



wwPDB X-ray Structure Validation Summary Report

Feb 14, 2017 – 09:10 pm GMT

PDB ID : 1DJZ
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

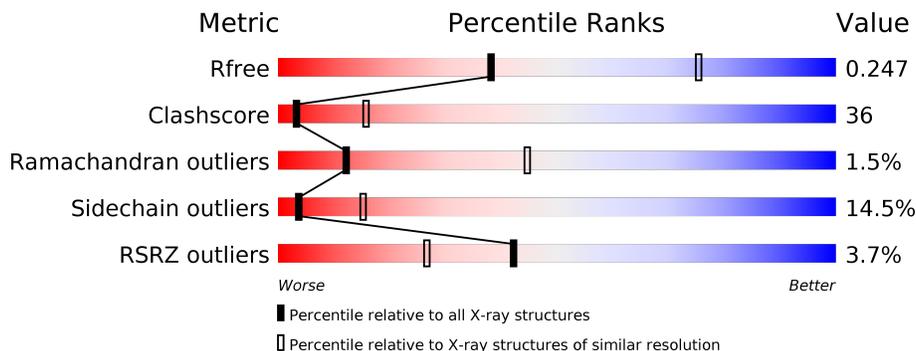
1 Overall quality at a glance

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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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. 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	 3% (red), 39% (green), 36% (yellow), 7% (orange), 18% (grey)
1	B	624	 3% (red), 40% (green), 43% (yellow), 6% (orange), 10% (grey)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IP2	A	1	-	-	-	X

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.

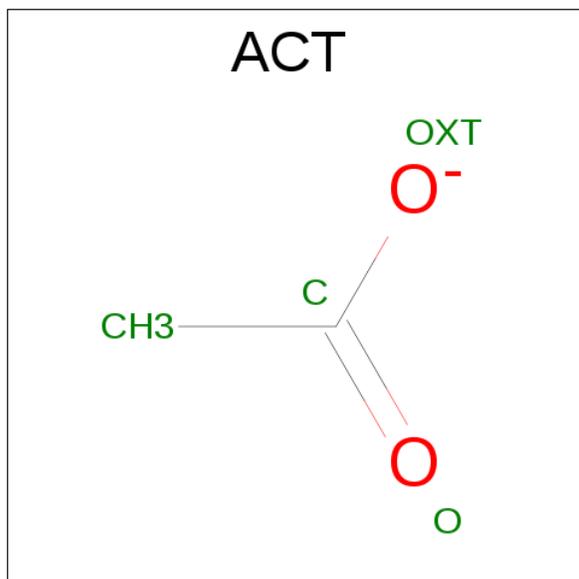
- Molecule 1 is a protein called PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

