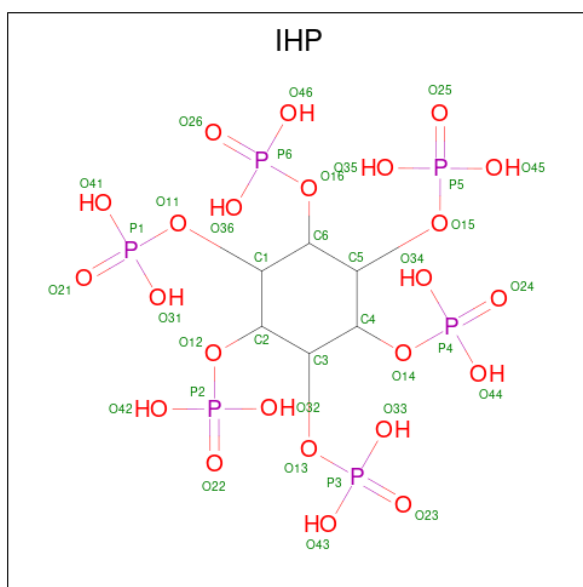
- Molecule 1 is a protein called RHO GTPase-activating protein RGD1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	283	4152	1351	2020	362	410	9	0	0	0
1	B	288	4209	1370	2035	368	427	9	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P38339
A	18	HIS	-	expression tag	UNP P38339
A	19	HIS	-	expression tag	UNP P38339
A	20	HIS	-	expression tag	UNP P38339
A	21	HIS	-	expression tag	UNP P38339
A	22	HIS	-	expression tag	UNP P38339
A	23	HIS	-	expression tag	UNP P38339
B	17	MET	-	initiating methionine	UNP P38339
B	18	HIS	-	expression tag	UNP P38339
B	19	HIS	-	expression tag	UNP P38339
B	20	HIS	-	expression tag	UNP P38339
B	21	HIS	-	expression tag	UNP P38339
B	22	HIS	-	expression tag	UNP P38339
B	23	HIS	-	expression tag	UNP P38339

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	2	Total	O	0	0
			2	2		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.99Å 74.11Å 105.73Å 90.00° 104.27° 90.00°	Depositor
Resolution (Å)	30.77 – 3.34 30.77 – 3.34	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.77-3.34) 97.9 (30.77-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 3.32Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.261 , 0.300 0.266 , 0.309	Depositor DCC
R_{free} test set	995 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtrriage
Anisotropy	0.200	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8441	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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	0.42	0/2161	0.70	3/2927 (0.1%)
1	B	0.38	1/2202 (0.0%)	0.65	0/2984
All	All	0.40	1/4363 (0.0%)	0.68	3/5911 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLN	CD-OE1	5.14	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	THR	CA-C-N	5.67	131.90	121.70
1	A	190	THR	C-N-CA	5.67	131.90	121.70
1	A	314	ASN	N-CA-C	5.29	116.86	111.14

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	2132	2020	2031	15	0
1	B	2174	2035	2036	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	6	0	0
2	B	36	0	6	1	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
All	All	4386	4055	4079	21	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 2.

All (21) 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:203:GLU:OE1	1:A:206:ARG:NH2	2.29	0.66
1:A:190:THR:OG1	1:A:191:LEU:HA	2.04	0.57
1:A:190:THR:HG23	1:A:191:LEU:CB	2.39	0.53
1:B:196:THR:OG1	1:B:197:THR:N	2.42	0.53
1:A:316:ASN:HD22	1:A:316:ASN:N	2.08	0.50
1:B:49:LEU:O	1:B:141:ARG:NH1	2.47	0.47
1:A:77:VAL:HG22	1:A:116:LYS:HB3	1.98	0.46
1:B:250:THR:O	1:B:253:THR:OG1	2.28	0.46
1:A:235:PRO:HA	1:A:238:VAL:HG22	1.98	0.45
1:A:190:THR:CB	1:A:191:LEU:HA	2.47	0.45
1:A:290:VAL:O	1:A:291:SER:OG	2.34	0.43
1:A:76:HIS:NE2	1:B:73:GLU:OE2	2.51	0.43
1:B:141:ARG:NH2	2:B:401:IHP:O34	2.51	0.42
1:B:195:LYS:CB	1:B:196:THR:HB	2.50	0.42
1:A:194:SER:OG	1:A:195:LYS:N	2.52	0.42
1:A:271:GLY:HA2	1:B:267:VAL:HG11	2.01	0.42
1:A:276:PRO:C	1:A:278:ASP:H	2.28	0.42
1:A:234:ARG:N	1:A:235:PRO:HD2	2.35	0.42
1:A:114:GLN:HG2	1:A:115:VAL:N	2.36	0.41
1:A:190:THR:HG23	1:A:191:LEU:CA	2.50	0.41
1:B:234:ARG:HB3	1:B:235:PRO:HD3	2.02	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	275/317 (87%)	263 (96%)	11 (4%)	1 (0%)	30	59
1	B	276/317 (87%)	255 (92%)	20 (7%)	1 (0%)	30	59
All	All	551/634 (87%)	518 (94%)	31 (6%)	2 (0%)	30	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	PHE
1	B	292	ASN

