



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2017 – 07:58 PM EST

PDB ID : 5J16
Title : Crystal structure of Inositol monophosphate bound SaIMPase-II
Authors : Dutta, A.; Bhattacharyya, S.; Das, A.K.
Deposited on : 2016-03-29
Resolution : 2.40 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.

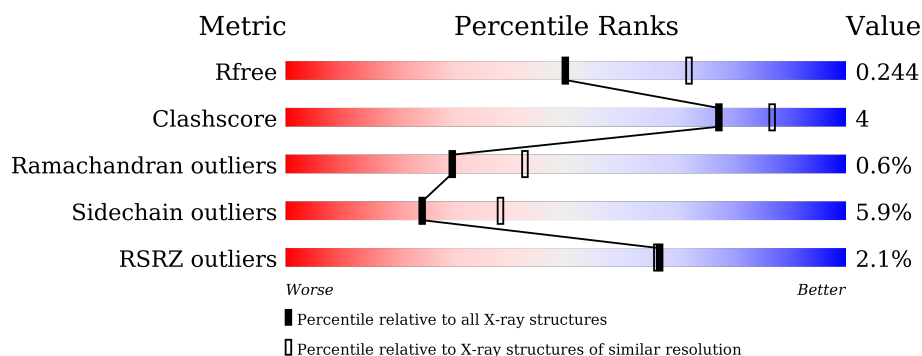
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20028442

i

X-RAY DIFFRACTION

A.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

Mol	Chain	Length	Quality of chain
1	A	283	<div> <div></div> <div>78%</div> <div>11%</div> <div>9%</div> </div>
1	B	283	<div> <div></div> <div>79%</div> <div>9%</div> <div>10%</div> </div>
1	C	283	<div> <div></div> <div>80%</div> <div>8%</div> <div>11%</div> </div>
1	D	283	<div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7985 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 monophosphatase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1970	1259	330	377	4			
1	B	254	Total	C	N	O	S	0	1	0
			1917	1224	322	367	4			
1	C	253	Total	C	N	O	S	0	0	0
			1936	1234	327	372	3			
1	D	254	Total	C	N	O	S	0	0	0
			1922	1230	325	364	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP A0A1I9GET0
A	-6	HIS	-	expression tag	UNP A0A1I9GET0
A	-5	HIS	-	expression tag	UNP A0A1I9GET0
A	-4	HIS	-	expression tag	UNP A0A1I9GET0
A	-3	HIS	-	expression tag	UNP A0A1I9GET0
A	-2	HIS	-	expression tag	UNP A0A1I9GET0
A	-1	GLY	-	expression tag	UNP A0A1I9GET0
A	0	SER	-	expression tag	UNP A0A1I9GET0
B	-7	HIS	-	expression tag	UNP A0A1I9GET0
B	-6	HIS	-	expression tag	UNP A0A1I9GET0
B	-5	HIS	-	expression tag	UNP A0A1I9GET0
B	-4	HIS	-	expression tag	UNP A0A1I9GET0
B	-3	HIS	-	expression tag	UNP A0A1I9GET0
B	-2	HIS	-	expression tag	UNP A0A1I9GET0
B	-1	GLY	-	expression tag	UNP A0A1I9GET0
B	0	SER	-	expression tag	UNP A0A1I9GET0
C	-7	HIS	-	expression tag	UNP A0A1I9GET0
C	-6	HIS	-	expression tag	UNP A0A1I9GET0
C	-5	HIS	-	expression tag	UNP A0A1I9GET0
C	-4	HIS	-	expression tag	UNP A0A1I9GET0
C	-3	HIS	-	expression tag	UNP A0A1I9GET0

