



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 07:24 PM EDT

PDB ID : 3UJ0 / pdb_00003uj0
Title : Crystal structure of the inositol 1,4,5-trisphosphate receptor with ligand bound form.
Authors : Ikura, M.; Seo, M.D.; Ishiyama, N.; Stathopulos, P.
Deposited on : 2011-11-07
Resolution : 3.60 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

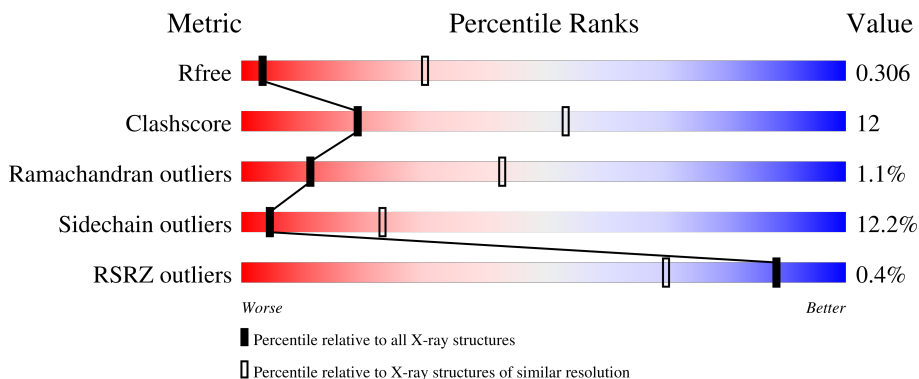
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	604	
1	B	604	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7779 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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	502	3850	2438	681	724	7	0	0	0
1	B	502	3872	2453	687	725	7	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

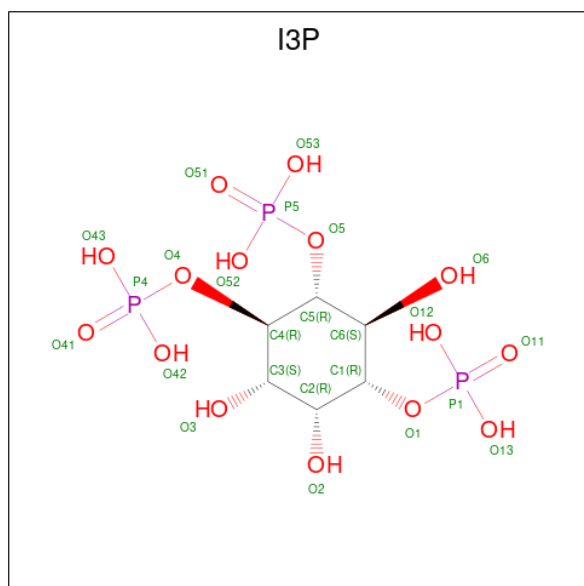
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	CYS	engineered mutation	UNP P29994
A	37	ALA	CYS	engineered mutation	UNP P29994
A	56	ALA	CYS	engineered mutation	UNP P29994
A	61	ALA	CYS	engineered mutation	UNP P29994
A	206	ALA	CYS	engineered mutation	UNP P29994
A	214	ALA	CYS	engineered mutation	UNP P29994
A	253	ALA	CYS	engineered mutation	UNP P29994
A	292	ALA	CYS	engineered mutation	UNP P29994
A	326	ALA	CYS	engineered mutation	UNP P29994
A	394	ALA	CYS	engineered mutation	UNP P29994
A	530	ALA	CYS	engineered mutation	UNP P29994
A	553	ALA	CYS	engineered mutation	UNP P29994
A	556	ALA	CYS	engineered mutation	UNP P29994
B	15	ALA	CYS	engineered mutation	UNP P29994
B	37	ALA	CYS	engineered mutation	UNP P29994
B	56	ALA	CYS	engineered mutation	UNP P29994
B	61	ALA	CYS	engineered mutation	UNP P29994
B	206	ALA	CYS	engineered mutation	UNP P29994
B	214	ALA	CYS	engineered mutation	UNP P29994
B	253	ALA	CYS	engineered mutation	UNP P29994
B	292	ALA	CYS	engineered mutation	UNP P29994
B	326	ALA	CYS	engineered mutation	UNP P29994
B	394	ALA	CYS	engineered mutation	UNP P29994
B	530	ALA	CYS	engineered mutation	UNP P29994
B	553	ALA	CYS	engineered mutation	UNP P29994