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	221/297 (74%)	197 (89%)	24 (11%)	6	24
1	B	226/297 (76%)	195 (86%)	31 (14%)	3	16
All	All	447/594 (75%)	392 (88%)	55 (12%)	4	20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	48	LEU
1	A	66	ILE
1	A	67	ARG

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Mol	Chain	Res	Type
1	A	70	TYR
1	A	90	ILE
1	A	109	ASP
1	A	114	GLN
1	A	123	LEU
1	A	130	ILE
1	A	133	LEU
1	A	137	MET
1	A	177	ASP
1	A	189	LEU
1	A	191	LEU
1	A	225	LEU
1	A	234	ARG
1	A	241	LEU
1	A	253	THR
1	A	255	GLN
1	A	272	VAL
1	A	290	VAL
1	A	303	TYR
1	A	316	ASN
1	B	26	LEU
1	B	43	VAL
1	B	56	LEU
1	B	59	CYS
1	B	66	ILE
1	B	81	SER
1	B	84	TYR
1	B	86	HIS
1	B	89	ASN
1	B	90	ILE
1	B	98	LEU
1	B	109	ASP
1	B	140	LEU
1	B	159	ILE
1	B	177	ASP
1	B	196	THR
1	B	197	THR
1	B	222	SER
1	B	225	LEU
1	B	228	THR
1	B	241	LEU
1	B	252	MET

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Mol	Chain	Res	Type
1	B	254	ILE
1	B	255	GLN
1	B	256	LEU
1	B	261	ILE
1	B	262	TRP
1	B	290	VAL
1	B	301	ASN
1	B	313	ILE
1	B	320	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	B	89	ASN
1	B	166	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 oligosaccharides 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
2	IHP	B	401	-	36,36,36	1.65	4 (11%)	60,60,60	0.51	0
2	IHP	A	401	-	36,36,36	1.66	4 (11%)	60,60,60	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IHP	B	401	-	-	0/30/54/54	0/1/1/1
2	IHP	A	401	-	-	0/30/54/54	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	IHP	P2-O22	3.58	1.61	1.50
2	A	401	IHP	P2-O22	3.55	1.61	1.50
2	B	401	IHP	P4-O24	3.54	1.61	1.50
2	A	401	IHP	P4-O24	3.54	1.61	1.50
2	A	401	IHP	P6-O26	3.54	1.61	1.50
2	B	401	IHP	P6-O26	3.53	1.61	1.50
2	B	401	IHP	P5-O25	3.53	1.61	1.50
2	A	401	IHP	P5-O25	3.49	1.61	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

