wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:29 AM GMT

PDB ID	:	2QUU
Title	:	Dihydroxyacetone phosphate Schiff base intermediate in mutant fructose-1,6-bisphosphate aldolase from rabbit muscle
Authors	:	St-Jean, M.; Sygusch, J.
Deposited on	:	2007-08-06
Resolution	:	1.98 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:

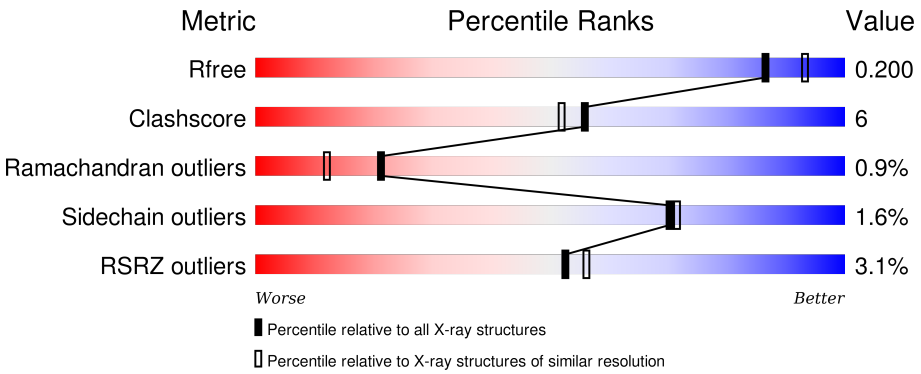
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	363	% 83% 13% •
1	B	363	3% 84% 13% •
1	C	363	4% 80% 17% •
1	D	363	4% 81% 18% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13086 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.

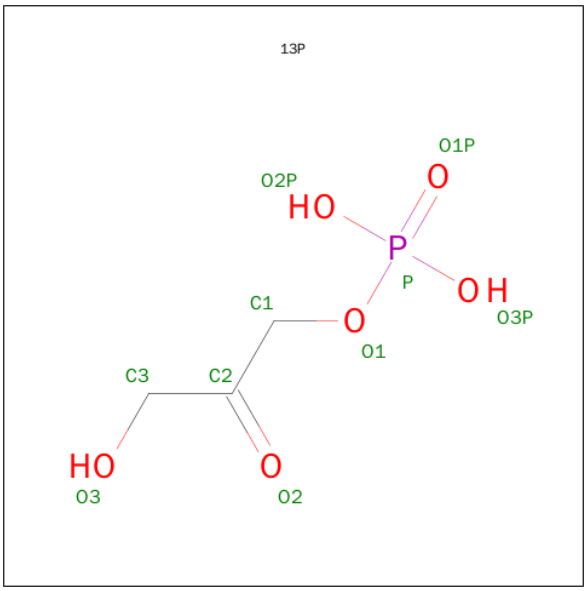
- Molecule 1 is a protein called Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2666	1676	473	505	12	0	0	0
1	B	351	2680	1685	475	508	12	0	0	0
1	C	353	2690	1689	478	511	12	0	0	0
1	D	363	2784	1749	493	530	12	0	8	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	LYS	ENGINEERED	UNP P00883
B	146	MET	LYS	ENGINEERED	UNP P00883
C	146	MET	LYS	ENGINEERED	UNP P00883
D	146	MET	LYS	ENGINEERED	UNP P00883

- Molecule 2 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	9	3	5	1	0	0
			Total	C	O	P		
2	B	1	9	3	5	1	0	0
			Total	C	O	P		
2	C	1	9	3	5	1	0	0
			Total	C	O	P		
2	D	1	9	3	5	1	0	0

- Molecule 3 is water.