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Chain	Residue	Modelled	Actual	Comment	Reference
B	556	ALA	CYS	engineered mutation	UNP P29994

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: $C_6H_{15}O_{15}P_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			P
2	A	1	Total	C	O	P	0	0
			24	6	15	3		
2	B	1	Total	C	O	P	0	0
			24	6	15	3		

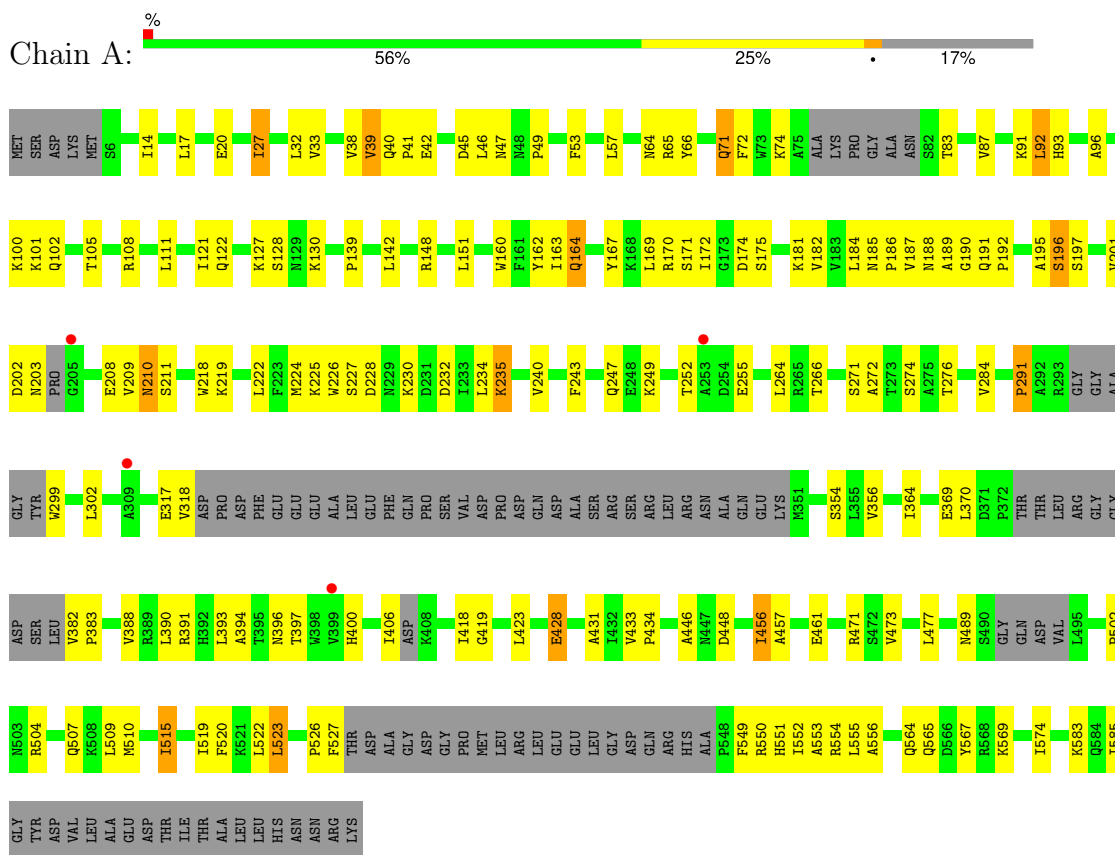
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	A	5	Total	O	0	0
			5	5		
3	B	4	Total	O	0	0
			4	4		

