wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:23 AM GMT

PDB ID	:	2AA3
Title	:	Crystal structure of Plasmodium vivax lactate dehydrogenase complex with APADH
Authors	:	Chaikuad, A.; Fairweather, V.; Conners, R.; Joseph-Horne, T.; Turgut-Balik, D.; Brady, R.L.
Deposited on	:	2005-07-13
Resolution	:	2.05 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

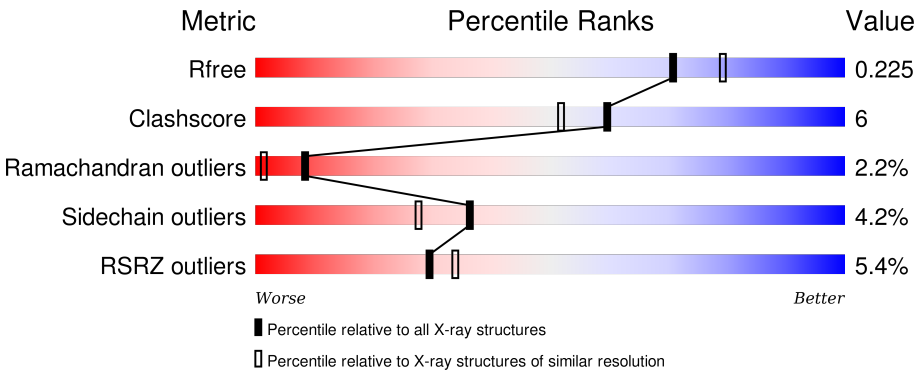
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 <=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	321	4% 87% 8% • •
1	B	321	5% 83% 12% • •
1	C	321	4% 89% 6% • ••
1	D	321	7% 80% 14% • •

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
3	AP0	A	1401	X	-	-	-
3	AP0	B	1407	X	-	-	-
3	AP0	C	1405	X	-	-	-
3	AP0	D	1403	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10302 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2408	1540	403	451	14	106	1	0
1	B	315	2398	1534	400	450	14	34	1	0
1	C	318	2433	1557	409	453	14	118	2	0
1	D	315	2398	1534	400	450	14	125	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	HIS	-	EXPRESSION TAG	GB 66967948
A	331	HIS	-	EXPRESSION TAG	GB 66967948
A	332	HIS	-	EXPRESSION TAG	GB 66967948
A	333	HIS	-	EXPRESSION TAG	GB 66967948
A	334	HIS	-	EXPRESSION TAG	GB 66967948
A	335	HIS	-	EXPRESSION TAG	GB 66967948
B	330	HIS	-	EXPRESSION TAG	GB 66967948
B	331	HIS	-	EXPRESSION TAG	GB 66967948
B	332	HIS	-	EXPRESSION TAG	GB 66967948
B	333	HIS	-	EXPRESSION TAG	GB 66967948
B	334	HIS	-	EXPRESSION TAG	GB 66967948
B	335	HIS	-	EXPRESSION TAG	GB 66967948
C	330	HIS	-	EXPRESSION TAG	GB 66967948
C	331	HIS	-	EXPRESSION TAG	GB 66967948
C	332	HIS	-	EXPRESSION TAG	GB 66967948
C	333	HIS	-	EXPRESSION TAG	GB 66967948
C	334	HIS	-	EXPRESSION TAG	GB 66967948
C	335	HIS	-	EXPRESSION TAG	GB 66967948
D	330	HIS	-	EXPRESSION TAG	GB 66967948
D	331	HIS	-	EXPRESSION TAG	GB 66967948
D	332	HIS	-	EXPRESSION TAG	GB 66967948

