



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 05:33 am GMT

PDB ID : 4AXD
Title : Inositol 1,3,4,5,6-pentakisphosphate 2-kinase in complex with AMPPNP
Authors : I Banos-Sanz, J.; Sanz-Aparicio, J.; Gonzalez, B.
Deposited on : 2012-06-12
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

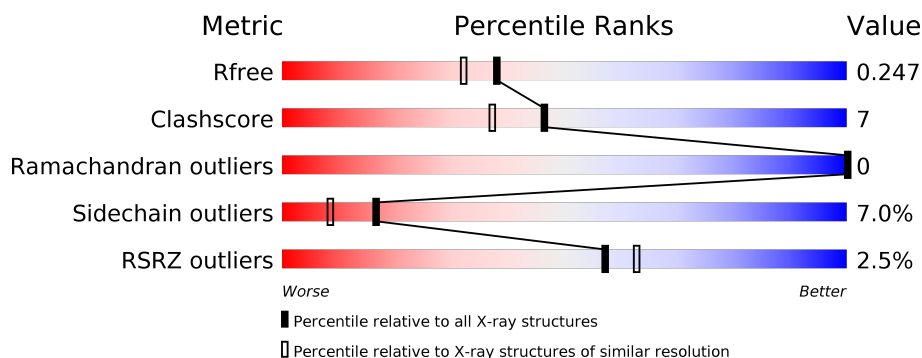
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	111664	1449 (2.04-2.04)
Clashscore	122126	1524 (2.04-2.04)
Ramachandran outliers	120053	1512 (2.04-2.04)
Sidechain outliers	120020	1512 (2.04-2.04)
RSRZ outliers	108989	1429 (2.04-2.04)

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	456	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3849 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.

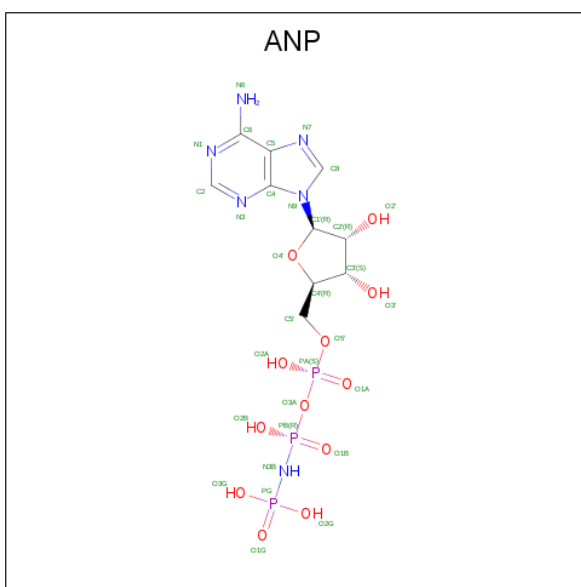
- Molecule 1 is a protein called INOSITOL-PENTAKISPHOSPHATE 2-KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3458	2192	589	663	14	0	4	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q93YN9
A	-3	GLU	-	expression tag	UNP Q93YN9
A	-2	PHE	-	expression tag	UNP Q93YN9
A	-1	GLU	-	expression tag	UNP Q93YN9
A	0	LEU	-	expression tag	UNP Q93YN9
A	54	SER	ALA	conflict	UNP Q93YN9
A	90	GLN	LYS	conflict	UNP Q93YN9
A	129	ALA	TRP	conflict	UNP Q93YN9
A	157	THR	SER	conflict	UNP Q93YN9
A	204	ILE	ASN	conflict	UNP Q93YN9
A	224	ARG	SER	conflict	UNP Q93YN9
A	321	CYS	SER	conflict	UNP Q93YN9
A	325	ILE	LEU	conflict	UNP Q93YN9
A	334	ARG	LYS	conflict	UNP Q93YN9
A	337	ARG	LYS	conflict	UNP Q93YN9