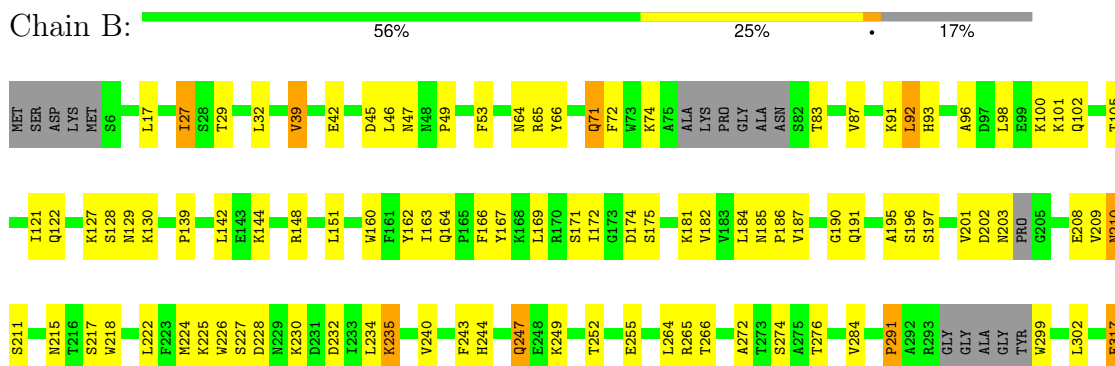
3 Residue-property plots [i](#)

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: Inositol 1,4,5-trisphosphate receptor type 1



- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



V318	ASP
V318	PRD
V318	ASP
V318	PHE
V318	GLU
V318	GLU
V318	ALA
V318	LEU
V318	GLU
V318	PHE
V318	GLN
V318	PRO
V318	SER
V318	VAL
V318	ASP
V318	PRO
V318	ASP
V318	GLN
V318	ASP
V318	ALA
V318	ALA
V318	SER
V318	ARG
V318	SER
V318	ARG
V318	LEU
V318	ASN
V318	ALA
V318	GLN
V318	GLU
V318	LYS
V318	M351
V318	V352
V318	Y353
V318	S354
V318	L355
V318	V356
V318	I364
V318	E369
V318	L370
V318	D371
V318	P372
V318	THR
V318	THR
V318	LEU
V318	ARG
V318	GLY
V318	GLY
V318	ASP
V318	SER
V318	LEU
V318	V382
V318	P383
V318	V388
V318	R389
L390	GLY
L391	H392
L392	L393
L393	ASP
L394	A394
L395	T395
L396	N396
L397	T397
H400	H400
I406	I406
K406	K406
I418	I418
G419	G419
L423	L423
E428	E428
A431	A431
I432	I432
V433	V433
P434	P434
V435	V435
S436	S436
E439	E439
V440	V440
R441	R441
D442	D442
L443	L443
D444	D444
F445	F445
A446	A446
N447	N447
D448	D448
K451	K451
I456	I456
L460	L460
I465	I465
R471	R471
S472	S472
V473	V473
L477	L477
L480	L480
V481	V481
Y482	Y482
G487	G487
T488	T488
N489	N489
S490	S490
GLY	GLY
GLN	GLN
ASP	ASP
VAL	VAL
I495	I495
R504	R504
E505	E505
R506	R506
Q507	Q507
M510	M510
I515	I515
L522	L522
L523	L523
F527	F527
THR	THR
ASP	ASP
ALA	ALA
GLY	GLY
ASP	ASP
GLY	GLY
PRO	PRO
MET	MET
LEU	LEU
ARG	ARG
LEU	LEU
LEU	LEU
GLU	GLU
LEU	LEU
LEU	LEU
GLY	GLY
ASP	ASP
GLN	GLN
ARG	ARG
HIS	HIS
ALA	ALA
F548	F548
F549	F549
I552	I552
A553	A553
R554	R554
L555	L555
V559	V559
Q564	Q564
Y567	Y567
R568	R568
K569	K569
I574	I574
K583	K583
G584	G584
I585	I585
TYR	TYR
ASP	ASP
VAL	VAL
LEU	LEU
ALA	ALA
GLU	GLU
ASP	ASP
THR	THR
ILE	ILE
THR	THR
ALA	ALA
LEU	LEU
LEU	LEU
HIS	HIS
ASN	ASN
ASN	ASN
ARG	ARG
LYS	LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.17Å 78.72Å 134.11Å 90.00° 124.49° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-3.60) 99.5 (50.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.57Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.258 , 0.308 0.247 , 0.306	Depositor DCC
R_{free} test set	981 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	110.6	Xtrriage
Anisotropy	0.446	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7779	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.80% 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: I3P