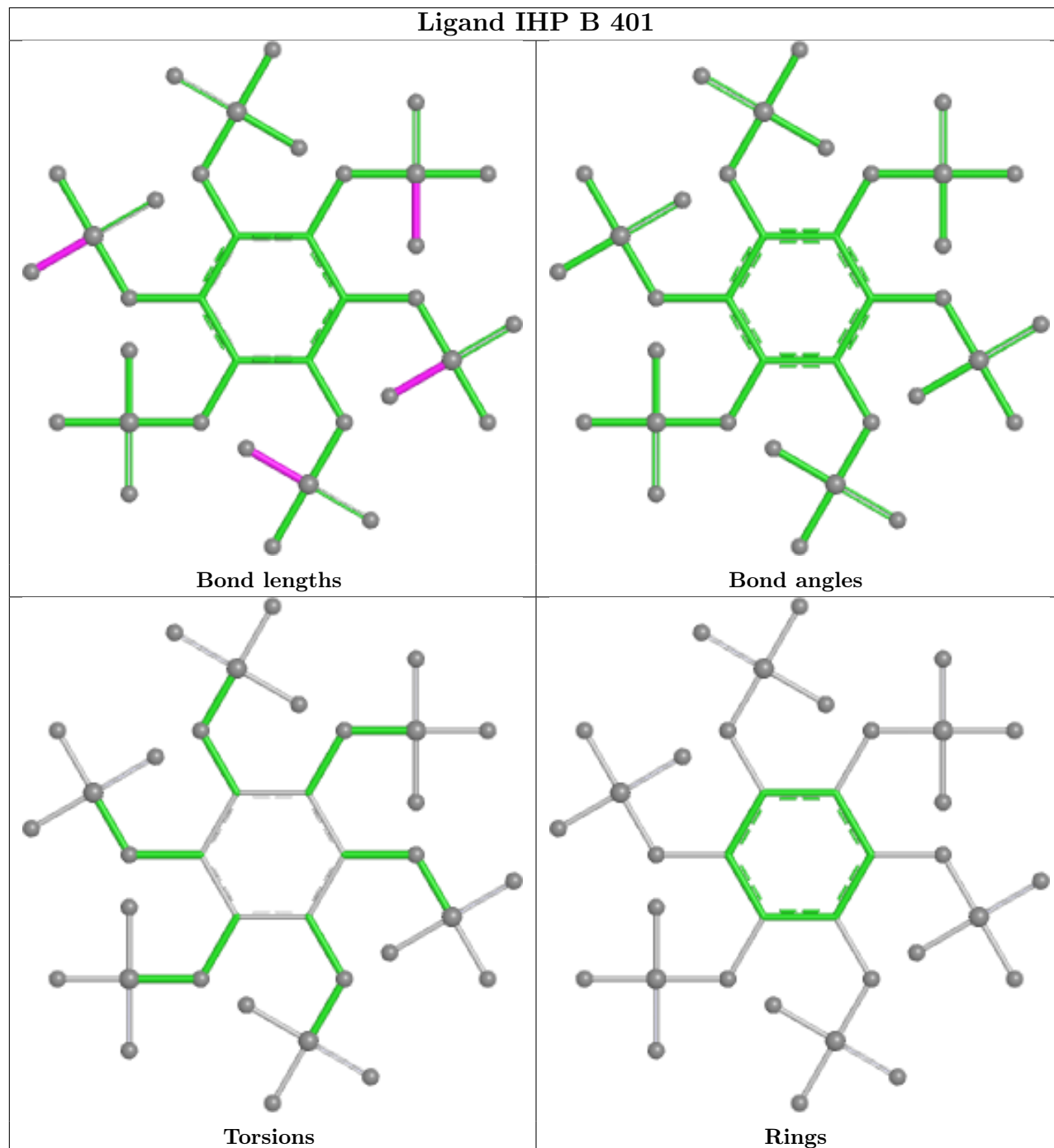
There are no ring outliers.

