



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 24, 2026 – 09:43 PM EDT

PDB ID : 1DJZ / pdb_00001djz
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH INOSITOL-4,5-BISPHOSPHATE
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-08-24
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

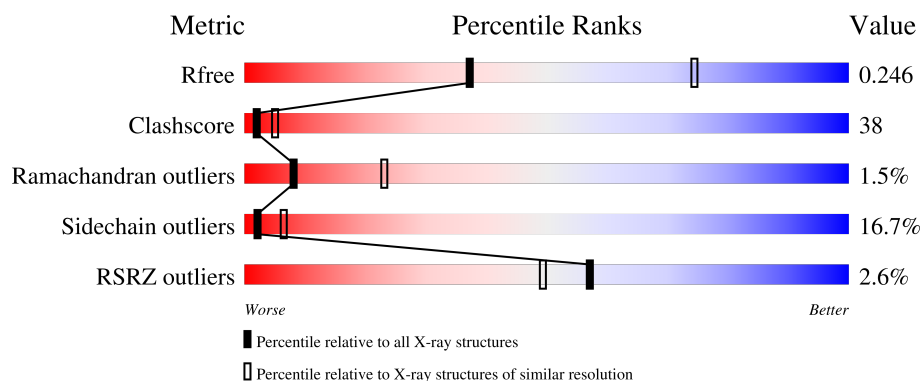
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	624	2% 34% 36% 11% • 18%
1	B	624	2% 36% 42% 10% • 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8840 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.

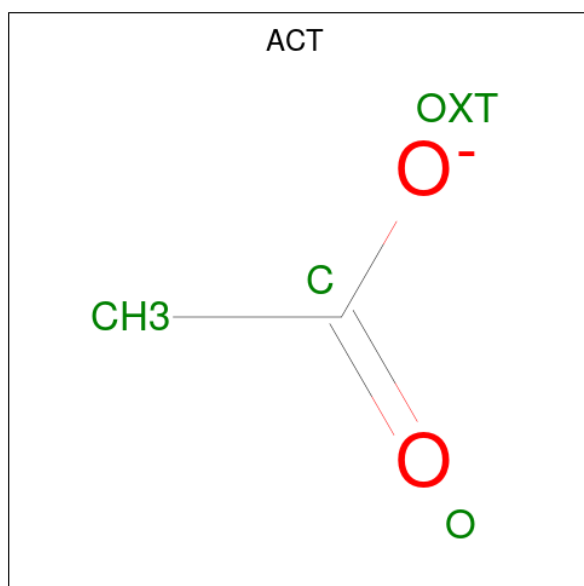
- Molecule 1 is a protein called PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	82	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	109	0	0
			4465	2818	776	847	24			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

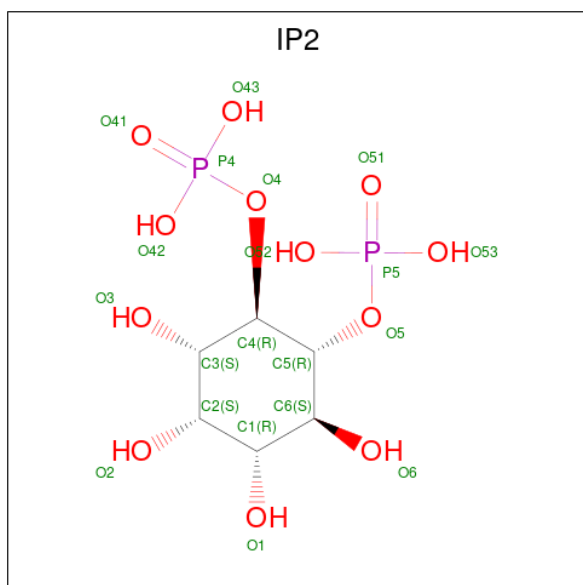
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is D-MYO-INOSITOL-4,5-BISPHOSPHATE (CCD ID: IP2) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		

