



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:17 pm GMT

PDB ID : 1A3W
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-
PLEXED WITH FBP, PG, MN2+ AND K+
Authors : Jurica, M.S.; Mesecar, A.; Heath, P.J.; Shi, W.; Nowak, T.; Stoddard, B.L.
Deposited on : 1998-01-26
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

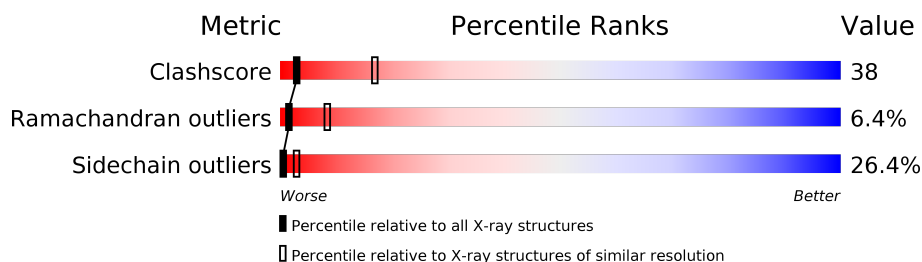
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	

2 Entry composition [i](#)

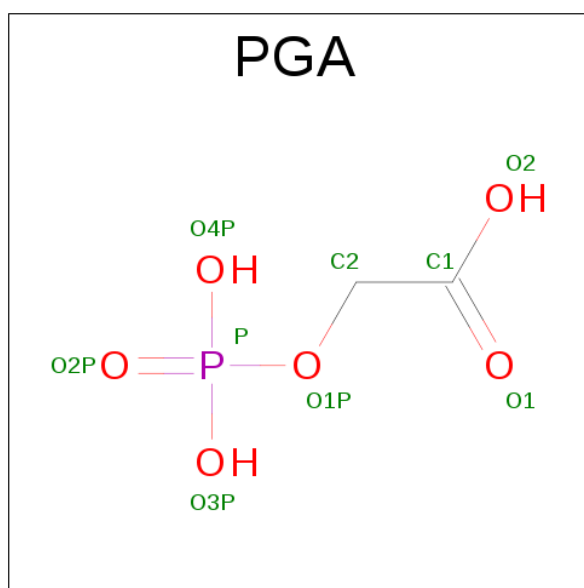
There are 5 unique types of molecules in this entry. The entry contains 7581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE KINASE.

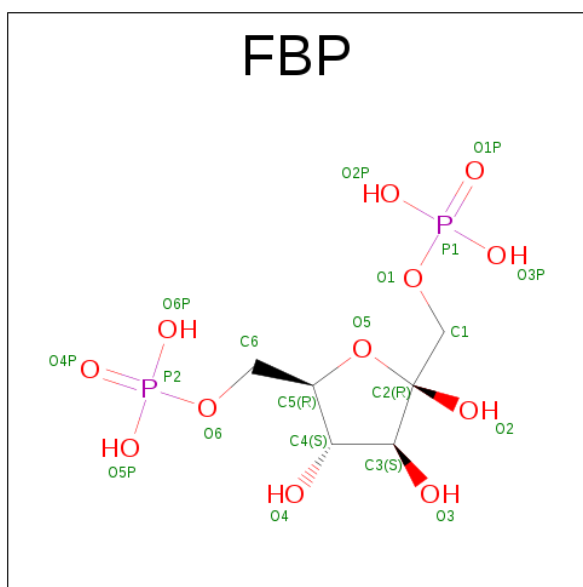
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3773	2380	650	726	17			
1	B	489	Total	C	N	O	S	0	0	0
			3746	2362	647	720	17			

- Molecule 2 is SUGAR (2-PHOSPHOGLYCOLIC ACID) (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is SUGAR (FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