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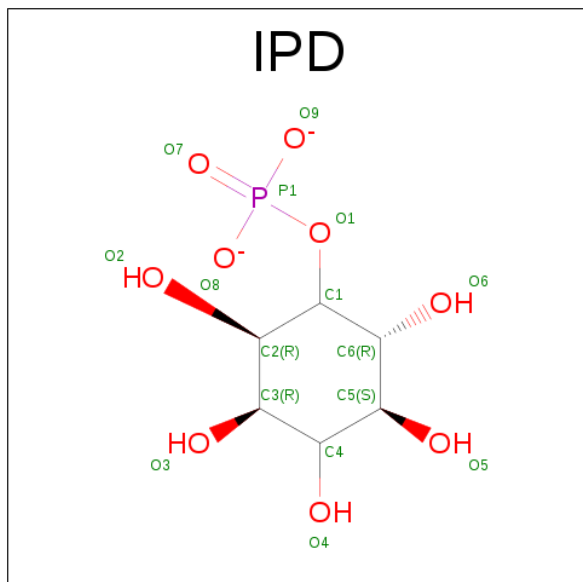
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP A0A1I9GET0
C	-1	GLY	-	expression tag	UNP A0A1I9GET0
C	0	SER	-	expression tag	UNP A0A1I9GET0
D	-7	HIS	-	expression tag	UNP A0A1I9GET0
D	-6	HIS	-	expression tag	UNP A0A1I9GET0
D	-5	HIS	-	expression tag	UNP A0A1I9GET0
D	-4	HIS	-	expression tag	UNP A0A1I9GET0
D	-3	HIS	-	expression tag	UNP A0A1I9GET0
D	-2	HIS	-	expression tag	UNP A0A1I9GET0
D	-1	GLY	-	expression tag	UNP A0A1I9GET0
D	0	SER	-	expression tag	UNP A0A1I9GET0

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

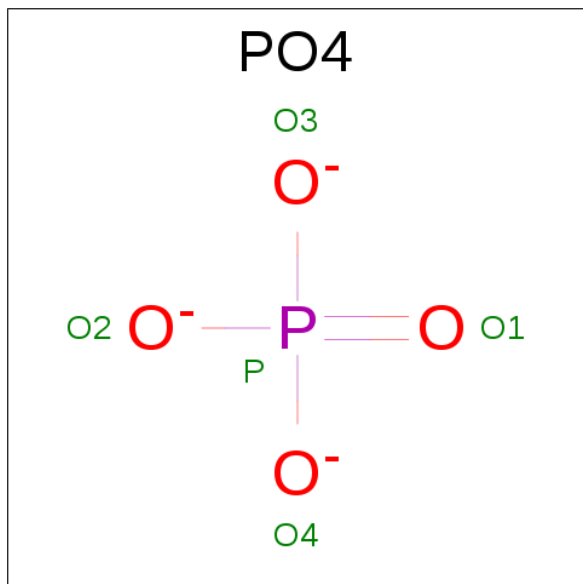
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ca 2 2	0	0
2	A	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0

- Molecule 3 is D-MYO-INOSITOL-1-PHOSPHATE (three-letter code: IPD) (formula: C₆H₁₁O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		

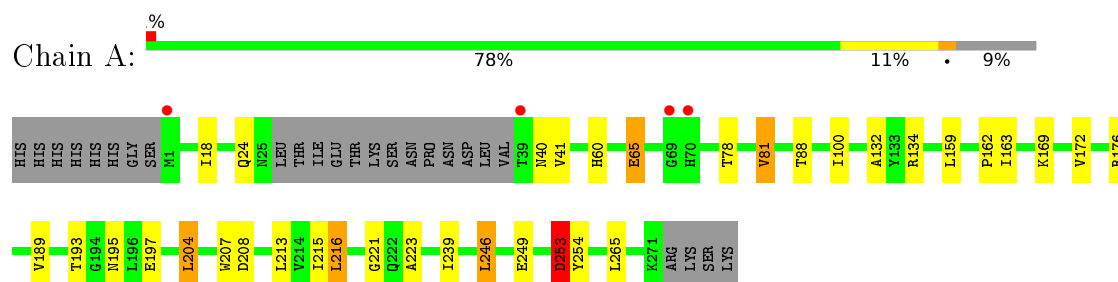
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	46	Total	O	0	0
			46	46		
5	C	38	Total	O	0	0
			38	38		
5	D	48	Total	O	0	0
			48	48		