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	0.65	0/3920	0.86	1/5309 (0.0%)
1	B	0.64	0/3943	0.85	1/5336 (0.0%)
All	All	0.64	0/7863	0.86	2/10645 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	LYS	N-CA-C	5.37	116.94	111.14
1	A	196	SER	N-CA-C	5.36	116.83	110.19

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	3850	0	3728	93	0
1	B	3872	0	3766	86	0
2	A	24	0	9	0	0
2	B	24	0	9	2	0
3	A	5	0	0	1	0
3	B	4	0	0	0	0
All	All	7779	0	7512	178	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 12.

The worst 5 of 178 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:564:GLN:HB3	1:A:574:ILE:HD12	1.53	0.90
1:B:196:SER:HB2	1:B:208:GLU:O	1.76	0.86
1:A:196:SER:HB2	1:A:208:GLU:O	1.77	0.85
1:A:49:PRO:HG2	1:A:291:PRO:HG2	1.59	0.83
1:B:171:SER:O	1:B:174:ASP:HB2	1.80	0.82

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	484/604 (80%)	420 (87%)	57 (12%)	7 (1%)	9	38
1	B	484/604 (80%)	423 (87%)	57 (12%)	4 (1%)	16	49
All	All	968/1208 (80%)	843 (87%)	114 (12%)	11 (1%)	11	43

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	ARG
1	A	226	TRP
1	B	226	TRP
1	A	53	PHE
1	A	189	ALA

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	399/520 (77%)	350 (88%)	49 (12%)	4	23
1	B	403/520 (78%)	354 (88%)	49 (12%)	5	23
All	All	802/1040 (77%)	704 (88%)	98 (12%)	5	23

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	GLN
1	B	210	ASN
1	B	121	ILE
1	B	172	ILE
1	B	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	396	ASN
1	B	564	GLN
1	B	403	ASN
1	B	507	GLN
1	A	403	ASN

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	I3P	B	1000	-	24,24,24	0.73	0	39,39,39	0.90	0
2	I3P	A	1000	-	24,24,24	0.68	0	39,39,39	0.98	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	I3P	B	1000	-	-	4/15/39/39	0/1/1/1
2	I3P	A	1000	-	-	4/15/39/39	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

