Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:35 PM GMT

PDB ID	:	1BL5
Title	:	ISOCITRATE DEHYDROGENASE FROM E. COLI SINGLE TURNOVER LAUE STRUCTURE OF RATE-LIMITED PRODUCT COMPLEX, 10 MSEC TIME RESOLUTION
Authors	:	Stoddard, B.L.; Cohen, B.; Brubaker, M.; Mesecar, A.; Koshland Junior, D.E.
Deposited on	:	1998-07-23
Resolution	:	2.50 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
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 (i)) were used in the production of this report:

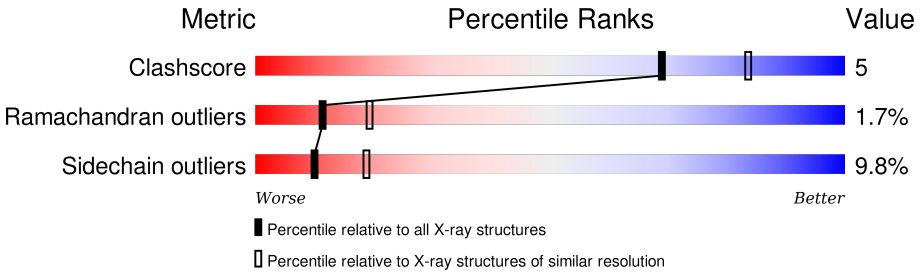
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	75% 18% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3317 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.

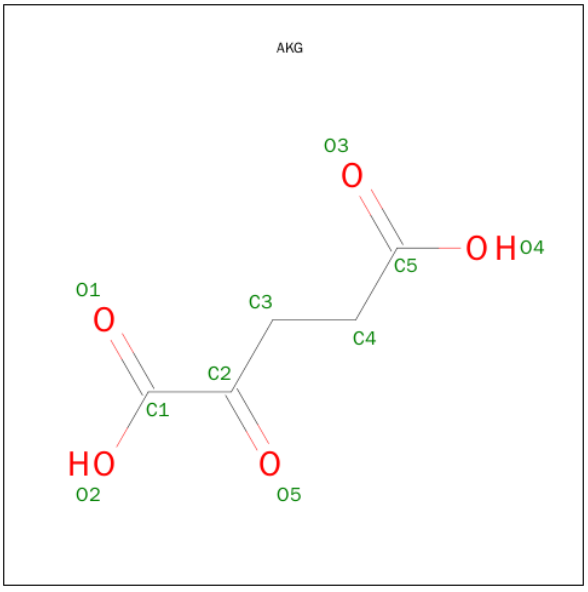
- Molecule 1 is a protein called ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3196	2035	538	605	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

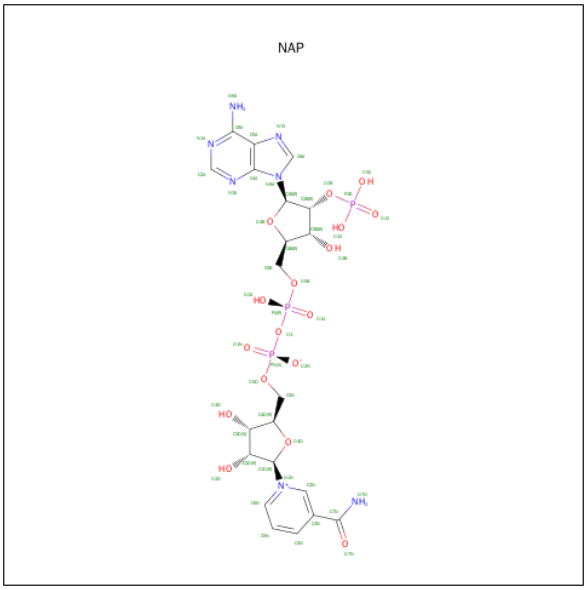
- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE

(three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		

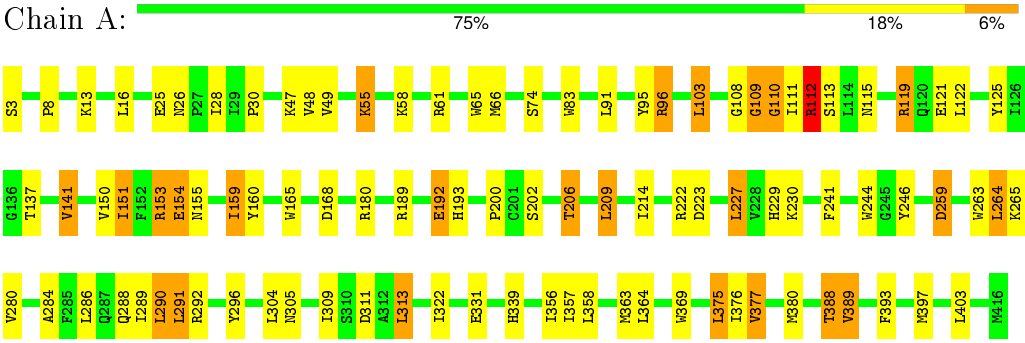
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: ISOCITRATE DEHYDROGENASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.10Å 106.10Å 151.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.8 (50.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.222 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3317	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, AKG, MG