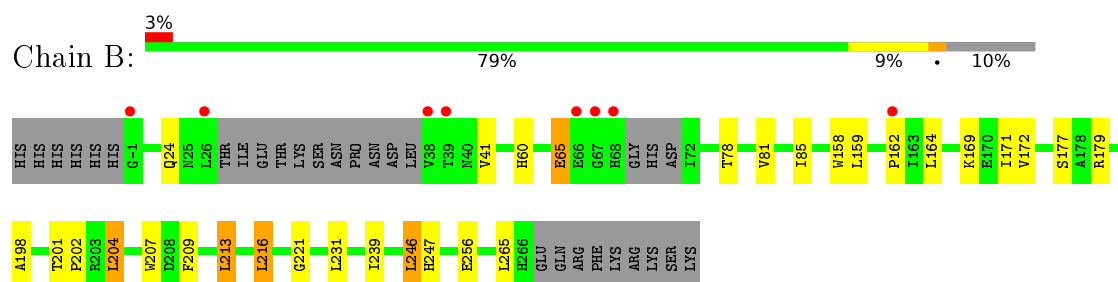
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

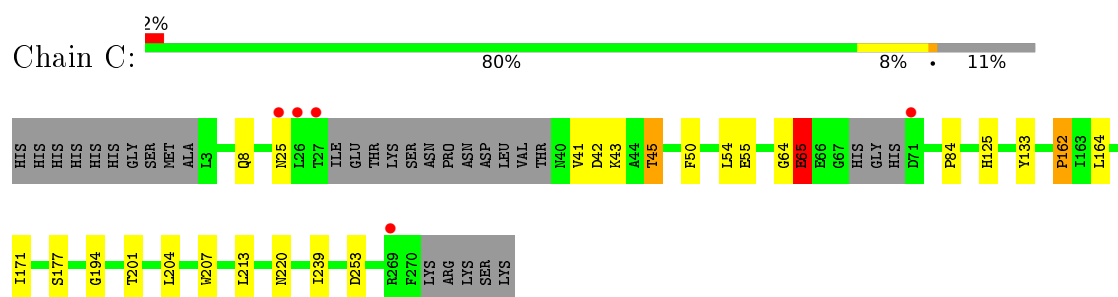
- Molecule 1: Inositol monophosphatase family protein



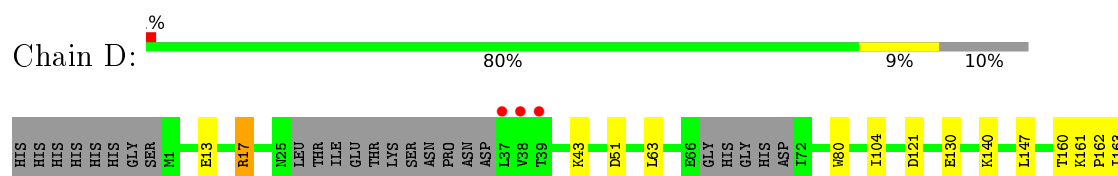
- Molecule 1: Inositol monophosphatase family protein



- Molecule 1: Inositol monophosphatase family protein



- Molecule 1: Inositol monophosphatase family protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.94Å 78.76Å 80.05Å 105.46° 102.28° 109.47°	Depositor
Resolution (Å)	72.79 – 2.40 19.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (72.79-2.40) 83.6 (19.75-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.237 0.187 , 0.244	Depositor DCC
R_{free} test set	2196 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7985	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: CA, PO4, IPD

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	0.71	0/2013	0.81	3/2739 (0.1%)
1	B	0.73	0/1959	0.88	2/2668 (0.1%)
1	C	0.71	0/1976	0.84	0/2687
1	D	0.71	0/1962	0.82	1/2674 (0.0%)
All	All	0.72	0/7910	0.84	6/10768 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	179	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	51	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	253	ASP	CB-CA-C	-5.57	99.25	110.40
1	A	176	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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	1970	0	1902	18	0
1	B	1917	0	1842	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1936	0	1859	10	0
1	D	1922	0	1849	15	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	16	0	11	0	0
3	B	16	0	10	0	0
3	C	16	0	11	0	0
4	D	5	0	0	0	0
5	A	47	0	0	1	0
5	B	46	0	0	0	0
5	C	38	0	0	1	0
5	D	48	0	0	0	0
All	All	7985	0	7484	56	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 4.