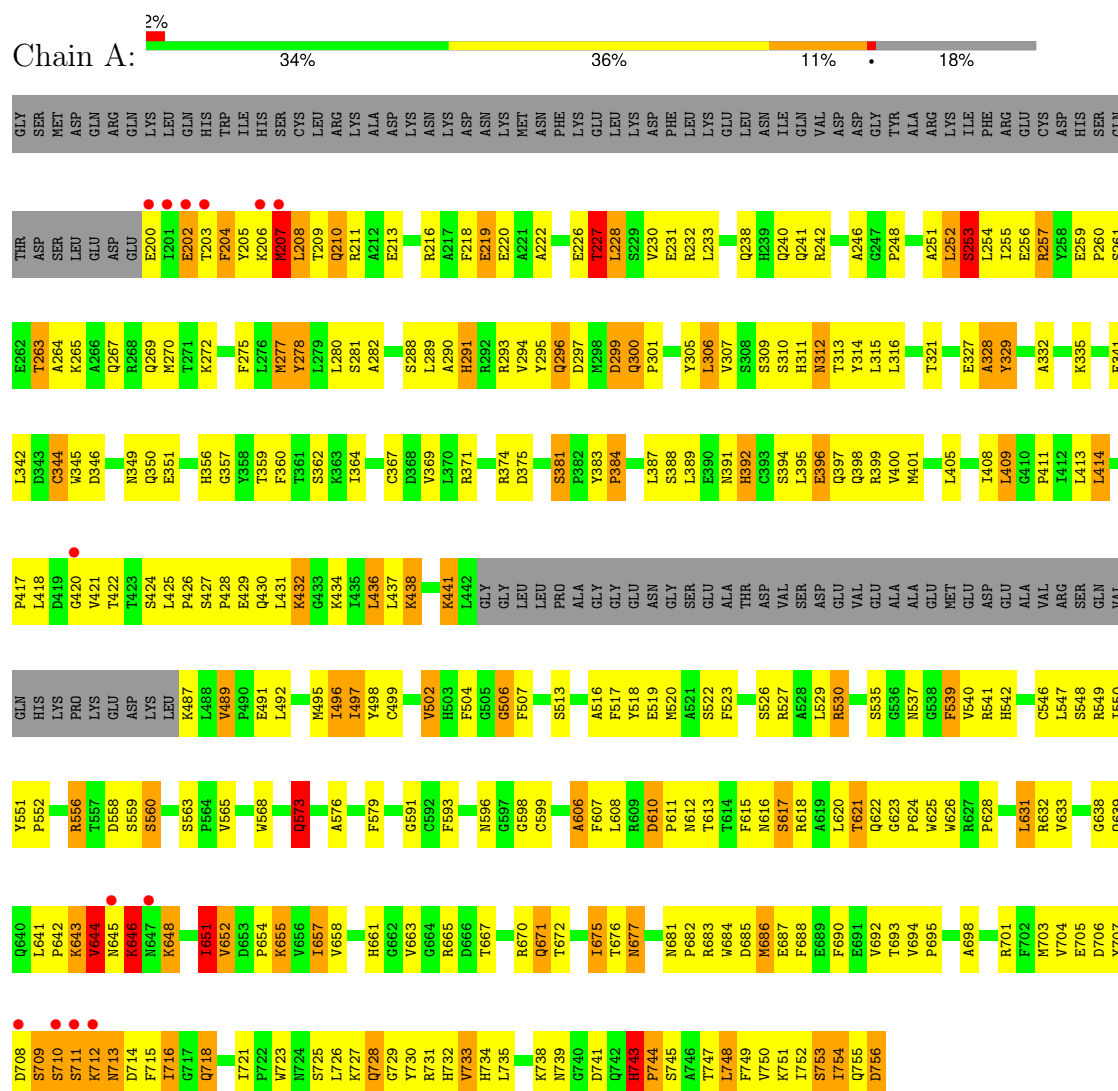
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	141	Total	O	0	0
			141	141		

3 Residue-property plots

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: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1



• Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1



D706	G638	L547	GLU	L418	C344	T263	T193	GLY
Y707	Q639	S548	D484	L421	W345	A264	D194	SER
D708	Q640	R549	K485	T422	D346	A265	S195	MET
S709	P642	I550	L486	T423		A266	L196	ASP
S710		P552	K487	T424	Q350	Q267	E197	GLN
			L488	S424	E351	Q268	E198	ARG
			W489	L425	P352	Q269	E199	GLN
			P490	P426	I353	K270	E200	LYS
			E491	S427		T271	T201	LEU
			L492		H356	K272	E202	GLN
			S493	L431	Q357		T203	HIS
			D494	K432	Y358		F204	TRP
			M495	G433	T359		Y205	ILE
			I496	K434			K266	HIS
			T497	L435	S362		M207	SER
			Y498	L436	K363			CYS
			K500	L437	I364		Q210	LEU
			K509	K438			R211	ARG
			S501	G439	V369		A212	LYS
			W502	K440	L370		E213	ALA
			H503	K441	R371		D214	ASP
			F504	L445			D215	LYS
			G505		R374		F218	ASN
			F507	LEU	D375			LYS
			S508	PRO	D376			ASP
			S509	ALA	A377		A221	H158
			P510	GLY	F378			K159
			G511	GLU	K379		E226	M160
			T512	ASN			T227	H161
			S513	GLY	Y383		L228	F162
			S514	SER	P384		S229	K163
			Q515	GLU	V385		V230	E164
			A516	ALA				L165
			F517	THR	S388		L233	K166
			Y518	ASP	K389		V234	D167
			E519	VAL	E390		T235	F168
			W520	SER	K391		F236	L169
				ASP	H392		L237	K170
				GLU	C393		Q238	E171
			F523	GLU	S394		H239	L172
			S524	VAL	L395		Q240	M173
			E525	GLU	E396		Q241	I174
			S526	ALA	Q397		R242	G175
			R527	ALA	Q398		E243	H176
			A528	GLU	R399		E244	D177
			L529	MET	V400		E245	D178
			R530	GLU	W401		A246	G179
			L531	ASP				Y180
			L532	GLU	L405		A251	A181
			Q533	ALA	A328		L252	R182
			S534	VAL	T408		S253	K183
			G535	ARG	L409		L254	I184
			G536	SER	G410		T255	F185
			N537	GLN	P411		E256	R186
				VAL	T412		R257	E187
			R541	GLN	L413		Y258	C188
			H542	HIS	L414		E259	D189
				LYS	D415		P260	H190
			S545	PRO	Q416		S261	S191
			C546	LYS	P417		E262	Q192

4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	396.49Å 396.49Å 396.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.95 10.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.95) 91.8 (10.00-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.89Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.212 , 0.270 0.194 , 0.246	Depositor DCC
R_{free} test set	2048 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 106.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8840	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: IP2, CA, ACT

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	1.32	23/4152 (0.6%)	1.36	39/5624 (0.7%)
1	B	1.31	15/4565 (0.3%)	1.35	41/6174 (0.7%)
All	All	1.31	38/8717 (0.4%)	1.35	80/11798 (0.7%)

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	692	VAL	CA-CB	-8.46	1.43	1.53
1	B	565	VAL	CA-CB	-8.34	1.44	1.54
1	B	520	MET	SD-CE	-8.04	1.59	1.79
1	B	330	ILE	CA-CB	-7.94	1.44	1.54
1	A	277	MET	SD-CE	7.92	1.99	1.79

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LEU	N-CA-C	-11.30	97.79	111.69
1	B	508	SER	N-CA-C	10.31	123.90	112.97
1	B	226	GLU	N-CA-C	-9.48	99.38	113.61
1	A	202	GLU	N-CA-C	-8.96	99.69	111.24
1	A	226	GLU	N-CA-C	-8.95	102.06	113.16

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	4057	0	3972	305	0
1	B	4465	0	4375	332	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	20	0	9	3	0
4	B	20	0	9	4	0
5	A	125	0	0	4	0
5	B	141	0	0	19	0
All	All	8840	0	8371	629	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 38.

The worst 5 of 629 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:B:196:LEU:HD22	1:B:200:GLU:HB3	1.28	1.14
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.38	1.03
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.23	1.01
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.41	1.00
1:B:728:GLN:NE2	1:B:754:ILE:H	1.59	1.00

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	509/624 (82%)	449 (88%)	51 (10%)	9 (2%)	6 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	557/624 (89%)	485 (87%)	65 (12%)	7 (1%)	9	26
All	All	1066/1248 (85%)	934 (88%)	116 (11%)	16 (2%)	8	23

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	VAL
1	A	646	LYS
1	A	712	LYS
1	B	173	ASN
1	B	645	ASN

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	444/545 (82%)	372 (84%)	72 (16%)	2	7
1	B	492/545 (90%)	408 (83%)	84 (17%)	2	5
All	All	936/1090 (86%)	780 (83%)	156 (17%)	2	6