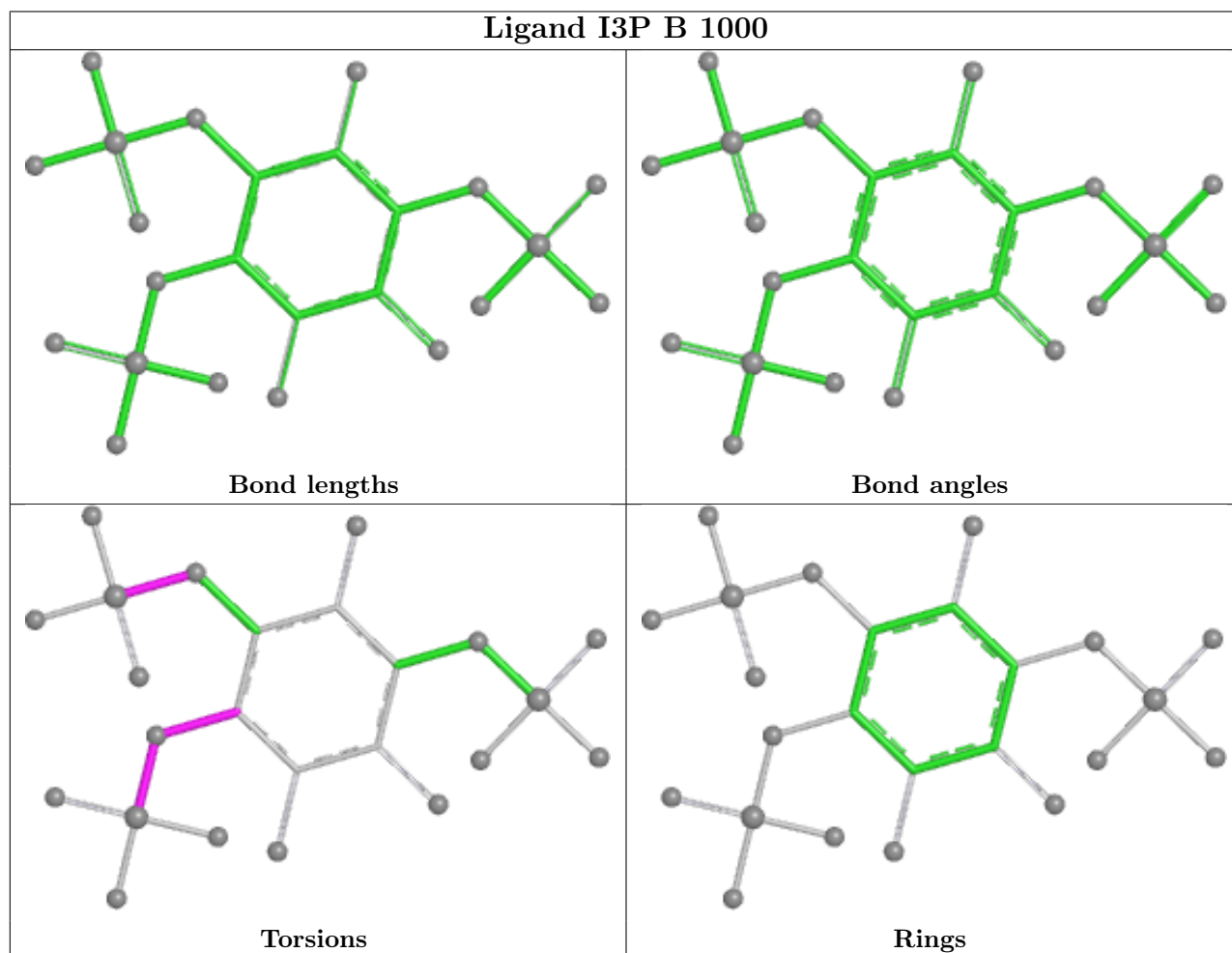
Mol	Chain	Res	Type	Atoms
2	B	1000	I3P	C3-C4-O4-P4
2	B	1000	I3P	C5-C4-O4-P4
2	A	1000	I3P	C5-O5-P5-O52
2	A	1000	I3P	C5-O5-P5-O51
2	A	1000	I3P	C4-O4-P4-O42