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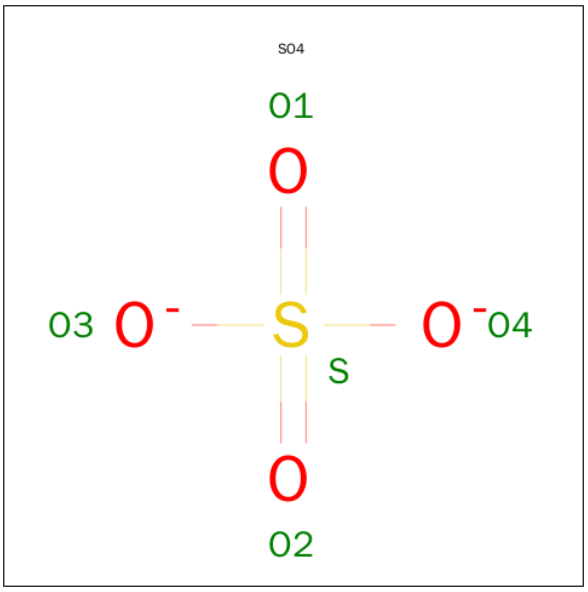
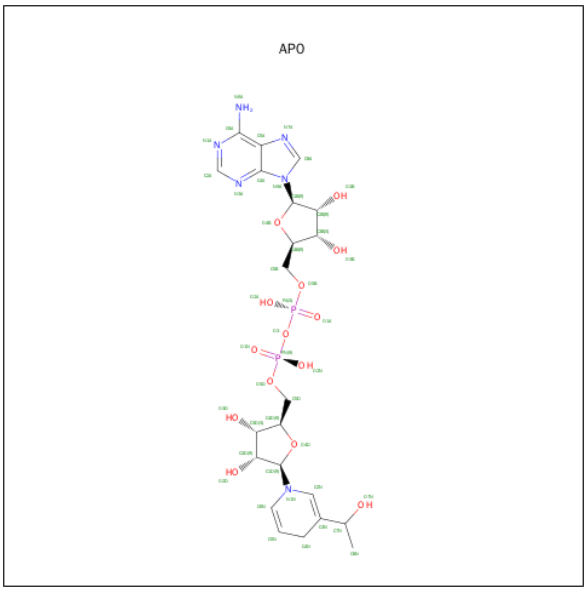
Chain	Residue	Modelled	Actual	Comment	Reference
D	333	HIS	-	EXPRESSION TAG	GB 66967948
D	334	HIS	-	EXPRESSION TAG	GB 66967948
D	335	HIS	-	EXPRESSION TAG	GB 66967948

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



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

- Molecule 3 is ACETYL PYRIDINE ADENINE DINUCLEOTIDE, REDUCED (three-letter code: AP0) (formula: $C_{22}H_{32}N_6O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	44	22	6	14	2	0	0
3	D	1	44	22	6	14	2	0	0
3	C	1	44	22	6	14	2	0	0
3	B	1	44	22	6	14	2	0	0

- Molecule 4 is water.

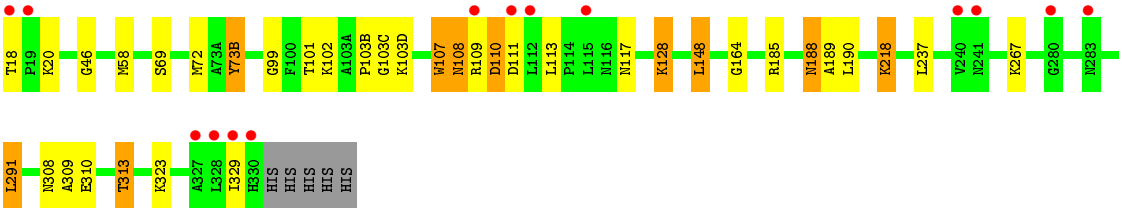
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	149	149	149	0	0
4	B	121	121	121	0	0
4	C	121	121	121	0	0
4	D	88	88	88	0	0

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 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.

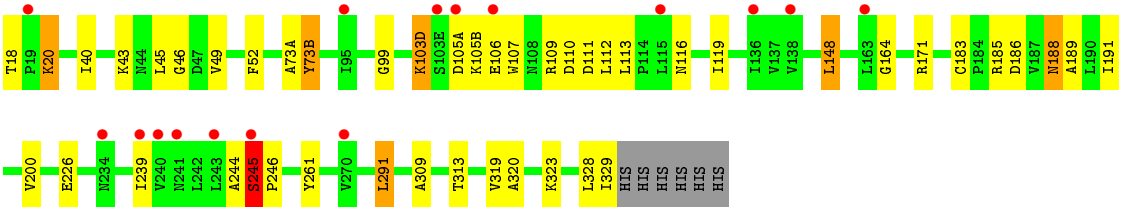
- Molecule 1: L-lactate dehydrogenase

Chain A:



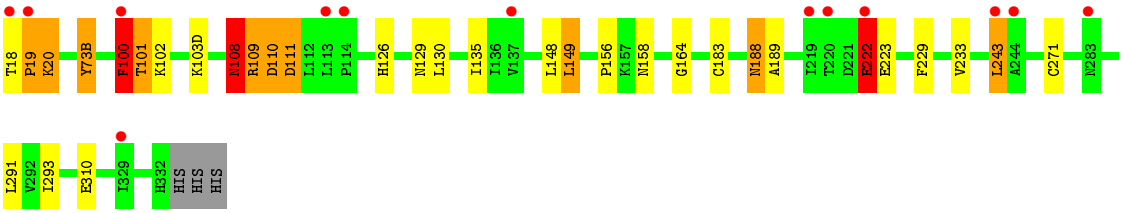
- Molecule 1: L-lactate dehydrogenase

Chain B:



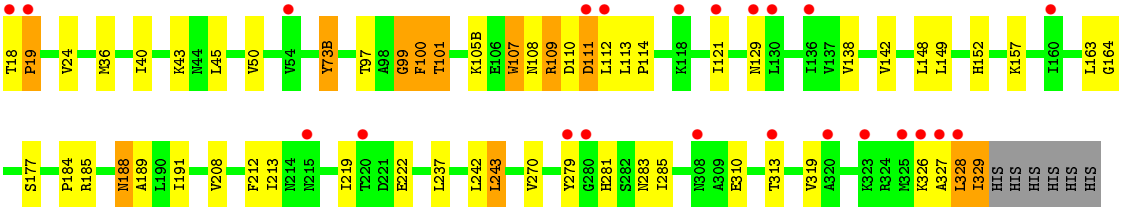
- Molecule 1: L-lactate dehydrogenase

Chain C:



- Molecule 1: L-lactate dehydrogenase

Chain D:


T18
P19
V24
M36
I40
K43
N44
L45
V50
V54
Y73B
T97
A98
G99
F100
T101
K105B
E106
W107
N108
R109
D110
D111
L112
L113
P114
K118
I121
N129
L130
I136
V137
V138
V142
L148
L149
H152
K157
I160
L163
G164
S177
P184
R185
N188
A189
L190
I191
V208
F212
I213
N214
N215
I219
T220
D221
E222
L237
L242
L243
V270
Y279
G280
H281
S282
N283
I285
N308
A309
E310
T313
V319
A320
K323
R324
M325
K326
A327
I328
I329
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.48Å 128.45Å 130.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.67 – 2.05 29.14 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.3 (91.67-2.05) 98.4 (29.14-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.226 0.191 , 0.225	Depositor DCC
R_{free} test set	4273 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.1	EDS
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 85446 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: AP0, 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	1.06	4/2448 (0.2%)	0.85	4/3315 (0.1%)
1	B	1.00	4/2437 (0.2%)	0.92	10/3300 (0.3%)
1	C	0.99	3/2478 (0.1%)	0.88	12/3356 (0.4%)
1	D	0.86	3/2437 (0.1%)	0.77	2/3300 (0.1%)
All	All	0.98	14/9800 (0.1%)	0.86	28/13271 (0.2%)

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	2
1	B	0	1
1	C	2	1
1	D	1	2
All	All	3	6

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	LYS	CE-NZ	15.30	1.87	1.49
1	C	222	GLU	CD-OE1	14.62	1.41	1.25
1	A	128	LYS	CE-NZ	14.36	1.84	1.49
1	C	222	GLU	CD-OE2	12.60	1.39	1.25
1	B	226	GLU	CD-OE1	12.25	1.39	1.25

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	106	GLU	CA-CB-CG	15.37	147.21	113.40
1	C	100	PHE	O-C-N	14.45	145.82	122.70
1	C	100	PHE	CA-C-N	-9.95	95.32	117.20
1	A	218	LYS	CD-CE-NZ	-9.86	89.02	111.70
1	B	107	TRP	CB-CA-C	-9.71	90.97	110.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	101	THR	CB,CA
1	D	110	ASP	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TRP	Peptide
1	A	108	ASN	Peptide
1	B	244	ALA	Peptide
1	C	108	ASN	Peptide
1	D	99	GLY	Mainchain

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	2408	0	2505	33	0
1	B	2398	0	2498	29	0
1	C	2433	0	2530	31	0
1	D	2398	0	2497	33	0
2	A	5	0	0	0	0
2	C	5	0	0	1	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
4	A	149	0	0	1	0
4	B	121	0	0	1	0
4	C	121	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	88	0	0	0	0
All	All	10302	0	10134	109	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 6.