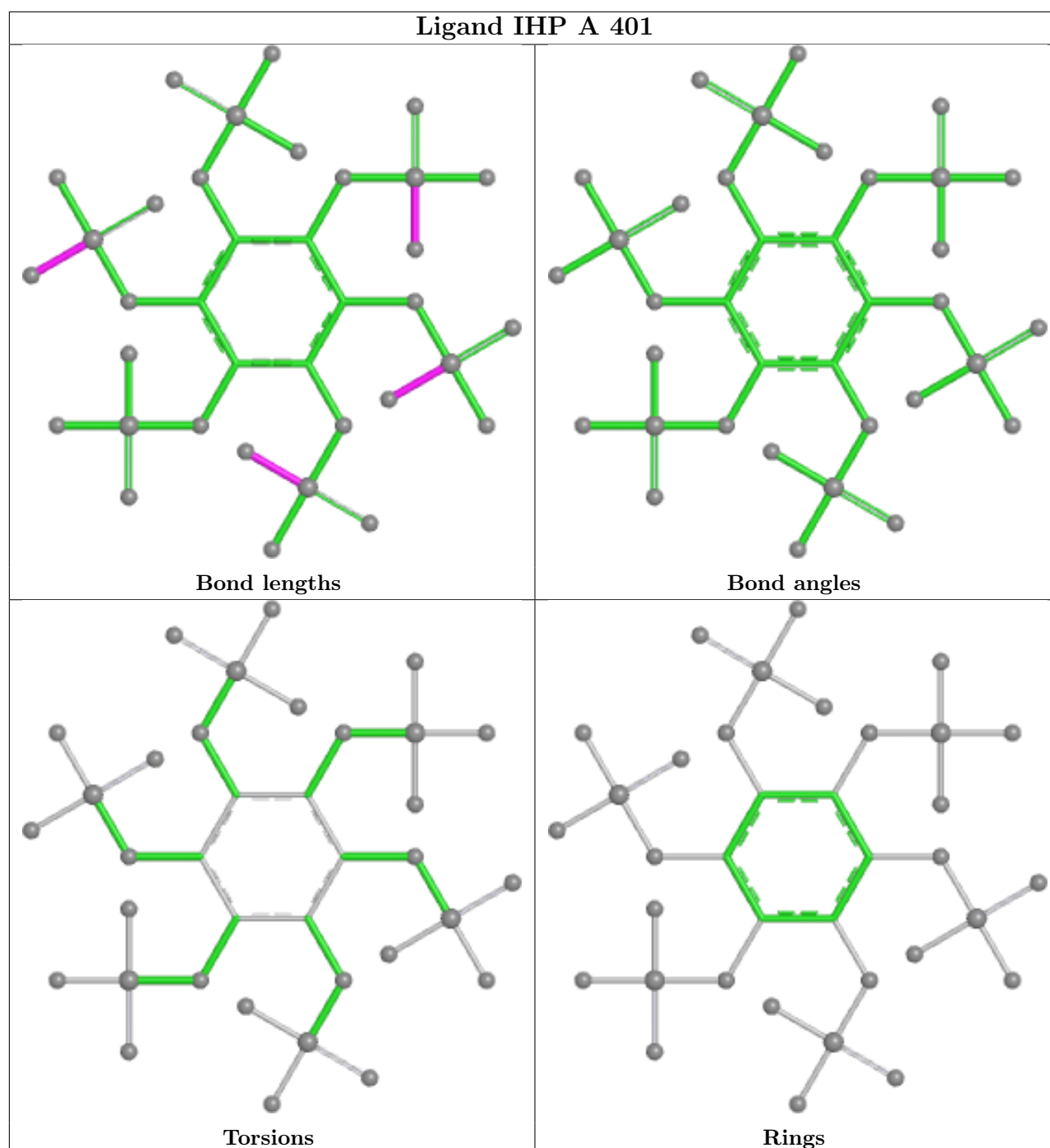
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	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

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	283/317 (89%)	0.75	27 (9%) 14 12	34, 62, 115, 163	0
1	B	288/317 (90%)	0.95	41 (14%) 6 6	35, 69, 121, 157	0
All	All	571/634 (90%)	0.85	68 (11%) 9 8	34, 65, 120, 163	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	ASP	11.5
1	A	95	ASN	8.7
1	B	85	LYS	5.8
1	B	42	ASP	5.0
1	A	314	ASN	5.0
1	B	171	SER	4.8
1	B	187	THR	4.4
1	B	25	ASP	4.4
1	B	173	CYS	4.4
1	A	326	PRO	4.1
1	B	192	ARG	4.1
1	B	326	PRO	3.8
1	B	193	GLY	3.6
1	A	30	PHE	3.6
1	A	91	GLN	3.5
1	A	186	LYS	3.4
1	B	295	ASP	3.4
1	B	84	TYR	3.3
1	B	298	SER	3.3
1	A	303	TYR	3.3
1	B	181	MET	3.3
1	B	33	PRO	3.2
1	A	188	LYS	3.2
1	B	88	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	325	HIS	3.1
1	B	90	ILE	3.1
1	A	305	GLN	3.0
1	B	170	ASN	3.0
1	B	257	GLN	2.9
1	A	315	LYS	2.8
1	A	70	TYR	2.8
1	A	42	ASP	2.8
1	A	277	LEU	2.7
1	B	108	PHE	2.7
1	B	297	TYR	2.7
1	A	316	ASN	2.7
1	B	82	LYS	2.7
1	B	301	ASN	2.6
1	A	106	LEU	2.6
1	B	175	ASP	2.6
1	B	32	THR	2.6
1	B	162	ALA	2.6
1	B	103	HIS	2.5
1	A	79	GLU	2.5
1	A	180	ARG	2.5
1	B	188	LYS	2.4
1	A	40	ASN	2.4
1	A	324	LYS	2.3
1	B	45	ILE	2.2
1	A	48	LEU	2.2
1	B	190	THR	2.2
1	B	179	LEU	2.2
1	A	312	LEU	2.2
1	B	195	LYS	2.2
1	B	180	ARG	2.2
1	B	325	HIS	2.2
1	B	47	ALA	2.2
1	B	303	TYR	2.1
1	A	317	LEU	2.1
1	A	44	ALA	2.1
1	B	34	GLU	2.1
1	B	169	TYR	2.1
1	A	96	SER	2.1
1	B	280	THR	2.1
1	A	82	LYS	2.1
1	A	35	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	96	SER	2.0
1	B	205	LEU	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](#)