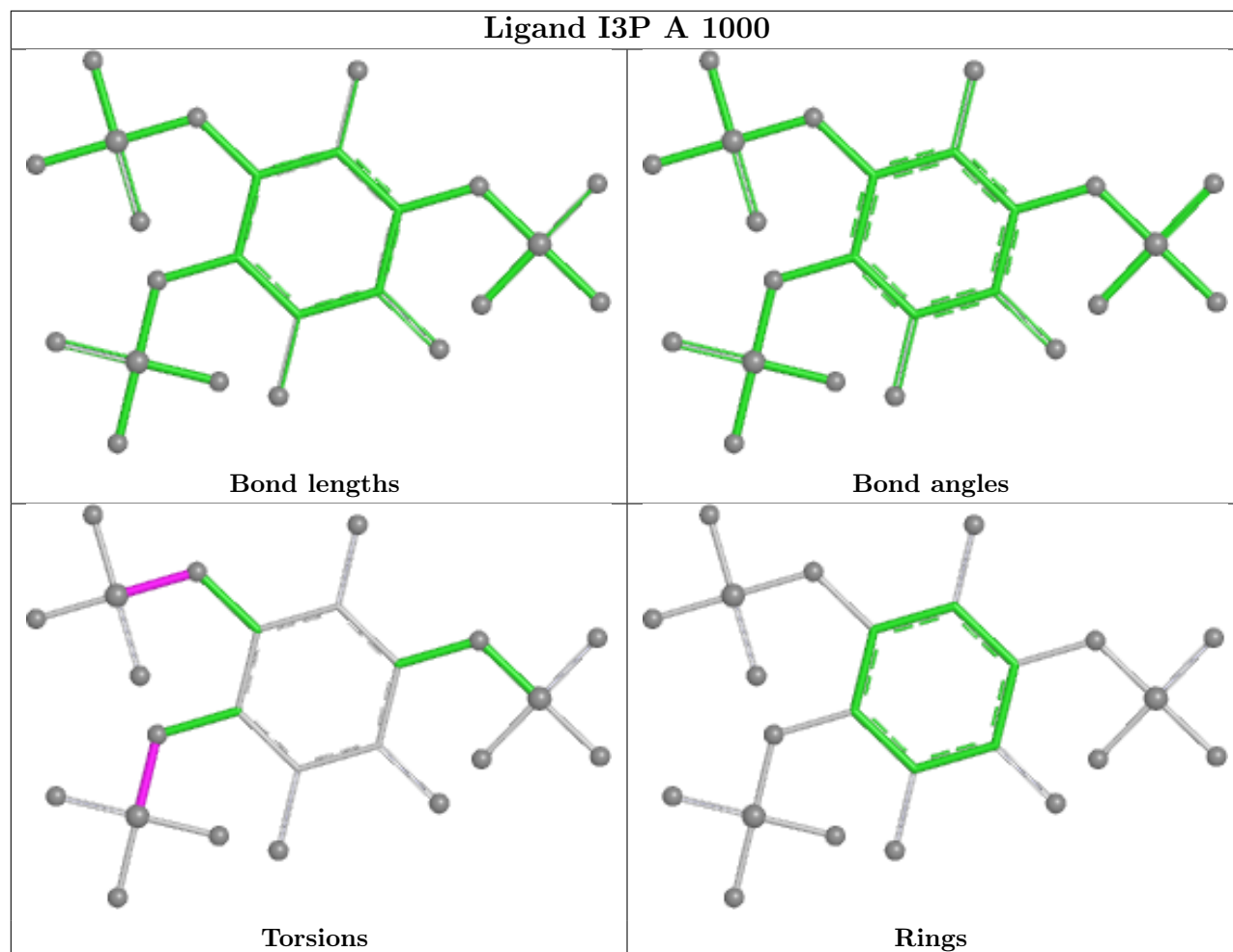
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	I3P	2	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	502/604 (83%)	-0.20	4 (0%) 82 58	80, 130, 185, 208	0
1	B	502/604 (83%)	-0.25	0 100 100	78, 130, 182, 210	0
All	All	1004/1208 (83%)	-0.22	4 (0%) 88 70	78, 130, 184, 210	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	3.0
1	A	205	GLY	2.9
1	A	309	ALA	2.6
1	A	399	VAL	2.5

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.