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	488	LEU
1	B	676	THR
1	B	508	SER
1	B	617	SER
1	B	715	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	291	HIS
1	B	349	ASN

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Mol	Chain	Res	Type
1	B	739	ASN
1	B	319	GLN
1	B	542	HIS

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IP2	B	1	2	20,20,20	2.19	8 (40%)	32,32,32	2.00	11 (34%)
3	ACT	B	5	-	3,3,3	1.03	0	3,3,3	1.00	0
3	ACT	A	5	-	3,3,3	0.97	0	3,3,3	0.91	0
4	IP2	A	1	2	20,20,20	2.16	9 (45%)	32,32,32	1.63	8 (25%)

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	IP2	B	1	2	-	1/10/34/34	0/1/1/1
4	IP2	A	1	2	-	1/10/34/34	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	IP2	P4-O4	4.65	1.67	1.59
4	A	1	IP2	P4-O4	4.25	1.67	1.59
4	B	1	IP2	P4-O41	4.12	1.63	1.50
4	A	1	IP2	P5-O51	3.88	1.62	1.50
4	A	1	IP2	P4-O41	3.82	1.62	1.50

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	IP2	C3-C2-C1	4.65	119.00	110.83
4	B	1	IP2	O1-C1-C2	-4.24	100.39	110.38
4	B	1	IP2	C1-C6-C5	3.81	118.32	109.68
4	A	1	IP2	O2-C2-C1	-3.61	101.86	110.38
4	B	1	IP2	O2-C2-C1	-3.30	102.60	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	IP2	C6-C5-O5-P5
4	B	1	IP2	C5-O5-P5-O53

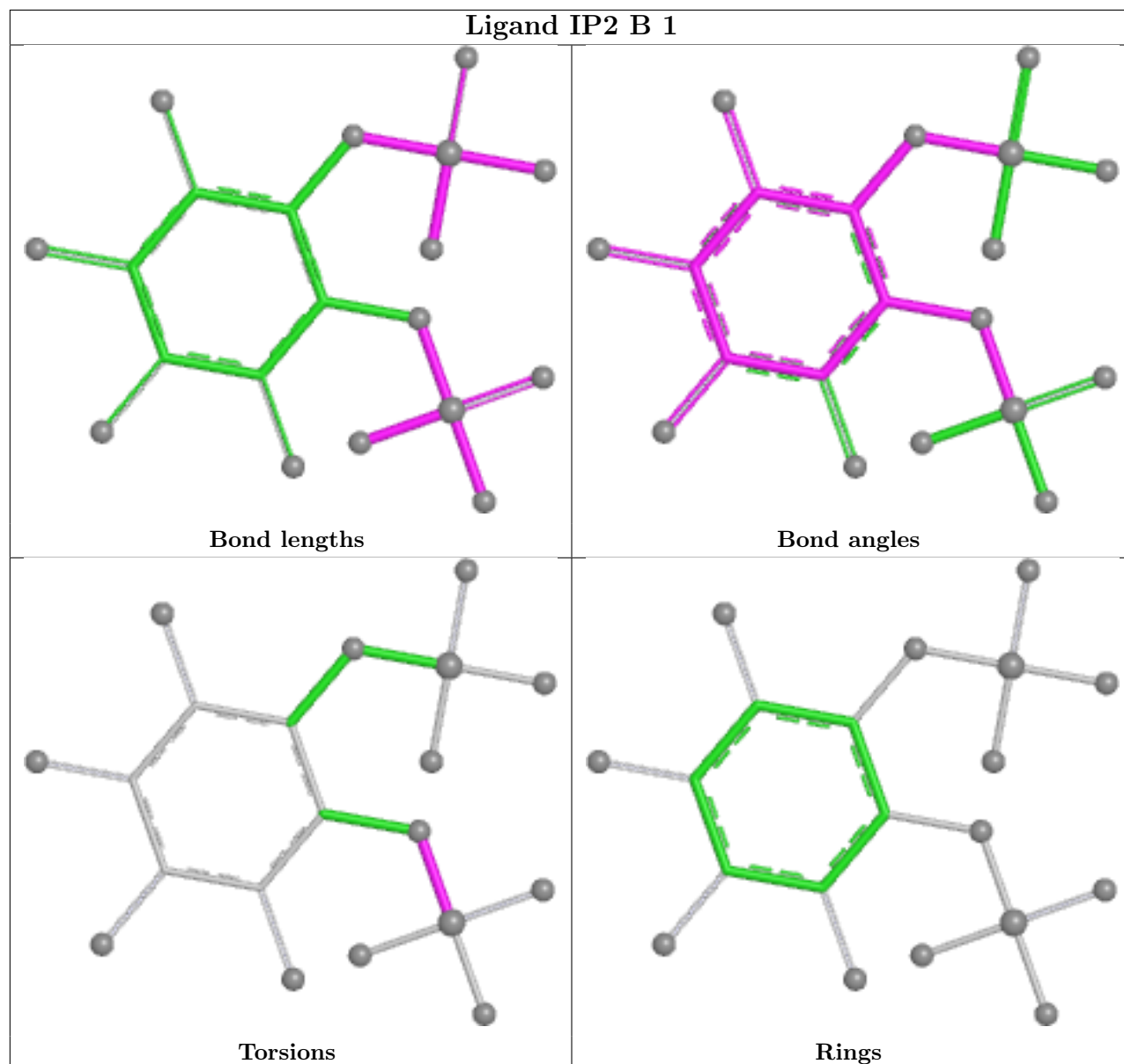
There are no ring outliers.

