wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 09:53 am BST

PDB ID	:	1YXM
Title	:	Crystal structure of peroxisomal trans 2-enoyl CoA reductase
Authors	:	Jansson, A.; Ng, S.; Arrowsmith, C.; Sharma, S.; Edwards, A.M.; Von Delft, F.; Sundstrom, M.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2005-02-22
Resolution	:	1.90 Å(reported)

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

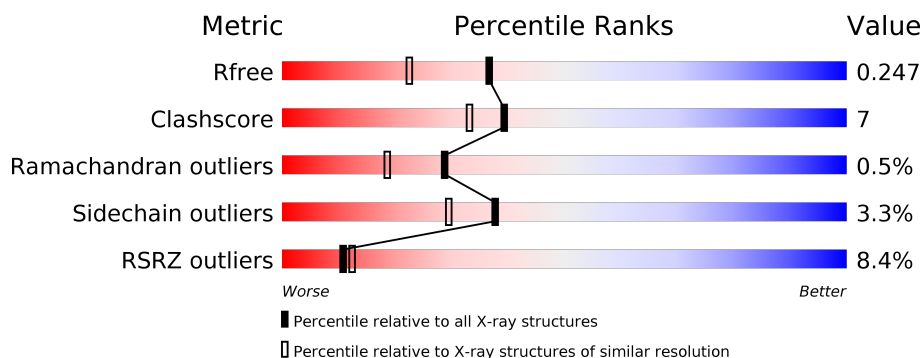|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		3.3%
RSRZ outliers		8.4%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 <=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	303	5% ▬ 86% 10% ··
1	B	303	3% ▬ 84% 8% · 7%
1	C	303	13% ▬ 72% 13% · 13%
1	D	303	11% ▬ 79% 15% ··

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8697 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 peroxisomal trans 2-enoyl CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	1	0
			2153	1376	366	403	8			
1	B	283	Total	C	N	O	S	0	2	0
			2102	1345	358	391	8			
1	C	264	Total	C	N	O	S	0	0	0
			1892	1210	322	352	8			
1	D	291	Total	C	N	O	S	0	1	0
			2141	1369	363	401	8			

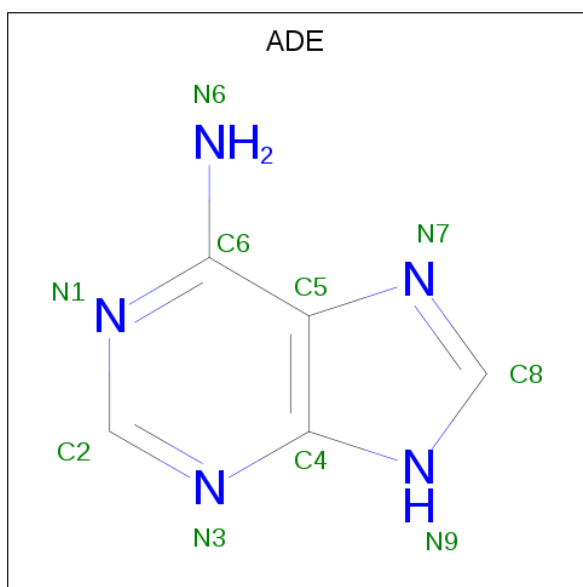- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

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

- Molecule 4 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).