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

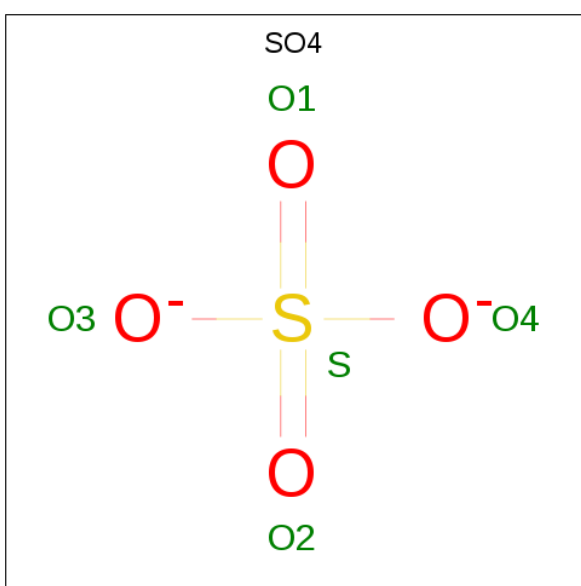


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

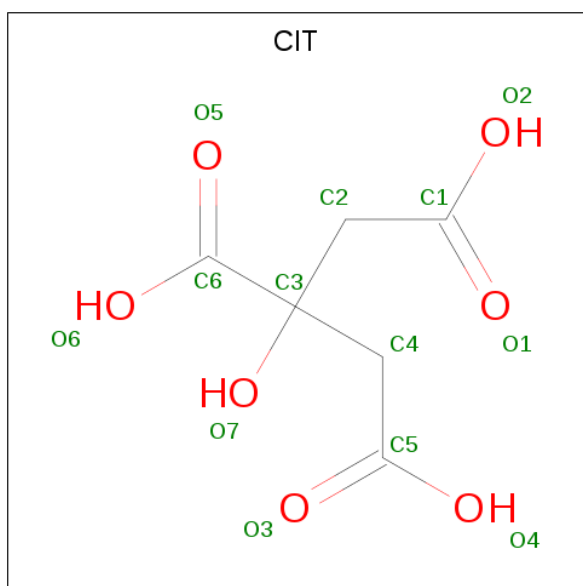
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0

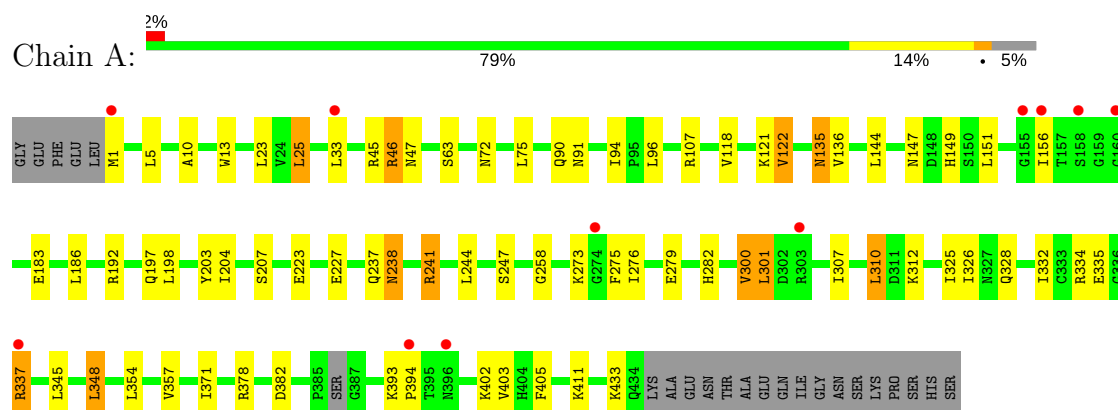
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	321	Total O 321 321	0	0

3 Residue-property plots [i](#)

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: INOSITOL-PENTAKISPHOSPHATE 2-KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.23Å 71.80Å 63.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.37 – 2.05 53.37 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.37-2.05) 99.9 (53.37-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.194 , 0.246 0.195 , 0.247	Depositor DCC
R_{free} test set	1483 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.6	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	0.94	EDS
Total number of atoms	3849	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ANP, SO4, CIT

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	0.50	1/3520 (0.0%)	0.68	5/4747 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	TRP	CD2-CE2	5.04	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	241	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	334	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	25	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	192	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3458	0	3476	48	0
2	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	25	0	0	1	0
5	A	13	0	5	5	0
6	A	321	0	0	7	0
All	All	3849	0	3494	48	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 7.