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	1.23	1/3257 (0.0%)	1.81	68/4405 (1.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	SER	CA-CB	-6.33	1.43	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	ARG	NE-CZ-NH1	12.33	126.47	120.30
1	A	112	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	A	119	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	A	61	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	A	165	TRP	CD1-CG-CD2	9.59	113.97	106.30
1	A	180	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	A	65	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	A	112	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	150	VAL	CG1-CB-CG2	-7.89	98.28	110.90
1	A	153	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	65	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	165	TRP	CE2-CD2-CG	-7.74	101.11	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	A	83	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	160	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	244	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	83	TRP	CD1-CG-CD2	7.13	112.01	106.30
1	A	389	VAL	N-CA-CB	-6.94	96.23	111.50
1	A	103	LEU	CA-CB-CG	6.92	131.21	115.30
1	A	55	LYS	CB-CG-CD	6.90	129.55	111.60
1	A	363	MET	CG-SD-CE	6.73	110.97	100.20
1	A	222	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	65	TRP	CB-CG-CD1	-6.58	118.44	127.00
1	A	280	VAL	CG1-CB-CG2	-6.58	100.37	110.90
1	A	13	LYS	CA-CB-CG	6.56	127.83	113.40
1	A	48	VAL	CG1-CB-CG2	-6.44	100.60	110.90
1	A	290	LEU	CB-CG-CD2	-6.42	100.08	111.00
1	A	223	ASP	CA-C-N	6.41	131.31	117.20
1	A	223	ASP	O-C-N	-6.39	112.48	122.70
1	A	112	ARG	CG-CD-NE	6.37	125.19	111.80
1	A	151	ILE	CG1-CB-CG2	-6.28	97.59	111.40
1	A	369	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	A	388	THR	CA-CB-OG1	-6.23	95.91	109.00
1	A	25	GLU	CA-CB-CG	6.15	126.94	113.40
1	A	263	TRP	CD1-CG-CD2	6.12	111.20	106.30
1	A	263	TRP	CE2-CD2-CG	-6.12	102.41	107.30
1	A	388	THR	CA-CB-CG2	6.08	120.92	112.40
1	A	244	TRP	CG-CD2-CE3	6.03	139.32	133.90
1	A	222	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	369	TRP	CD1-CG-CD2	6.00	111.10	106.30
1	A	13	LYS	CB-CA-C	-5.96	98.48	110.40
1	A	165	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	A	277	ILE	N-CA-C	-5.84	95.22	111.00
1	A	180	ARG	CG-CD-NE	5.81	124.01	111.80
1	A	112	ARG	CD-NE-CZ	5.71	131.59	123.60
1	A	292	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	267	LYS	CA-CB-CG	5.63	125.79	113.40
1	A	291	LEU	CB-CA-C	-5.62	99.52	110.20
1	A	16	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	377	VAL	CA-C-N	5.60	129.52	117.20
1	A	113	SER	N-CA-C	-5.59	95.91	111.00
1	A	322	ILE	O-C-N	-5.50	113.90	122.70
1	A	65	TRP	CG-CD2-CE3	5.46	138.82	133.90
1	A	125	TYR	CB-CG-CD1	-5.39	117.77	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	LEU	N-CA-CB	-5.30	99.79	110.40
1	A	200	PRO	CA-C-N	5.27	128.79	117.20
1	A	65	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	131	VAL	CA-C-N	-5.25	105.65	117.20
1	A	376	ILE	CA-C-N	5.25	128.75	117.20
1	A	222	ARG	CA-CB-CG	5.23	124.91	113.40
1	A	265	LYS	CA-CB-CG	5.23	124.90	113.40
1	A	229	HIS	CA-C-N	5.19	128.62	117.20
1	A	209	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	A	141	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	A	259	ASP	CA-C-N	5.06	126.32	116.20
1	A	227	LEU	CA-CB-CG	5.05	126.93	115.30
1	A	388	THR	N-CA-CB	-5.05	100.71	110.30
1	A	49	VAL	CG1-CB-CG2	-5.02	102.86	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain
1	A	95	TYR	Sidechain

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	3196	0	3222	30	0
2	A	1	0	0	0	0
3	A	10	0	4	1	0
4	A	27	0	11	2	0
5	A	83	0	0	1	0
All	All	3317	0	3237	30	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 5.