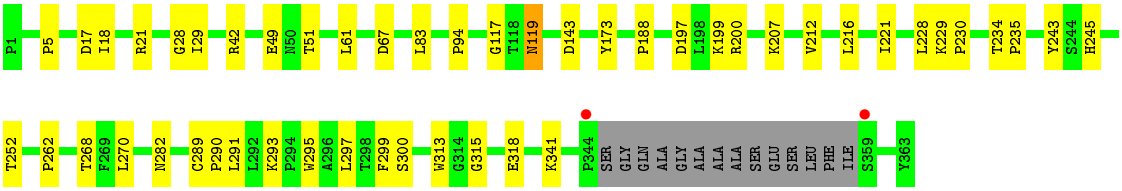
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	583	583	583	0	0
			Total	O		
3	B	555	555	555	0	0
			Total	O		
3	C	524	524	524	0	0
			Total	O		
3	D	568	568	568	0	14

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.

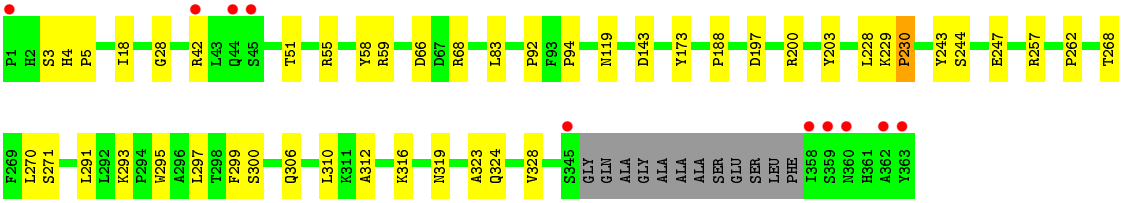
- Molecule 1: Fructose-bisphosphate aldolase A

Chain A:



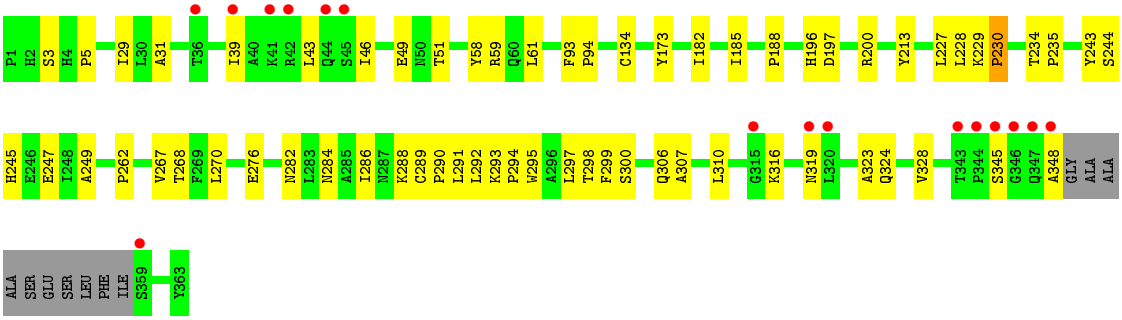
- Molecule 1: Fructose-bisphosphate aldolase A

Chain B:



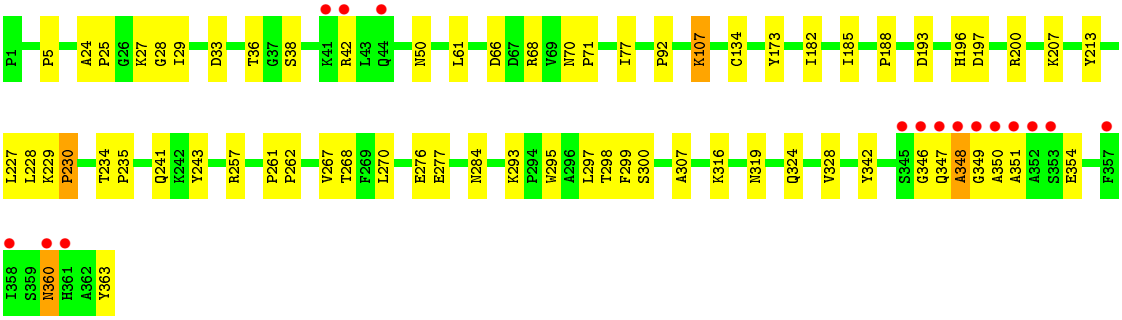
- Molecule 1: Fructose-bisphosphate aldolase A