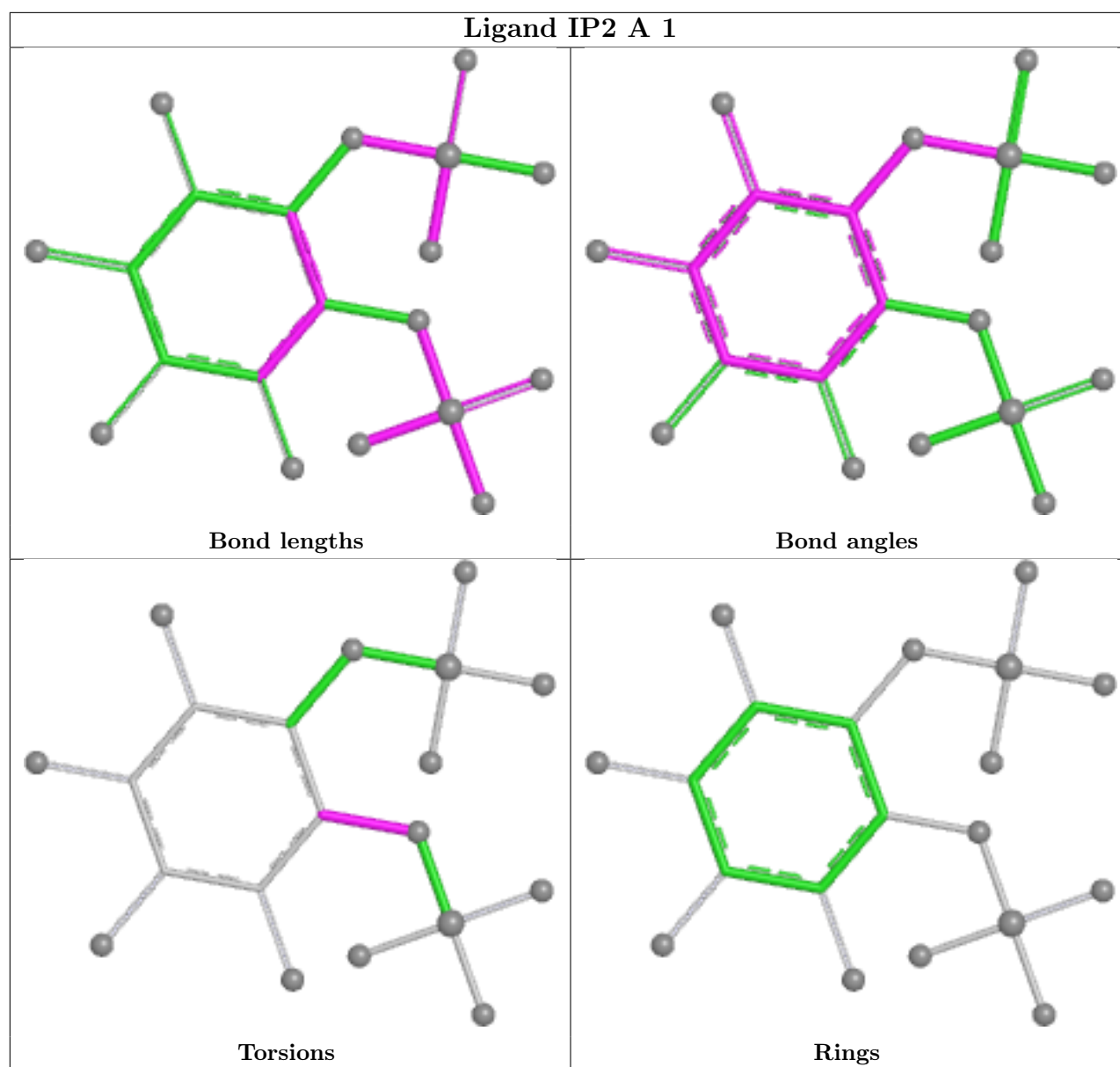
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	IP2	4	0
4	A	1	IP2	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	508/624 (81%)	-0.48	13 (2%)	57 49	4, 22, 77, 127	14 (2%)
1	B	558/624 (89%)	-0.47	15 (2%)	56 48	4, 23, 74, 118	23 (4%)
All	All	1066/1248 (85%)	-0.48	28 (2%)	57 49	4, 23, 76, 127	37 (3%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LYS	6.2
1	B	514	GLY	5.7
1	B	649	ASN	5.0
1	A	201	ILE	4.7
1	A	647	ASN	4.2

