



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

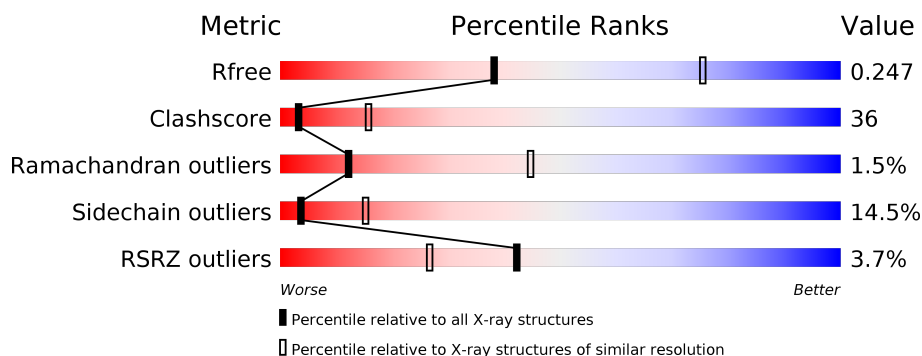
1 Overall quality at a glance

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	<div> <div>3%</div> <div> <div></div> <div>39%</div> <div>36%</div> <div>7%</div> <div>18%</div> </div> </div>
1	B	624	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>43%</div> <div>6%</div> <div>10%</div> </div> </div>

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.

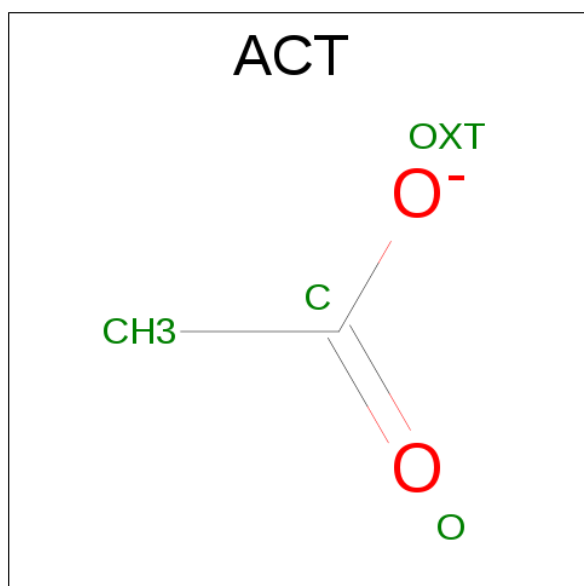
- Molecule 1 is a protein called PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 (three-letter code: CA) (formula: Ca).

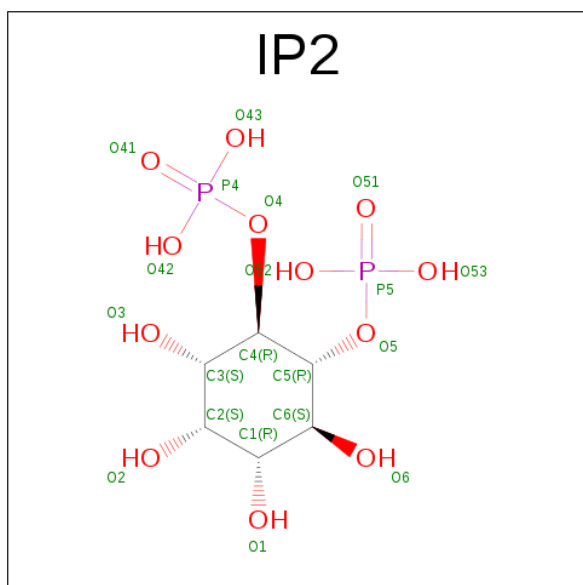
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETATE ION (three-letter code: 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 (three-letter code: 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		

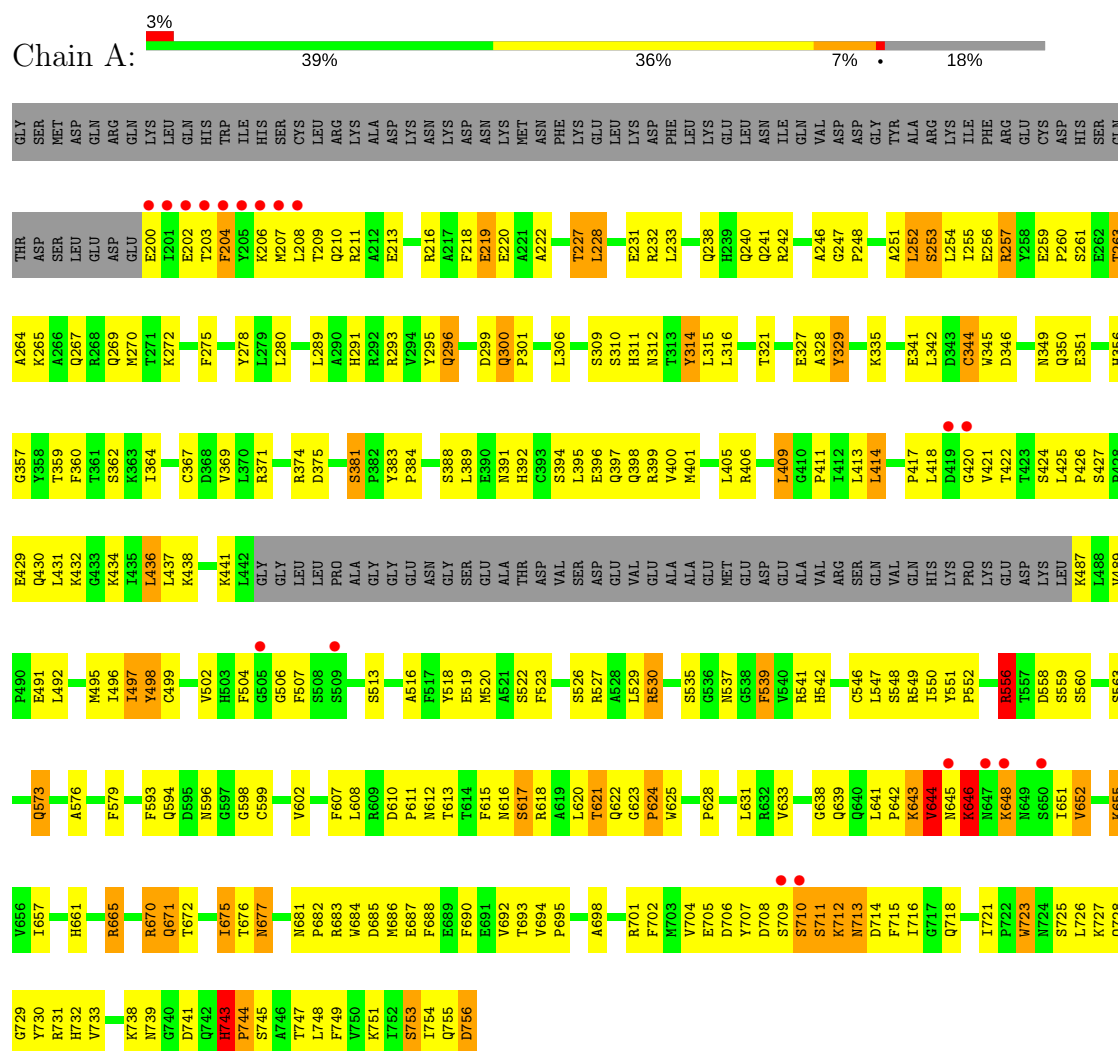
- Molecule 5 is water.