All (48) 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:135:ASN:HD22	1:A:136[B]:VAL:H	1.16	0.93
1:A:135:ASN:HD22	1:A:136[A]:VAL:H	1.19	0.90
1:A:197:GLN:HE22	1:A:237:GLN:HE22	1.22	0.84
1:A:149:HIS:ND1	5:A:1440:CIT:H42	1.97	0.80
1:A:72:ASN:HD21	1:A:91:ASN:HD22	1.31	0.75
1:A:107:ARG:HD3	6:A:2071:HOH:O	1.87	0.74
1:A:301:LEU:HD11	1:A:371[A]:ILE:CD1	2.21	0.71
1:A:46:ARG:O	1:A:47:ASN:HB2	1.94	0.68
1:A:135:ASN:ND2	1:A:136[B]:VAL:H	1.92	0.65
1:A:273:LYS:HE3	6:A:2239:HOH:O	1.95	0.65
1:A:301:LEU:HD11	1:A:371[A]:ILE:HD11	1.79	0.64
1:A:332:ILE:O	1:A:335:GLU:HB2	1.98	0.63
1:A:135:ASN:ND2	1:A:136[A]:VAL:H	1.94	0.62
1:A:393:LYS:N	1:A:394:PRO:HD2	2.16	0.61
1:A:135:ASN:HD22	1:A:136[A]:VAL:N	1.94	0.59
1:A:238:ASN:H	1:A:238:ASN:HD22	1.50	0.59
1:A:135:ASN:HD22	1:A:136[B]:VAL:N	1.93	0.58
1:A:223:GLU:O	1:A:227[B]:GLU:HG2	2.05	0.56
1:A:118:VAL:O	1:A:122:VAL:HG13	2.08	0.54
1:A:325:ILE:HD11	1:A:354:LEU:HA	1.89	0.54
1:A:371[B]:ILE:HG13	1:A:371[B]:ILE:O	2.06	0.54
1:A:72:ASN:HD22	1:A:75:LEU:HB2	1.72	0.54
1:A:72:ASN:ND2	1:A:75:LEU:HB2	2.24	0.52
1:A:411:LYS:NZ	6:A:2305:HOH:O	2.34	0.51
1:A:275:PHE:N	6:A:2132:HOH:O	2.42	0.51
1:A:204:ILE:O	1:A:204:ILE:HD12	2.11	0.51
1:A:326:ILE:HG13	1:A:328:GLN:HG2	1.91	0.51
1:A:402:LYS:NZ	5:A:1440:CIT:H21	2.28	0.48
1:A:325:ILE:HD12	1:A:357:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:H	1:A:337:ARG:HG2	1.48	0.48
1:A:275:PHE:HD2	1:A:276:ILE:HD12	1.80	0.47
1:A:238:ASN:N	1:A:238:ASN:HD22	2.11	0.45
1:A:10:ALA:O	1:A:121:LYS:HE3	2.17	0.45
1:A:402:LYS:HD3	5:A:1440:CIT:H21	1.99	0.45
1:A:345:LEU:O	1:A:348:LEU:HB2	2.17	0.44
1:A:307:ILE:O	1:A:310:LEU:HB2	2.18	0.44
1:A:402:LYS:HZ3	5:A:1440:CIT:C2	2.32	0.42
1:A:300:VAL:HG11	1:A:403:VAL:HG11	2.00	0.42
1:A:147:ASN:CB	5:A:1440:CIT:O7	2.67	0.42
1:A:279:GLU:HG3	1:A:282:HIS:CD2	2.55	0.42
1:A:371[B]:ILE:HG22	1:A:405:PHE:CD1	2.55	0.42
1:A:90:GLN:HA	1:A:94:ILE:HD12	2.01	0.41
1:A:183:GLU:HB2	6:A:2157:HOH:O	2.19	0.41
1:A:63:SER:HB3	4:A:1437:SO4:O2	2.20	0.41
1:A:258:GLY:HA2	6:A:2178:HOH:O	2.20	0.41
1:A:378:ARG:NH2	1:A:382:ASP:HB3	2.36	0.41
1:A:203:TYR:O	1:A:204:ILE:HG13	2.21	0.40
1:A:227[B]:GLU:HG3	6:A:2198:HOH:O	2.21	0.40