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](#)

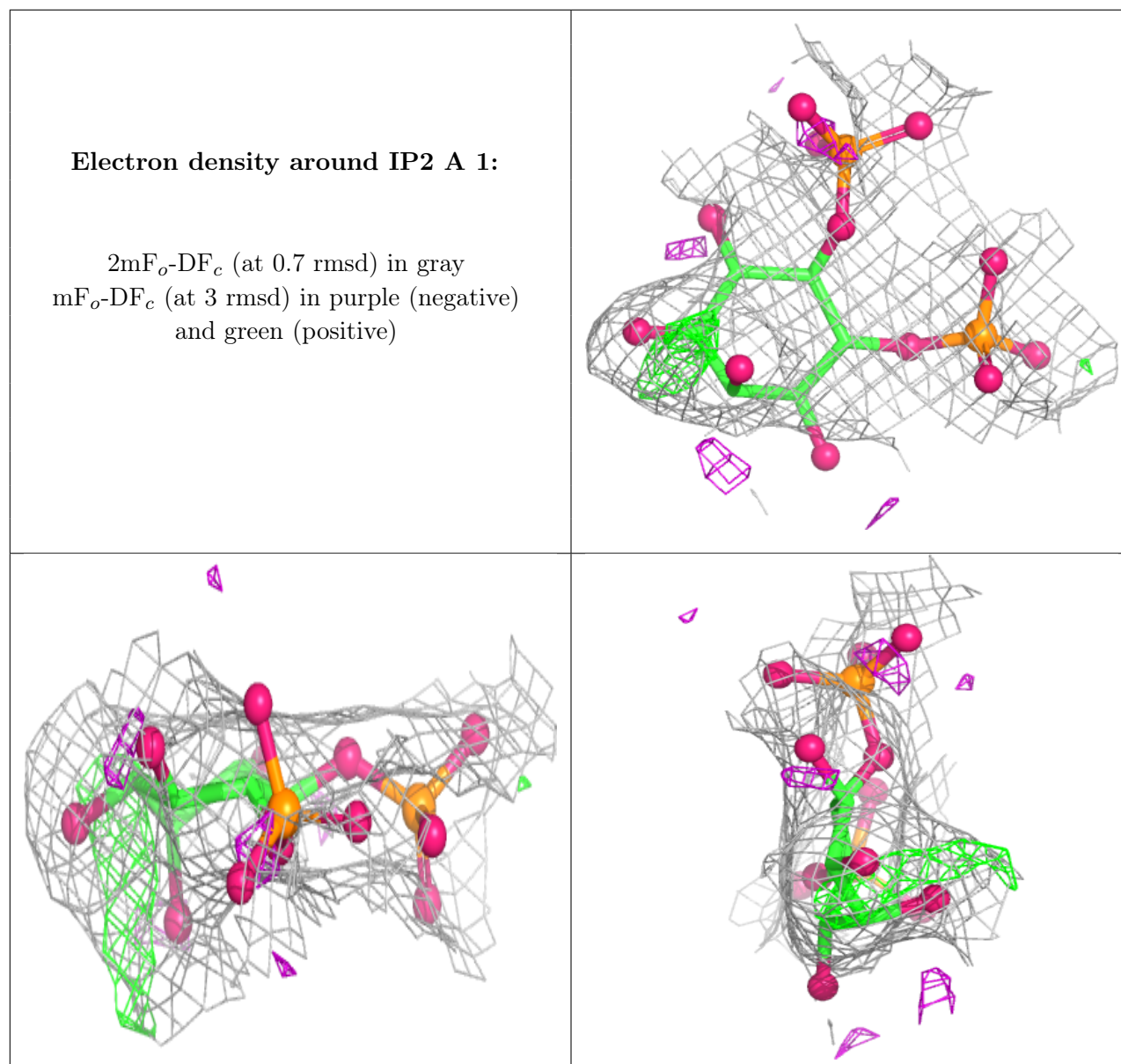
There are no oligosaccharides in this entry.