The worst 5 of 109 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:128:LYS:CE	1:A:128:LYS:NZ	1.84	1.39
1:A:218:LYS:CE	1:A:218:LYS:NZ	1.87	1.37
1:D:18:THR:HA	1:D:19:PRO:O	1.27	1.27
1:A:109:ARG:HB2	1:A:110:ASP:HB3	1.33	1.08
1:D:18:THR:HA	1:D:19:PRO:C	1.66	1.06

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	315/321 (98%)	296 (94%)	11 (4%)	8 (2%)	7 1
1	B	314/321 (98%)	302 (96%)	10 (3%)	2 (1%)	30 18
1	C	318/321 (99%)	294 (92%)	17 (5%)	7 (2%)	8 1
1	D	314/321 (98%)	291 (93%)	12 (4%)	11 (4%)	4 0
All	All	1261/1284 (98%)	1183 (94%)	50 (4%)	28 (2%)	8 1

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS

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Mol	Chain	Res	Type
1	A	103(C)	GLY
1	A	108	ASN
1	B	245	SER
1	C	20	LYS

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	269/273 (98%)	260 (97%)	9 (3%)	45	37
1	B	268/273 (98%)	256 (96%)	12 (4%)	34	25
1	C	272/273 (100%)	260 (96%)	12 (4%)	35	26
1	D	268/273 (98%)	252 (94%)	16 (6%)	24	13
All	All	1077/1092 (99%)	1028 (96%)	49 (4%)	36	25

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	73(B)[B]	TYR
1	C	110	ASP
1	D	237	LEU
1	C	102	LYS
1	C	111	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	210(B)	GLN
1	C	140	ASN
1	D	210(B)	GLN
1	C	126	HIS
1	C	152	HIS

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	A	1001	-	4,4,4	0.43	0	6,6,6	0.56	0
3	AP0	A	1401	-	39,48,48	2.38	9 (23%)	49,73,73	2.76	13 (26%)
3	AP0	B	1407	-	39,48,48	2.06	8 (20%)	49,73,73	2.47	14 (28%)
2	SO4	C	1002	-	4,4,4	0.18	0	6,6,6	0.21	0
3	AP0	C	1405	-	39,48,48	2.07	10 (25%)	49,73,73	2.53	15 (30%)
3	AP0	D	1403	-	39,48,48	2.29	10 (25%)	49,73,73	2.57	17 (34%)

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
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	AP0	A	1401	-	3/3/13/16	0/24/72/72	0/5/5/5
3	AP0	B	1407	-	3/3/13/16	0/24/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
3	AP0	C	1405	-	3/3/13/16	0/24/72/72	0/5/5/5
3	AP0	D	1403	-	3/3/13/16	0/24/72/72	0/5/5/5

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1403	AP0	C2D-C1D	-6.04	1.33	1.53
3	D	1403	AP0	O7N-C7N	-6.01	1.21	1.42
3	A	1401	AP0	O7N-C7N	-6.01	1.21	1.42
3	A	1401	AP0	C2D-C1D	-5.89	1.34	1.53
3	B	1407	AP0	O7N-C7N	-5.88	1.22	1.42

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1401	AP0	N3A-C2A-N1A	-9.90	121.31	128.89
3	D	1403	AP0	N3A-C2A-N1A	-9.48	121.63	128.89
3	C	1405	AP0	N3A-C2A-N1A	-9.37	121.72	128.89
3	B	1407	AP0	N3A-C2A-N1A	-8.45	122.42	128.89
3	A	1401	AP0	O3D-C3D-C2D	-4.54	97.05	111.83

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1407	AP0	C7N
3	B	1407	AP0	C1D
3	B	1407	AP0	C2D
3	C	1405	AP0	C7N
3	C	1405	AP0	C1D

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1407	AP0	1	0
2	C	1002	SO4	1	0
3	D	1403	AP0	2	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	303/321 (94%)	0.03	14 (4%)	36	41	9, 17, 29, 43	19 (6%)
1	B	315/321 (98%)	0.15	16 (5%)	32	36	11, 19, 34, 47	32 (10%)
1	C	304/321 (94%)	0.04	13 (4%)	39	44	9, 20, 30, 42	36 (11%)
1	D	300/321 (93%)	0.42	23 (7%)	16	19	12, 24, 39, 49	40 (13%)
All	All	1222/1284 (95%)	0.16	66 (5%)	29	34	9, 20, 36, 49	127 (10%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	LEU	10.4
1	D	18	THR	8.5
1	A	18	THR	7.3
1	C	18	THR	6.1
1	A	330	HIS	5.1

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(Å^2)	Q<0.9
3	AP0	B	1407	44/44	0.93	0.13	0.00	17,23,34,36	0
3	AP0	C	1405	44/44	0.95	0.11	-0.19	14,22,28,33	0
3	AP0	D	1403	44/44	0.94	0.12	-0.24	24,31,38,39	0
3	AP0	A	1401	44/44	0.96	0.09	-0.61	14,19,27,28	0
2	SO4	C	1002	5/5	0.86	0.25	-	35,38,39,40	5
2	SO4	A	1001	5/5	0.94	0.14	-	29,29,31,32	5

6.5 Other polymers (i)

There are no such residues in this entry.