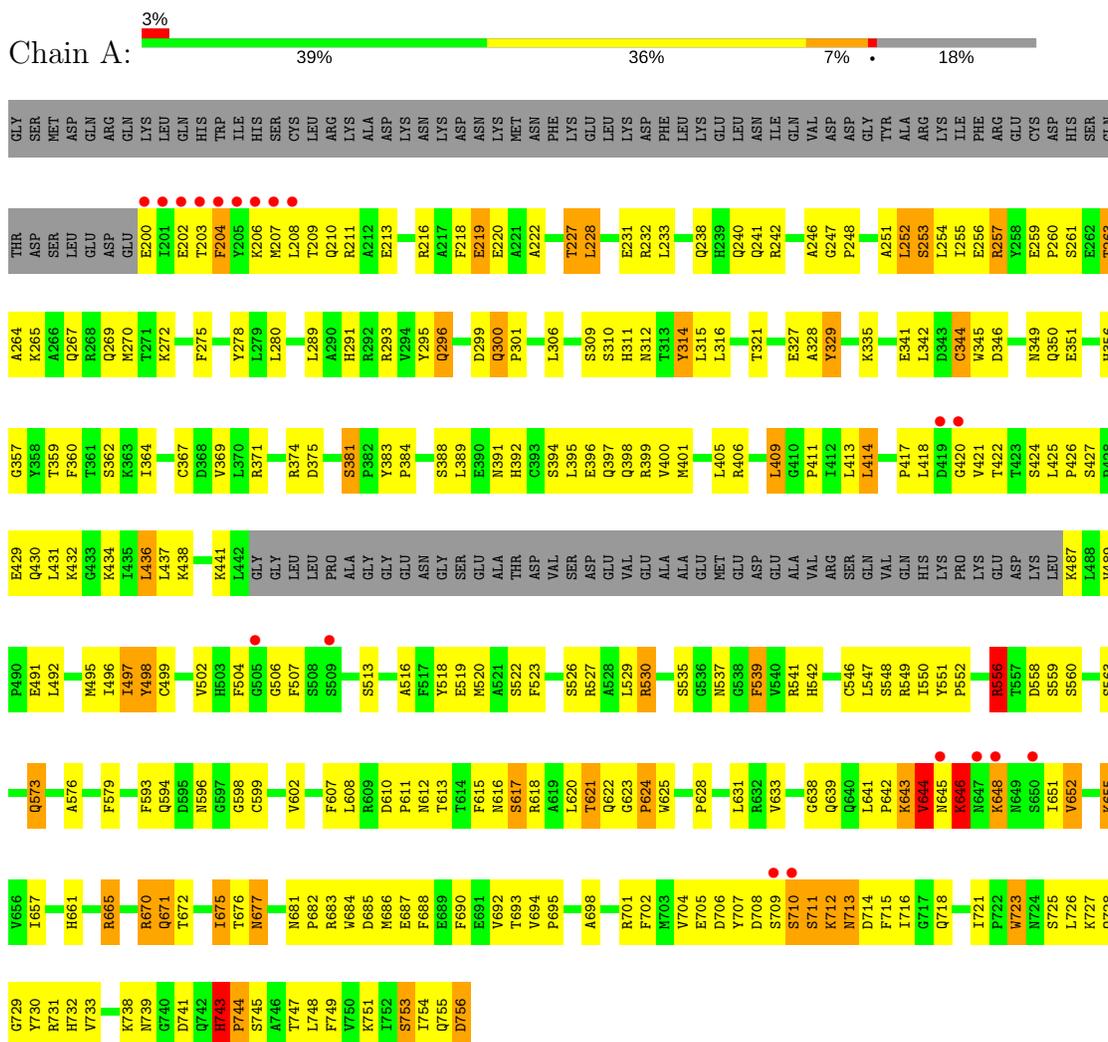
- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



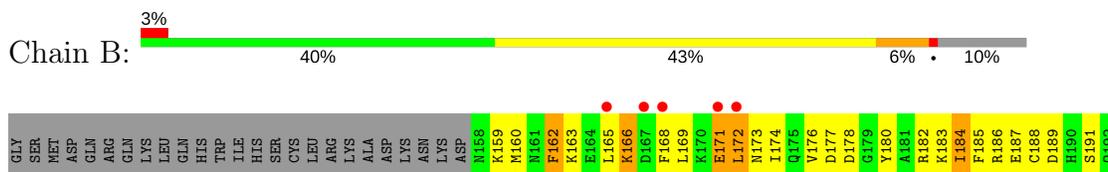
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