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.

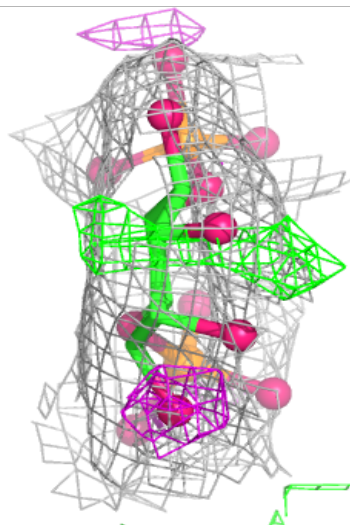
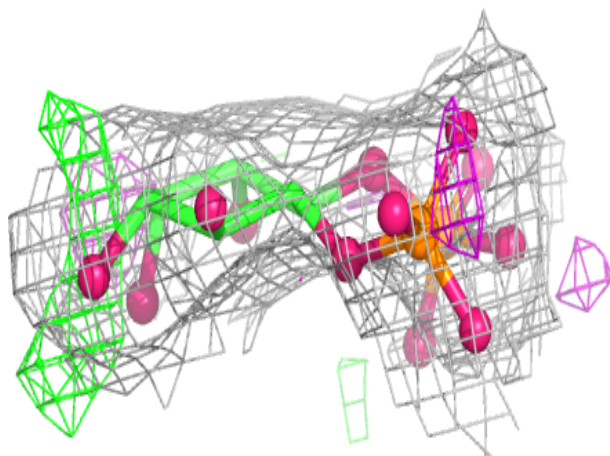
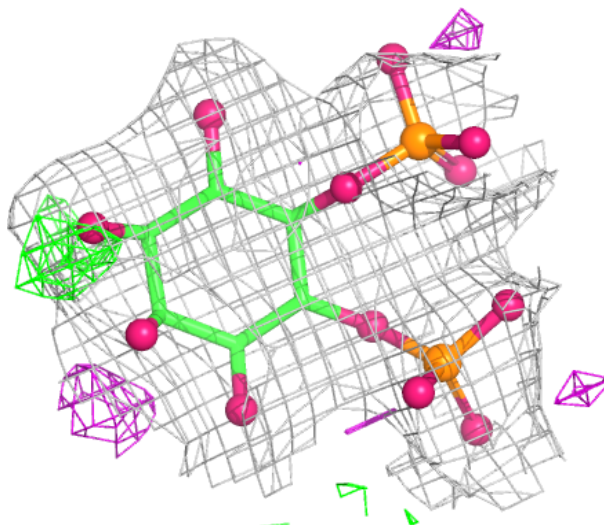
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IP2	A	1	20/20	0.84	0.16	70,97,136,136	0
4	IP2	B	1	20/20	0.84	0.12	53,74,108,110	0
3	ACT	A	5	4/4	0.92	0.11	36,38,38,39	0
2	CA	A	2	1/1	0.92	0.05	59,59,59,59	0
2	CA	B	3	1/1	0.92	0.04	74,74,74,74	0
2	CA	A	3	1/1	0.94	0.07	66,66,66,66	0
3	ACT	B	5	4/4	0.97	0.06	25,26,27,29	0
2	CA	B	2	1/1	0.99	0.02	37,37,37,37	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 IP2 B 1:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.