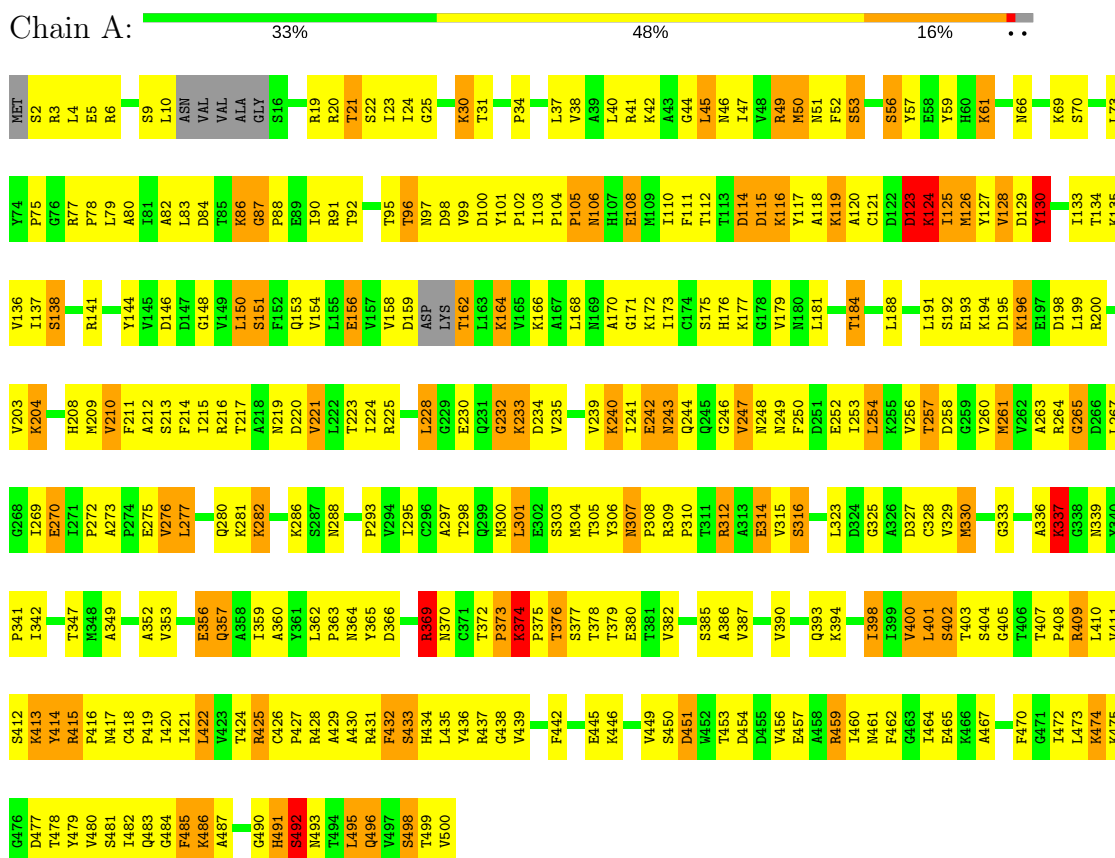
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		

3 Residue-property plots

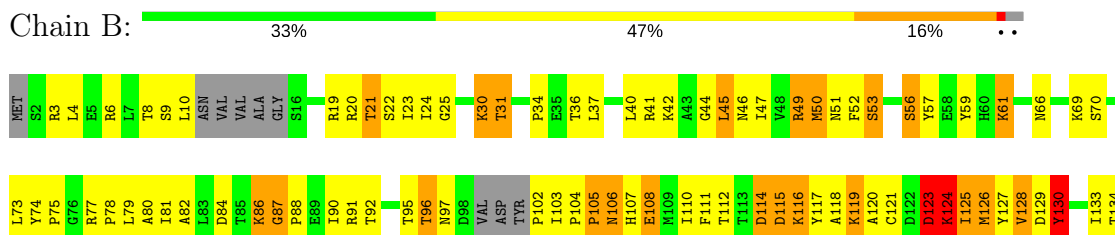
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



• Molecule 1: PYRUVATE KINASE



S481	K135	K204	T347	M417	G490	G490	T424	E386	V353	A352	P272	H208	K136
I482	V136		M348	C418	H491	H491	T424	Q357	V353	A352	P272	H208	I137
Q483	S138		A349	P419	S492	S492	R425	A358	V353	A352	P272	M209	
G484				T420	T493	T493	R425	I359	V353	A352	P272	V210	
F485				T421	T494	T494	R425	A360	V353	A352	P272	F211	R141
K486				L422	T495	T495	R425	Y361	V353	A352	P272	A212	
A487				V423	T496	T496	R425	L362	V353	A352	P272	S213	
				G423	T497	T497	R425	P363	V353	A352	P272	F214	Y144
				T424	T498	T498	R425	N364	V353	A352	P272	I215	Y145
				R425	T499	T499	R425	D366	V353	A352	P272	R216	D146
					T500	T500	R425		V353	A352	P272	T217	D147
							R425		V353	A352	P272	A218	Y149
							R425		V353	A352	P272	L150	
							R425		V353	A352	P272	F152	S151
							R425		V353	A352	P272	Q153	
							R425		V353	A352	P272	V154	
							R425		V353	A352	P272	L155	
							R425		V353	A352	P272	E156	
							R425		V353	A352	P272	V157	
							R425		V353	A352	P272	V158	
							R425		V353	A352	P272	D159	
							R425		V353	A352	P272	E230	
							R425		V353	A352	P272	Q231	LYS
							R425		V353	A352	P272	Q232	T162
							R425		V353	A352	P272	K233	L163
							R425		V353	A352	P272	D234	K164
							R425		V353	A352	P272	V235	V165
							R425		V353	A352	P272	K166	
							R425		V353	A352	P272	A167	
							R425		V353	A352	P272	L168	
							R425		V353	A352	P272	N169	
							R425		V353	A352	P272	A170	
							R425		V353	A352	P272	G171	
							R425		V353	A352	P272	K172	
							R425		V353	A352	P272	I173	
							R425		V353	A352	P272	G174	
							R425		V353	A352	P272	S175	
							R425		V353	A352	P272	H176	
							R425		V353	A352	P272	K177	
							R425		V353	A352	P272	G178	
							R425		V353	A352	P272	F250	
							R425		V353	A352	P272	D251	V179
							R425		V353	A352	P272	E252	N180
							R425		V353	A352	P272	I253	L181
							R425		V353	A352	P272	K254	
							R425		V353	A352	P272	V255	
							R425		V353	A352	P272	T256	T184
							R425		V353	A352	P272	D257	
							R425		V353	A352	P272	G258	L191
							R425		V353	A352	P272	E259	S192
							R425		V353	A352	P272	V260	E193
							R425		V353	A352	P272	M261	K194
							R425		V353	A352	P272	D195	D195
							R425		V353	A352	P272	V262	K196
							R425		V353	A352	P272	A263	E197
							R425		V353	A352	P272	R264	D198
							R425		V353	A352	P272	G265	L199
							R425		V353	A352	P272	D266	R200
							R425		V353	A352	P272	L267	
							R425		V353	A352	P272	G268	V203