ADE

N6

NH_2

C6

N7

N1 N

C5

N

N3

C2

N

C4

N

H

N9

C8

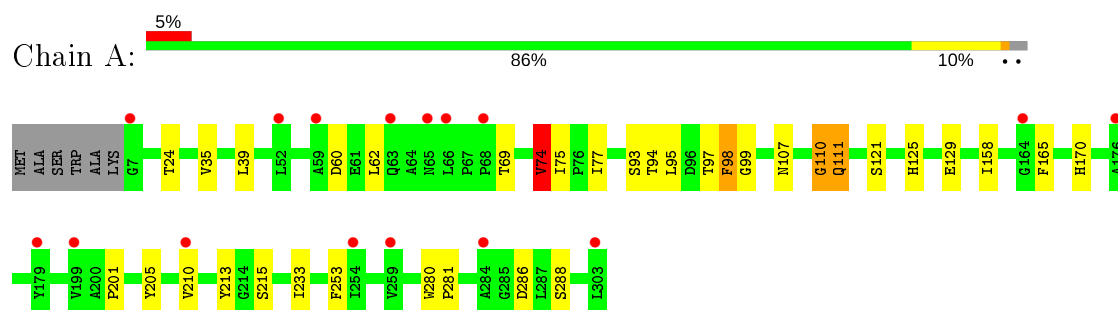| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			10	5	5		

- Molecule 5 is water.

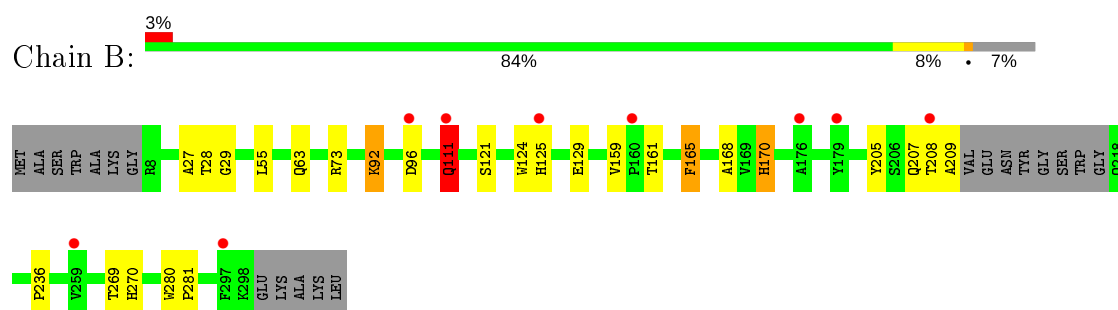| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	96	Total	O	0	0
			96	96		
5	C	70	Total	O	0	0
			70	70		
5	D	107	Total	O	0	0
			107	107		

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.
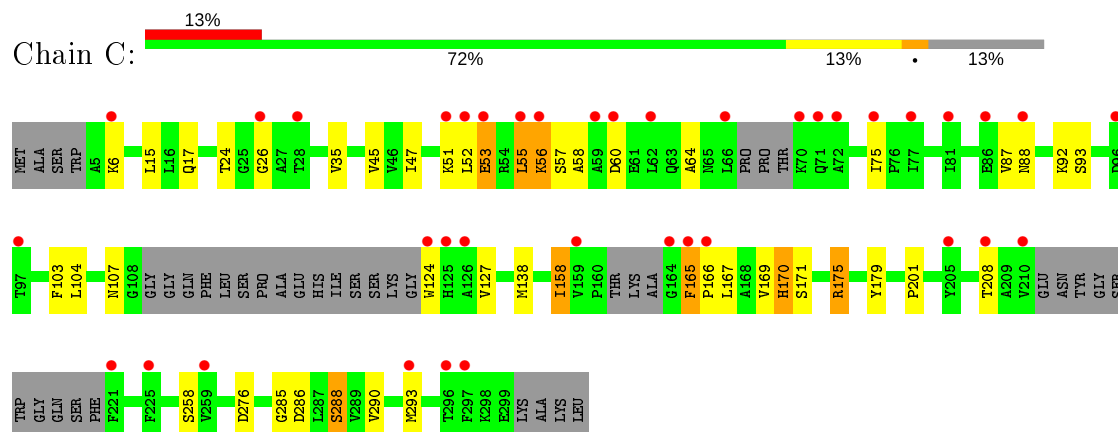
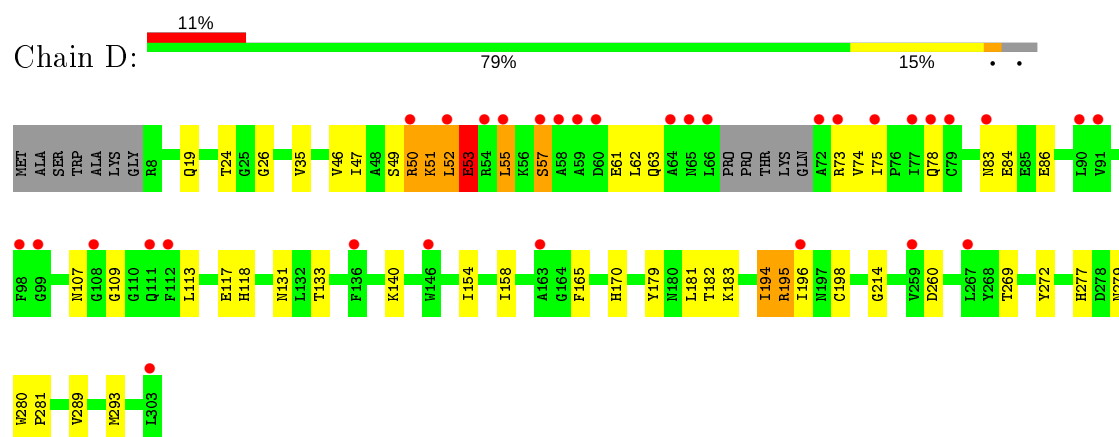• Molecule 1: peroxisomal trans 2-enoyl CoA reductase