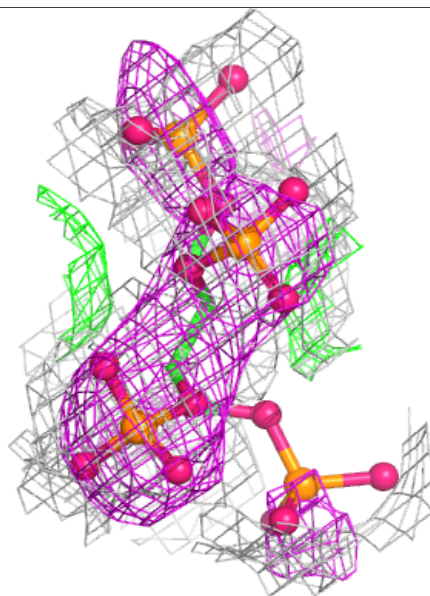
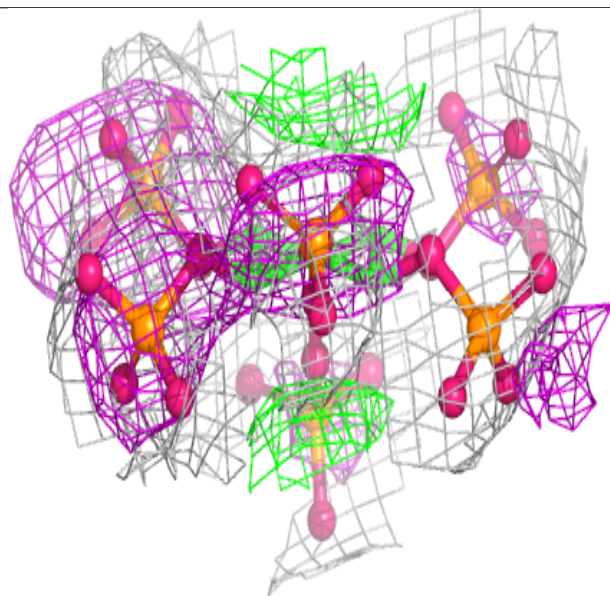
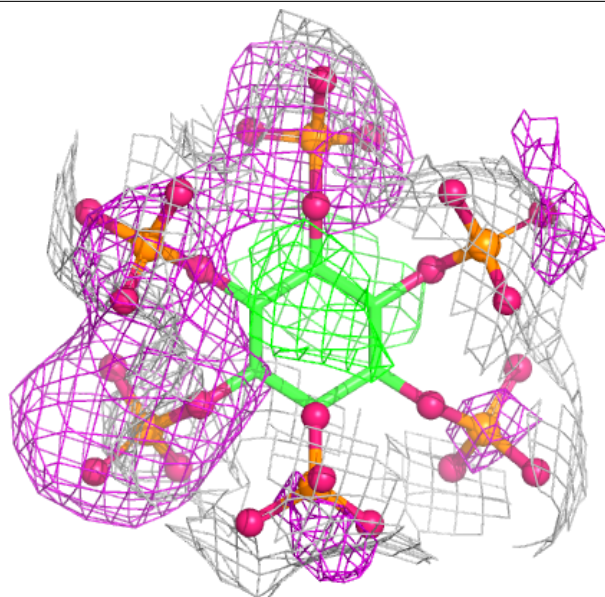
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