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

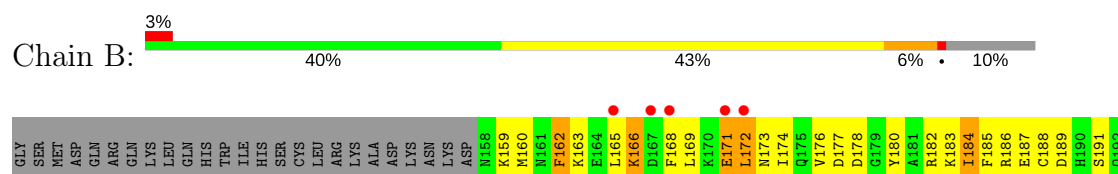
3 Residue-property plots

These plots are drawn for all protein, RNA 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



T193	K265	P352	P426	E491	R556	P654	Q728
D194	A266	I353	S427	L492	S560	K655	G729
S195	Q287	H356	L431	S493	N561	V656	R730
L196	R268	H356	L431	D494	S561	V657	Y731
E197	Q269	G357	K434	M495	Y562	V658	H732
D198	M270	Y358	L435	M495	S563	V659	V733
E199	T271	T359	L435	L497	Q573	T660	H734
E200	K272	S362	L436	Y498	Q573	H661	L735
1201	F275	K363	L437	C499	A576	R665	L736
E202	L276	I364	K438	K500	L577	K665	S737
T203	M277	L364	K439	S501	N578	Q671	K738
F204	L280	V369	K440	V502	N578	Q671	N739
M207	L280	L370	K441	H503	D587	V674	G740
Q210	G284	R371	L445	F504	L590	T675	D741
R211	F287	R371	LEU	G505	L590	T676	Q742
A212	H291	D375	PRO	F507	F593	N677	P744
E213	R292	R375	ALA	S508	Q594	N678	T747
T214	K293	Y376	GLY	S509	D595	N681	L748
D215	V294	A377	GLY	P510	N596	P682	F749
F218	R293	K379	GLU	G511	G597	R683	V750
A221	Y295	Y383	ASN	S512	G598	W684	K751
T227	Q296	P384	GLY	S513	C599	D685	I752
L228	D297	P384	SER	G514	Q515	W686	S753
R232	M298	S388	GLU	A516	F517	E687	I754
L233	M298	L389	ALA	F517	Y518	V692	Q755
V234	P301	E390	THR	Y518	E519	T693	D756
T235	Y305	N391	ASP	M520	M520	V694	
F236	L306	H392	ASP	F523	T613	P695	
L237	L306	C393	GLU	S524	T614	D696	
H239	S309	L395	VAL	E525	F615	L697	
Q240	H311	E396	ALA	S526	N616	A698	
Q241	N312	Q397	ALA	R527	R618		
R242	T313	Q398	GLU	A528	T621		
E243	Y314	R399	MET	L529	Q622		
L244	L315	V400	GLU	R530	G623		
E245	L316	M401	ASP	L531	P624		
A246	E327	L405	GLU	L532	W625		
G247	A328	R406	VAL	Q533	W626		
A251	Y329	L409	ARG	E534	R632		
L252	T330	G410	SER	G535	G638		
S253	R331	P411	GLN	G536	Q639		
L254	L333	I412	VAL	N537	P642		
T255	L340	L413	GLN	F539	P642		
E256	L342	A332	HIS	V540	R645		
R257	L342	L414	LYS	R541	K646		
E259	W345	D415	PRO	H542	N647		
P260	D346	Q416	LYS	C546	K648		
S261	Q350	L418	LYS	L547	R649		
T262	E351	V421	D484	S548	N650		
A264	E351	T422	L486	I550	I651		
		T423	K487	P552	W652		
		L425	V488		D653		
			P490				

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)	Xtriage
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	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 100.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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	1.08	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 ⓘ

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(Å²)	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

There are no such residues in this entry.