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.40Å 102.70Å 110.90Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	75.9 (100.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.218 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: K, FBP, PGA, MN

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	0.29	0/3834	0.63	7/5196 (0.1%)
1	B	0.31	0/3805	0.65	8/5153 (0.2%)
All	All	0.30	0/7639	0.64	15/10349 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ARG	NE-CZ-NH2	-12.25	114.17	120.30
1	B	369	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	A	369	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	A	369	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	B	409	ARG	NE-CZ-NH2	-10.42	115.09	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	3773	0	3844	296	0
1	B	3746	0	3822	298	0
2	A	9	0	2	1	0
2	B	9	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	10	3	0
3	B	20	0	10	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	7581	0	7690	579	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 38.

The worst 5 of 579 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:B:374:LYS:H	1:B:375:PRO:HA	1.16	1.11
1:A:374:LYS:H	1:A:375:PRO:HA	1.19	1.05
1:B:398:ILE:HD11	1:B:482:ILE:HD11	1.43	1.01
1:A:242:GLU:HG3	1:A:263:ALA:CB	1.95	0.96
1:B:242:GLU:HG3	1:B:263:ALA:CB	1.97	0.95

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	486/500 (97%)	398 (82%)	56 (12%)	32 (7%)	1	8
1	B	481/500 (96%)	394 (82%)	57 (12%)	30 (6%)	2	10
All	All	967/1000 (97%)	792 (82%)	113 (12%)	62 (6%)	1	8

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	99	VAL
1	A	106	ASN
1	A	170	ALA
1	A	337	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	417/423 (99%)	307 (74%)	110 (26%)	0	3
1	B	414/423 (98%)	305 (74%)	109 (26%)	0	3
All	All	831/846 (98%)	612 (74%)	219 (26%)	0	3

5 of 219 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	ASP
1	B	50	MET
1	B	422	LEU
1	A	461	ASN
1	B	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	HIS
1	B	106	ASN
1	B	434	HIS
1	A	483	GLN
1	B	46	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, 4 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$
2	PGA	A	1005	5,4	5,8,8	2.35	2 (40%)	6,11,11	3.72	3 (50%)
3	FBP	A	1007	-	18,20,20	1.00	0	23,32,32	0.67	0
2	PGA	B	1006	5,4	5,8,8	2.28	2 (40%)	6,11,11	3.54	3 (50%)
3	FBP	B	1008	-	18,20,20	1.05	1 (5%)	23,32,32	0.82	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
2	PGA	A	1005	5,4	-	0/4/6/6	0/0/0/0
3	FBP	A	1007	-	-	0/13/32/32	0/1/1/1
2	PGA	B	1006	5,4	-	0/4/6/6	0/0/0/0
3	FBP	B	1008	-	-	0/13/32/32	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	P-O2P	2.28	1.58	1.50
2	B	1006	PGA	P-O2P	2.37	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1008	FBP	O5-C2	2.40	1.46	1.43
2	A	1005	PGA	P-O3P	3.81	1.70	1.54
2	B	1006	PGA	P-O3P	3.91	1.70	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	PGA	O4P-P-O1P	-2.41	100.32	106.73
2	B	1006	PGA	O4P-P-O1P	-2.11	101.13	106.73
2	A	1005	PGA	O3P-P-O1P	2.97	114.64	106.73
2	B	1006	PGA	O3P-P-O1P	3.09	114.94	106.73
2	B	1006	PGA	O1P-P-O2P	7.30	126.95	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	PGA	1	0
3	A	1007	FBP	3	0
3	B	1008	FBP	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.