• Molecule 1: peroxisomal trans 2-enoyl CoA reductase

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• Molecule 1: peroxisomal trans 2-enoyl CoA reductase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.15Å 119.01Å 119.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 1.90 47.34 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.00-1.90) 97.5 (47.34-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.245 0.212 , 0.247	Depositor DCC
R_{free} test set	4438 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8697	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, ADE, SO4

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	0.80	1/2200 (0.0%)	0.79	5/2996 (0.2%)
1	B	0.82	0/2152	0.76	1/2926 (0.0%)
1	C	0.75	2/1926 (0.1%)	0.83	5/2617 (0.2%)
1	D	0.89	4/2185 (0.2%)	0.93	6/2972 (0.2%)
All	All	0.82	7/8463 (0.1%)	0.83	17/11511 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	3	5
All	All	3	13

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	194	ILE	C-N	-15.25	0.98	1.34
1	D	195	ARG	C-N	9.89	1.56	1.34
1	A	111	GLN	C-N	-8.52	1.14	1.34
1	D	198	CYS	CB-SG	-6.13	1.71	1.82
1	D	195	ARG	CD-NE	-5.84	1.36	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	195	ARG	NE-CZ-NH2	-18.18	111.21	120.30
1	D	195	ARG	O-C-N	-17.14	95.28	122.70
1	D	195	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	C	285	GLY	O-C-N	-10.11	106.53	122.70
1	C	285	GLY	C-N-CA	10.07	146.88	121.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	52	LEU	CA
1	D	53	GLU	CA
1	D	54	ARG	CA

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLY	Mainchain
1	A	97	THR	Peptide
1	A	98	PHE	Peptide
1	B	111	GLN	Mainchain
1	B	207	GLN	Peptide

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	2153	0	2077	16	0
1	B	2102	0	2089	21	0
1	C	1892	0	1838	42	0
1	D	2141	0	2090	49	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	10	0	0	0	0
3	B	5	0	0	0	0
4	B	10	0	4	0	0
5	A	101	0	0	1	0
5	B	96	0	0	1	0
5	C	70	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	107	0	0	4	0
All	All	8697	0	8098	122	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.