The worst 5 of 56 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:204:LEU:HD22	1:A:239:ILE:HG13	1.64	0.78
1:B:204:LEU:HD22	1:B:239:ILE:HG13	1.64	0.77
1:C:204:LEU:HD22	1:C:239:ILE:HG13	1.70	0.72
1:C:41:VAL:O	1:C:45:THR:HG23	1.91	0.71
1:A:163:ILE:HG23	1:A:265:LEU:HD11	1.74	0.70

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	254/283 (90%)	243 (96%)	10 (4%)	1 (0%)	39	56
1	B	249/283 (88%)	239 (96%)	9 (4%)	1 (0%)	39	56
1	C	247/283 (87%)	234 (95%)	10 (4%)	3 (1%)	16	23
1	D	248/283 (88%)	243 (98%)	4 (2%)	1 (0%)	39	56
All	All	998/1132 (88%)	959 (96%)	33 (3%)	6 (1%)	30	43

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	65	GLU
1	C	55	GLU
1	C	162	PRO
1	A	162	PRO
1	D	162	PRO

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	204/239 (85%)	195 (96%)	9 (4%)	35	53
1	B	196/239 (82%)	182 (93%)	14 (7%)	18	28
1	C	200/239 (84%)	186 (93%)	14 (7%)	19	29
1	D	196/239 (82%)	186 (95%)	10 (5%)	29	46
All	All	796/956 (83%)	749 (94%)	47 (6%)	24	38

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	256	GLU
1	C	43	LYS
1	D	161	LYS
1	C	8	GLN
1	C	45	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 8 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	$\# Z > 2$
3	IPD	A	303	2	16,16,16	2.50	4 (25%)	24,25,25	1.29	4 (16%)
3	IPD	B	303	2	16,16,16	2.10	5 (31%)	24,25,25	1.44	3 (12%)
3	IPD	C	303	2	16,16,16	2.11	2 (12%)	24,25,25	1.39	3 (12%)
4	PO4	D	303	2	4,4,4	0.43	0	6,6,6	0.27	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
3	IPD	A	303	2	-	0/5/29/29	0/1/1/1
3	IPD	B	303	2	-	0/5/29/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPD	C	303	2	-	0/5/29/29	0/1/1/1
4	PO4	D	303	2	-	0/0/0/0	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	IPD	O4-C4	-2.87	1.36	1.43
3	B	303	IPD	O5-C5	-2.06	1.38	1.43
3	B	303	IPD	O2-C2	2.01	1.47	1.43
3	A	303	IPD	C6-C5	2.34	1.58	1.52
3	A	303	IPD	P1-O1	2.49	1.67	1.62

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	IPD	O9-P1-O7	-3.41	104.48	112.72
3	A	303	IPD	O9-P1-O8	-2.46	106.97	112.80
3	B	303	IPD	C6-C1-C2	-2.42	108.17	110.93
3	A	303	IPD	O4-C4-C5	-2.11	105.61	110.36
3	C	303	IPD	O5-C5-C6	-2.03	105.78	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	258/283 (91%)	-0.36	4 (1%) 74 74	22, 35, 63, 81	0
1	B	254/283 (89%)	-0.30	8 (3%) 52 52	19, 32, 62, 77	0
1	C	253/283 (89%)	-0.16	5 (1%) 68 68	21, 39, 70, 87	0
1	D	254/283 (89%)	-0.32	4 (1%) 74 74	21, 34, 62, 73	0
All	All	1019/1132 (90%)	-0.29	21 (2%) 67 66	19, 35, 65, 87	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	ASP	3.8
1	B	39	THR	3.7
1	A	1	MET	3.6
1	B	26	LEU	3.6
1	B	162	PRO	3.3

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
3	IPD	C	303	16/16	0.96	0.14	0.16	29,37,43,44	0
3	IPD	A	303	16/16	0.97	0.11	-0.25	34,39,47,51	0
4	PO4	D	303	5/5	0.97	0.10	-0.79	39,40,43,45	0
3	IPD	B	303	16/16	0.97	0.09	-0.87	30,36,40,40	7
2	CA	A	302	1/1	0.99	0.09	-1.26	40,40,40,40	0
2	CA	B	301	1/1	0.99	0.04	-1.89	30,30,30,30	0
2	CA	B	302	1/1	0.99	0.04	-2.07	38,38,38,38	0
2	CA	C	302	1/1	0.99	0.03	-2.38	37,37,37,37	0
2	CA	D	301	1/1	0.99	0.04	-2.51	31,31,31,31	0
2	CA	C	301	1/1	1.00	0.03	-2.56	30,30,30,30	0
2	CA	D	302	1/1	0.98	0.02	-3.32	45,45,45,45	0
2	CA	A	301	1/1	0.99	0.04	-4.71	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.