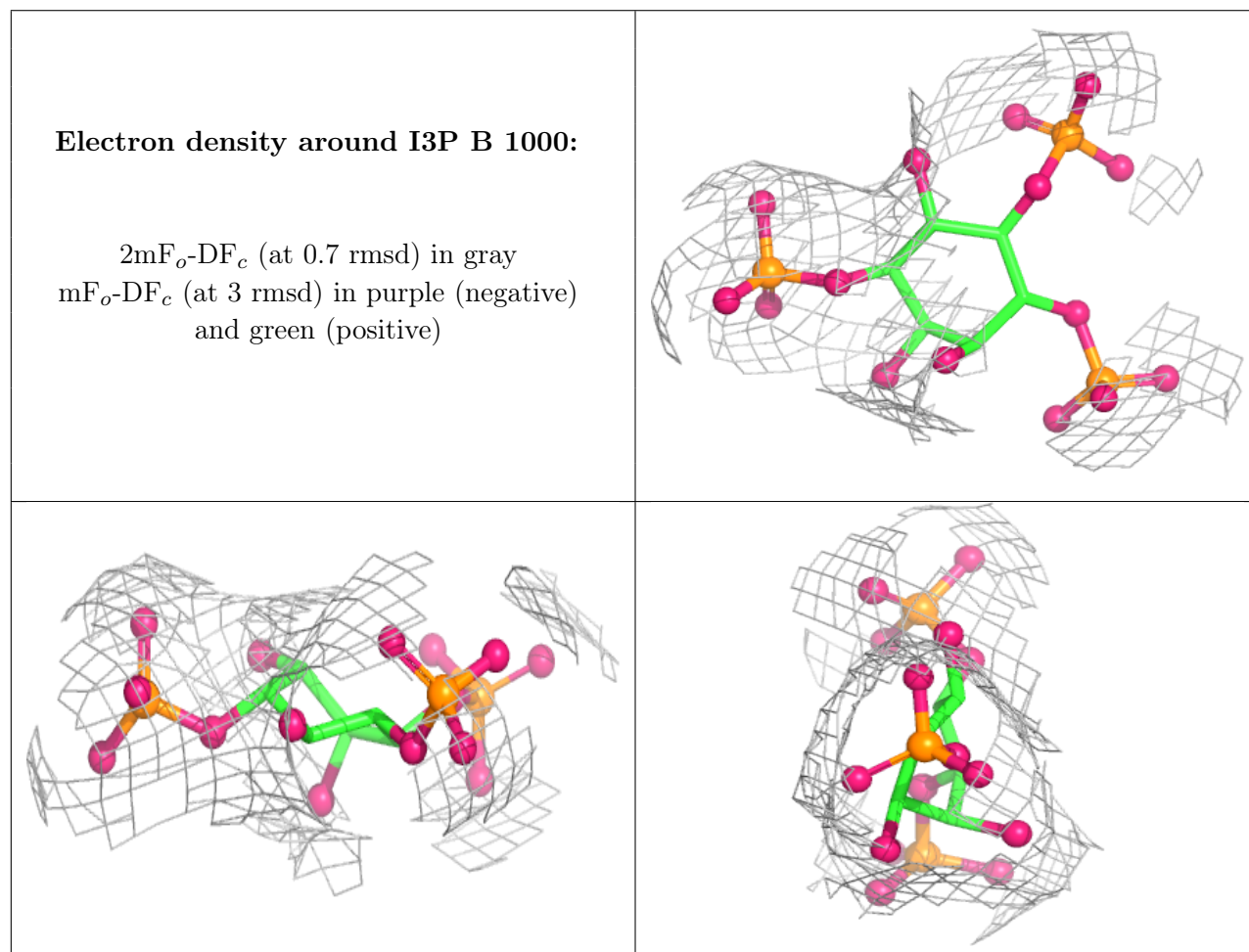
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	I3P	B	1000	24/24	0.86	0.07	141,148,156,162	0