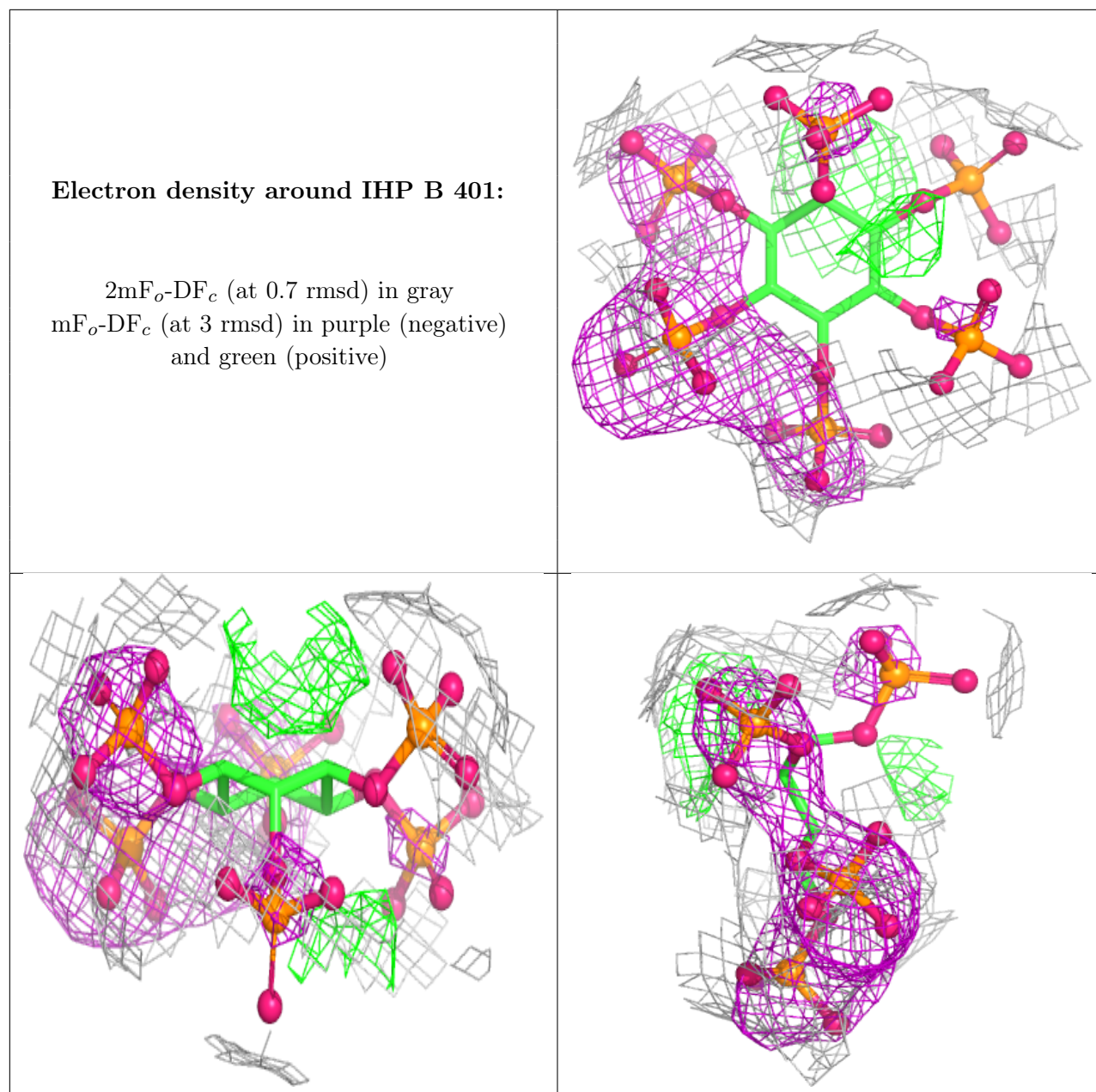
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IHP	A	401	36/36	0.44	0.17	98,98,98,98	0
2	IHP	B	401	36/36	0.44	0.16	98,98,98,98	0

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

Electron density around IHP A 401:

$2mF_o-DF_c$ (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.