The worst 5 of 122 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:D:52:LEU:CA	1:D:53:GLU:HG3	1.65	1.26
1:C:52:LEU:HB3	1:C:53:GLU:HA	1.30	1.12
1:D:52:LEU:N	1:D:53:GLU:HA	1.49	1.09
1:B:208:THR:HG23	5:B:4085:HOH:O	1.51	1.08
1:C:52:LEU:HD23	1:C:55:LEU:H	1.15	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	296/303 (98%)	284 (96%)	11 (4%)	1 (0%)	41	31
1	B	281/303 (93%)	271 (96%)	10 (4%)	0	100	100
1	C	254/303 (84%)	240 (94%)	11 (4%)	3 (1%)	13	4
1	D	288/303 (95%)	276 (96%)	10 (4%)	2 (1%)	22	12
All	All	1119/1212 (92%)	1071 (96%)	42 (4%)	6 (0%)	29	18

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	LYS

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Mol	Chain	Res	Type
1	D	53	GLU
1	C	55	LEU
1	A	111	GLN
1	C	158	ILE

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	215/245 (88%)	207 (96%)	8 (4%)	34	25
1	B	221/245 (90%)	217 (98%)	4 (2%)	59	55
1	C	191/245 (78%)	184 (96%)	7 (4%)	34	25
1	D	219/245 (89%)	210 (96%)	9 (4%)	30	21
All	All	846/980 (86%)	818 (97%)	28 (3%)	38	29

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	LEU
1	C	165	PHE
1	D	113	LEU
1	C	75	ILE
1	C	93	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	HIS
1	D	277	HIS
1	D	118	HIS
1	B	111	GLN
1	D	80	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)

6 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	SO4	D	1001	-	4,4,4	0.24	0	6,6,6	0.58	0
2	SO4	D	2001	-	4,4,4	0.20	0	6,6,6	0.52	0
3	PO4	B	3001	-	4,4,4	0.68	0	6,6,6	0.57	0
4	ADE	B	4002	-	9,11,11	1.74	2 (22%)	7,15,15	2.71	3 (42%)
2	SO4	A	304	-	4,4,4	0.27	0	6,6,6	0.39	0
2	SO4	B	4001	-	4,4,4	0.33	0	6,6,6	0.44	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
4	ADE	B	4002	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4002	ADE	C2-N3	4.19	1.38	1.32
4	B	4002	ADE	C4-N9	2.12	1.38	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4002	ADE	N3-C2-N1	-5.80	119.62	128.68
4	B	4002	ADE	C2-N3-C4	3.24	121.03	113.45
4	B	4002	ADE	C4-C5-N7	-2.11	107.20	109.40

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	111:GLN	C	112:PHE	N	1.14
1	D	194:ILE	C	195:ARG	N	0.99

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	297/303 (98%)	0.49	16 (5%)	25	29	22, 34, 53, 59	1 (0%)
1	B	283/303 (93%)	0.37	9 (3%)	47	50	20, 33, 48, 53	0
1	C	264/303 (87%)	0.86	38 (14%)	2	2	24, 38, 56, 60	0
1	D	291/303 (96%)	0.63	32 (10%)	5	6	25, 37, 55, 60	1 (0%)
All	All	1135/1212 (93%)	0.58	95 (8%)	11	12	20, 35, 53, 60	2 (0%)

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	LEU	6.8
1	C	296	THR	6.8
1	A	52	LEU	6.1
1	D	57	SER	6.0
1	D	50	ARG	5.6

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($\mathring{A}^2$)	Q<0.9
3	PO4	B	3001	5/5	0.85	0.28	56,56,57,57	0
4	ADE	B	4002	10/10	0.85	0.18	47,48,49,49	0
2	SO4	D	1001	5/5	0.95	0.09	50,53,57,59	0
2	SO4	A	304	5/5	0.95	0.15	53,56,56,56	0
2	SO4	D	2001	5/5	0.96	0.12	60,60,64,64	0
2	SO4	B	4001	5/5	0.98	0.08	33,35,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.