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	433/456 (95%)	417 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	387/402 (96%)	360 (93%)	27 (7%)	16 8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	23	LEU
1	A	25	LEU
1	A	33	LEU
1	A	45	ARG
1	A	46	ARG
1	A	96	LEU
1	A	122	VAL
1	A	135	ASN
1	A	144	LEU
1	A	151	LEU
1	A	156	ILE
1	A	186	LEU
1	A	198	LEU
1	A	207	SER
1	A	238	ASN
1	A	241	ARG
1	A	244	LEU
1	A	247	SER
1	A	300	VAL
1	A	301	LEU
1	A	310	LEU
1	A	312	LYS
1	A	337	ARG
1	A	348	LEU
1	A	433	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	66	GLN
1	A	72	ASN
1	A	135	ASN
1	A	147	ASN
1	A	237	GLN
1	A	238	ASN
1	A	282	HIS
1	A	379	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, 1 is monoatomic - leaving 7 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	SO4	A	1435	-	4,4,4	1.12	0	6,6,6	0.59	0
4	SO4	A	1436	-	4,4,4	0.40	0	6,6,6	0.24	0
4	SO4	A	1437	-	4,4,4	0.42	0	6,6,6	0.13	0
4	SO4	A	1438	-	4,4,4	0.45	0	6,6,6	0.25	0
4	SO4	A	1439	-	4,4,4	1.09	0	6,6,6	0.80	0
5	CIT	A	1440	-	3,12,12	0.99	0	3,17,17	4.04	3 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	A	600	-	29,33,33	2.80	5 (17%)	29,52,52	1.74	5 (17%)

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	SO4	A	1435	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1436	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1437	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1438	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1439	-	-	0/0/0/0	0/0/0/0
5	CIT	A	1440	-	-	0/6/16/16	0/0/0/0
2	ANP	A	600	-	-	0/13/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ANP	PG-O3G	-2.63	1.49	1.56
2	A	600	ANP	C5-C4	2.81	1.46	1.40
2	A	600	ANP	PG-N3B	3.64	1.73	1.63
2	A	600	ANP	PB-N3B	3.83	1.73	1.63
2	A	600	ANP	PG-O1G	12.60	1.60	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ANP	N3-C2-N1	-6.08	123.66	128.86
2	A	600	ANP	C4-C5-N7	-2.87	106.64	109.41
2	A	600	ANP	PA-O3A-PB	-2.85	122.39	132.40
5	A	1440	CIT	C3-C2-C1	-2.48	111.22	114.95
2	A	600	ANP	O3G-PG-O1G	-2.30	107.59	113.43
2	A	600	ANP	O1B-PB-N3B	2.69	115.82	111.79
5	A	1440	CIT	C3-C4-C5	2.85	119.23	114.95
5	A	1440	CIT	C4-C3-C2	5.89	124.29	109.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1437	SO4	1	0
5	A	1440	CIT	5	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	433/456 (94%)	0.03	11 (2%) 57 63	12, 22, 43, 59	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ILE	4.7
1	A	274	GLY	4.5
1	A	1	MET	4.1
1	A	158	SER	3.4
1	A	337	ARG	3.1
1	A	33	LEU	3.0
1	A	160	GLY	2.5
1	A	396	ASN	2.4
1	A	155	GLY	2.4
1	A	394	PRO	2.3
1	A	303	ARG	2.0

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. 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(\AA^2)	Q<0.9
5	CIT	A	1440	13/13	0.67	0.38	43,46,50,51	0
4	SO4	A	1437	5/5	0.76	0.29	74,75,77,78	0
4	SO4	A	1438	5/5	0.92	0.17	48,53,55,57	0
4	SO4	A	1436	5/5	0.94	0.20	46,48,49,51	0
4	SO4	A	1439	5/5	0.95	0.12	54,55,58,58	0
2	ANP	A	600	31/31	0.97	0.11	14,16,28,30	0
3	ZN	A	700	1/1	0.98	0.06	24,24,24,24	0
4	SO4	A	1435	5/5	0.98	0.09	41,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.