All (30) 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:192:GLU:N	1:A:192:GLU:OE1	2.06	0.88
1:A:192:GLU:CA	1:A:192:GLU:OE1	2.41	0.67
1:A:246:TYR:HD1	1:A:264:LEU:HD22	1.60	0.67
1:A:202:SER:O	1:A:206:THR:HG23	1.99	0.63
1:A:339:HIS:CD2	4:A:2:NAP:H61A	2.20	0.60
1:A:305:ASN:O	1:A:309:ILE:HG12	2.03	0.57
1:A:151:ILE:HD11	1:A:313:LEU:HD23	1.89	0.54
1:A:119:ARG:HG2	1:A:155:ASN:ND2	2.22	0.54
1:A:284:ALA:O	1:A:288:GLN:HG2	2.11	0.51
1:A:127:CYS:HB3	1:A:153:ARG:HB3	1.91	0.51
1:A:115:ASN:O	1:A:119:ARG:HD3	2.10	0.51
1:A:30:PRO:HA	1:A:66:MET:O	2.12	0.49
1:A:8:PRO:HD2	1:A:28:ILE:HD13	1.94	0.49
1:A:109:GLY:O	1:A:111:ILE:HG22	2.13	0.49
1:A:339:HIS:CD2	4:A:2:NAP:N6A	2.81	0.48
1:A:108:GLY:O	1:A:110:GLY:N	2.49	0.46
1:A:159:ILE:HG21	1:A:304:LEU:HD22	1.98	0.46
1:A:246:TYR:CD1	1:A:264:LEU:HD22	2.47	0.46
1:A:115:ASN:HD22	3:A:1:AKG:C5	2.29	0.46
1:A:137:THR:HG23	1:A:393:PHE:CZ	2.53	0.44
1:A:214:ILE:HG21	1:A:214:ILE:HD13	1.77	0.44
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.83	0.43
1:A:154:GLU:HA	1:A:209:LEU:HD13	2.01	0.42
1:A:289:ILE:HD12	1:A:313:LEU:HD13	2.00	0.42
1:A:356:ILE:HG21	1:A:356:ILE:HD13	1.83	0.42
1:A:357:ILE:HG21	1:A:357:ILE:HD13	1.80	0.42
1:A:331:GLU:HG2	5:A:463:HOH:O	2.20	0.42
1:A:206:THR:HB	1:A:241:PHE:CD1	2.55	0.42
1:A:159:ILE:HD12	1:A:159:ILE:HA	1.73	0.41
1:A:168:ASP:OD2	1:A:193:HIS:HD2	2.03	0.41

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	412/414 (100%)	387 (94%)	18 (4%)	7 (2%)	11 19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLY
1	A	110	GLY
1	A	112	ARG
1	A	159	ILE
1	A	58	LYS
1	A	96	ARG
1	A	259	ASP

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	336/336 (100%)	303 (90%)	33 (10%)	10 19

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	26	ASN
1	A	47	LYS
1	A	55	LYS
1	A	91	LEU
1	A	96	ARG
1	A	103	LEU
1	A	112	ARG
1	A	121	GLU
1	A	131	VAL
1	A	135	GLN
1	A	141	VAL
1	A	154	GLU
1	A	189	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	192	GLU
1	A	206	THR
1	A	227	LEU
1	A	230	LYS
1	A	264	LEU
1	A	286	LEU
1	A	290	LEU
1	A	291	LEU
1	A	311	ASP
1	A	313	LEU
1	A	358	LEU
1	A	364	LEU
1	A	375	LEU
1	A	377	VAL
1	A	380	MET
1	A	388	THR
1	A	389	VAL
1	A	397	MET
1	A	403	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	193	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	AKG	A	1	2	3,9,9	8.14	2 (66%)	4,11,11	6.48	4 (100%)
4	NAP	A	2	-	24,29,52	1.46	4 (16%)	29,45,80	1.68	8 (27%)

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	AKG	A	1	2	-	0/3/9/9	0/0/0/0
4	NAP	A	2	-	-	0/11/31/67	0/3/3/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	AKG	C3-C2	-10.33	1.34	1.51
4	A	2	NAP	P2B-O3X	2.28	1.62	1.54
4	A	2	NAP	PA-O5B	2.95	1.70	1.60
4	A	2	NAP	O4B-C1B	3.07	1.45	1.41
4	A	2	NAP	PA-O3	3.29	1.66	1.54
3	A	1	AKG	O5-C2	9.40	1.38	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	AKG	C3-C2-C1	-6.38	106.20	121.51
3	A	1	AKG	C3-C4-C5	-3.53	106.28	112.75
4	A	2	NAP	C3B-C2B-C1B	-3.28	96.38	102.73
4	A	2	NAP	O2B-C2B-C1B	-3.19	97.59	110.02
4	A	2	NAP	C1B-N9A-C4A	-2.35	123.39	126.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2	NAP	O4B-C1B-N9A	2.14	112.59	108.10
4	A	2	NAP	O2A-PA-O1A	2.23	117.77	110.58
4	A	2	NAP	O4B-C4B-C5B	2.29	117.51	109.32
4	A	2	NAP	O2X-P2B-O1X	3.26	121.09	110.58
4	A	2	NAP	O5B-C5B-C4B	3.33	121.38	109.12
3	A	1	AKG	C4-C3-C2	4.64	124.71	112.98
3	A	1	AKG	O5-C2-C3	9.66	138.53	120.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	AKG	1	0
4	A	2	NAP	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.