Q728	P654	R556	E491	R426	P352	K265	T193
G729	K655	S560	L492	S427	I353	A266	D194
Y730	V656	S561	S493	L431	H356	Q287	S195
R731	I657	N561	D494	M495	G357	R268	L196
H732	V658	Y562	M495	K434	G357	Q269	E197
W733	E659	S563	I496	K434	Y358	M270	D198
H734	T660	S563	I497	L435	T359	T271	E199
L735	H661	Q573	Y498	L436	S362	E200	E200
L736	R665	A576	C499	L437	K363	I201	I201
S737	L577	K500	K500	K438	L276	F275	E202
K738	L577	S501	K438	G439	M277	L276	E203
N739	Q671	V502	K440	K441	L280	F204	F204
G740	V674	D587	H503	K441	L370	M207	M207
D741	L675	L590	F504	L445	R371	Q210	Q210
Q742	T676	F507	G505	LEU	G284	R211	R211
P744	N677	F507	F507	PRO	R374	A212	A212
T747	N678	F593	S508	ALA	D375	E213	E213
L748	M681	Q594	S509	GLY	Y376	I214	I214
F749	P682	D595	P510	GLY	A377	D215	D215
W750	R683	G597	G511	GLU	F378	R291	R291
K751	M684	G598	T512	ASN	K379	R292	R292
I752	M685	C599	S513	GLY	Y383	V294	V294
S753	D686	F607	G514	SER	P384	Y295	Y295
I754	M686	F607	Q515	GLU	Q296	Q296	Q296
Q755	E687	D610	A516	ALA	D297	D297	D297
D756	V692	F517	F517	THR	S388	M298	T228
	T693	Y518	Y518	ASP	L389	L228	L228
	V694	M519	M519	VAL	D299	Q300	Q300
	P695	M520	M520	SER	N391	P301	R232
	D696	T613	T613	ASP	H392	L233	L233
	L697	T614	T614	GLU	C393	V234	V234
	A698	F615	S524	VAL	S394	T235	T235
	R701	N616	E525	GLU	L395	F236	F236
	F702	R618	S526	ALA	E396	L237	L237
	M703	R618	R527	ALA	Q397	Q238	Q238
	V704	T621	A528	GLU	Q398	H239	H239
	E705	Q622	L529	MET	R399	Q240	Q240
	D706	Q623	R530	GLU	V400	Q241	Q241
	Y707	P624	L531	ASP	M401	R242	R242
	D708	W625	Q533	GLU	L405	E243	E243
	S709	W626	M534	ALA	L316	E244	E244
	S710	R632	S535	VAL	R406	E245	E245
	N713	G638	G536	ARG	E327	A246	A246
	D714	Q639	N537	SER	A328	G247	G247
	F715	P642	M537	GLN	G410	A251	A251
	I716	R645	G638	VAL	P411	L252	L252
	G717	N647	F539	GLN	I412	S253	S253
	Q718	K648	V540	HIS	L413	L254	L254
	S719	N649	R541	LYS	L414	T255	T255
	T720	S650	H542	PRO	D415	E256	E256
	I721	I651	C546	LYS	Q416	L340	L340
	P722	I651	K646	GLU	P417	E341	E341
	S725	I651	N647	D484	L418	R257	R257
	L726	I651	K648	L485	L342	E258	E258
	K727	I651	N649	K487	L342	E259	E259
		I651	S650	L488	L342	P260	P260
		I651	I651	V421	L342	S261	S261
		I651	I651	T422	L342	E262	E262
		I651	I651	T423	L342	T263	T263
		I651	I651	S424	L342	Q350	Q350
		I651	I651	P490	L342	E351	E351

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 24.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.95) 94.2 (24.64-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.89Å)	Xtrriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.212 , 0.270 0.195 , 0.247	Depositor DCC
R_{free} test set	2048 reflections (4.01%)	DCC
Wilson B-factor (Å ²)	56.6	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 100.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	1.08	17/4152 (0.4%)	1.01	6/5624 (0.1%)
1	B	1.07	14/4565 (0.3%)	1.01	6/6174 (0.1%)
All	All	1.07	31/8717 (0.4%)	1.01	12/11798 (0.1%)

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	TYR	CE2-CZ	-11.14	1.24	1.38
1	A	329	TYR	CE2-CZ	-9.95	1.25	1.38
1	A	329	TYR	CG-CD1	-9.44	1.26	1.39
1	A	329	TYR	CE1-CZ	-8.93	1.26	1.38
1	B	498	TYR	CE1-CZ	-8.74	1.27	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	HIS	C-N-CD	-14.12	89.52	120.60
1	A	743	HIS	C-N-CD	-14.12	89.54	120.60
1	B	247	GLY	C-N-CD	-7.20	104.77	120.60
1	A	247	GLY	C-N-CD	-6.97	105.26	120.60
1	A	644	VAL	CB-CA-C	5.94	122.68	111.40

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	290	0
1	B	4465	0	4375	313	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	595	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 36.