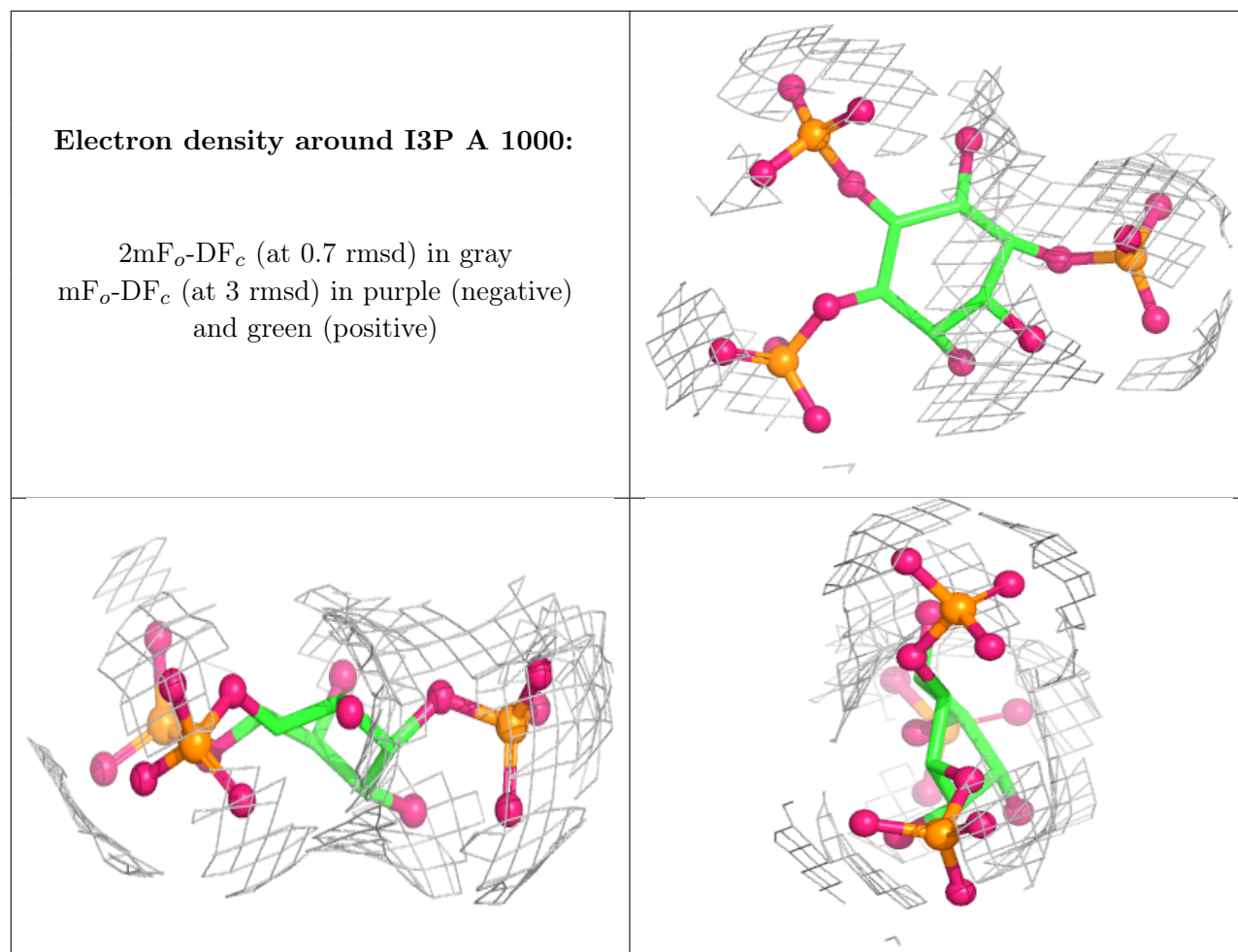
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	I3P	A	1000	24/24	0.88	0.06	136,156,165,168	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.