The worst 5 of 595 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:504:PHE:HB3	1:A:527:ARG:HH22	1.23	1.01
1:B:728:GLN:NE2	1:B:754:ILE:H	1.59	1.00
1:A:548:SER:H	1:A:573:GLN:NE2	1.61	0.96
1:A:613:THR:HG22	1:A:615:PHE:H	1.28	0.95

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%)	10 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	557/624 (89%)	485 (87%)	65 (12%)	7 (1%)	14	48
All	All	1066/1248 (85%)	934 (88%)	116 (11%)	16 (2%)	12	45

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 [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	444/545 (82%)	381 (86%)	63 (14%)	4	16
1	B	492/545 (90%)	419 (85%)	73 (15%)	3	14
All	All	936/1090 (86%)	800 (86%)	136 (14%)	4	15

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	753	SER
1	B	232	ARG
1	B	685	ASP
1	B	159	LYS
1	B	178	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	GLN
1	B	312	ASN

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Mol	Chain	Res	Type
1	B	743	HIS
1	B	291	HIS
1	B	349	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 carbohydrates 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	A	1	2	20,20,20	2.04	6 (30%)	30,32,32	1.67	7 (23%)
3	ACT	A	5	-	1,3,3	3.94	1 (100%)	0,3,3	0.00	-
4	IP2	B	1	2	20,20,20	2.06	7 (35%)	30,32,32	2.02	9 (30%)
3	ACT	B	5	-	1,3,3	4.31	1 (100%)	0,3,3	0.00	-

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	A	1	2	-	0/10/34/34	0/1/1/1
3	ACT	A	5	-	-	0/0/0/0	0/0/0/0
4	IP2	B	1	2	-	0/10/34/34	0/1/1/1
3	ACT	B	5	-	-	0/0/0/0	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	IP2	P4-O42	2.00	1.63	1.54
4	B	1	IP2	P5-O53	2.06	1.63	1.54
4	B	1	IP2	P5-O52	2.11	1.63	1.54
4	A	1	IP2	C6-C5	2.27	1.58	1.52
4	A	1	IP2	P5-O5	2.42	1.63	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	IP2	O1-C1-C2	-4.58	100.39	110.36
4	A	1	IP2	O2-C2-C1	-3.90	101.86	110.36
4	B	1	IP2	O2-C2-C1	-3.57	102.60	110.36
4	B	1	IP2	O3-C3-C2	-3.13	103.55	110.36
4	A	1	IP2	C3-C2-C1	-3.09	105.39	110.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	IP2	3	0
4	B	1	IP2	4	0

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%)	-0.46	19 (3%)	42 27	4, 22, 82, 127	14 (2%)
1	B	558/624 (89%)	-0.40	20 (3%)	43 27	4, 23, 78, 118	23 (4%)
All	All	1066/1248 (85%)	-0.43	39 (3%)	42 27	4, 23, 81, 127	37 (3%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	SER	7.9
1	B	649	ASN	7.4
1	A	201	ILE	6.7
1	B	509	SER	6.0
1	B	514	GLY	5.7

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	IP2	A	1	20/20	0.77	0.31	3.67	70,97,136,136	0
4	IP2	B	1	20/20	0.81	0.22	1.56	53,74,108,110	0
3	ACT	B	5	4/4	0.98	0.12	0.12	25,26,27,29	0
3	ACT	A	5	4/4	0.95	0.13	-0.03	36,38,38,39	0
2	CA	B	3	1/1	0.94	0.15	-0.63	74,74,74,74	0
2	CA	B	2	1/1	0.95	0.07	-2.70	37,37,37,37	0
2	CA	A	2	1/1	0.91	0.09	-	59,59,59,59	0
2	CA	A	3	1/1	0.78	0.12	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.