Chain C:



- Molecule 1: Fructose-bisphosphate aldolase A

Chain D:


P1
P5
A24
P25
G26
K27
G28
I29
D33
T36
G37
S38
K41
R42
L43
Q44
N50
L61
D66
D67
R68
V69
N70
P71
I77
P92
K107
C134
Y173
I182
I185
P188
D193
H196
D197
R200
K207
Y213
L227
L228
K229
P230
T234
P235
Q241
K242
Y243
R257
P261
P262
V267
T268
F269
L270
E276
E277
N284
K293
P294
W295
A296
L297
T298
F299
S300
A307
K316
N319
Q324
V328
Y342
S345
G346
Q347
A348
G349
A350
A351
A352
S353
E354
F357
I358
S359
N360
H361
A362
Y363

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.86Å 103.72Å 84.88Å 90.00° 98.77° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 48.54 – 1.84	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-1.98) 84.0 (48.54-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.157 , 0.195 0.162 , 0.200	Depositor DCC
R_{free} test set	9341 reflections (9.99%)	DCC
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.0	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 109915 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13086	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: 13P

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	0.30	0/2718	0.57	0/3682
1	B	0.30	0/2732	0.57	0/3701
1	C	0.30	0/2742	0.55	0/3714
1	D	0.29	0/2838	0.56	0/3844
All	All	0.30	0/11030	0.56	0/14941

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	213	TYR	Sidechain
1	D	213	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	2666	0	2682	31	0
1	B	2680	0	2698	27	0
1	C	2690	0	2703	36	0
1	D	2784	0	2799	47	0
2	A	9	0	5	0	0
2	B	9	0	5	1	0
2	C	9	0	5	1	0
2	D	9	0	5	3	0
3	A	583	0	0	9	0
3	B	555	0	0	2	0
3	C	524	0	0	1	0
3	D	568	0	0	9	0
All	All	13086	0	10902	135	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 135 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:C:49:GLU:HG2	1:C:51:THR:HG23	1.69	0.73
1:D:347:GLN:HG2	1:D:348:ALA:H	1.55	0.70
1:D:36:THR:HG22	1:D:50:ASN:HD21	1.59	0.68
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.76	0.66
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.77	0.66

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	345/363 (95%)	333 (96%)	9 (3%)	3 (1%)	21	12
1	B	347/363 (96%)	331 (95%)	14 (4%)	2 (1%)	30	21
1	C	349/363 (96%)	335 (96%)	12 (3%)	2 (1%)	30	21
1	D	365/363 (101%)	344 (94%)	16 (4%)	5 (1%)	14	5
All	All	1406/1452 (97%)	1343 (96%)	51 (4%)	12 (1%)	21	12

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	349	GLY
1	B	5	PRO
1	D	188	PRO
1	A	5	PRO
1	A	67	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	283/291 (97%)	280 (99%)	3 (1%)	80	82
1	B	285/291 (98%)	280 (98%)	5 (2%)	66	67
1	C	285/291 (98%)	281 (99%)	4 (1%)	74	75
1	D	294/291 (101%)	287 (98%)	7 (2%)	57	55
All	All	1147/1164 (98%)	1128 (98%)	19 (2%)	70	69

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	59	ARG
1	C	230	PRO
1	D	193	ASP

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Mol	Chain	Res	Type
1	B	295	TRP
1	D	230	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	119	ASN
1	B	319	ASN
1	D	284	ASN
1	B	136	GLN
1	B	179	GLN

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)

4 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	13P	A	3001	1	8,8,9	0.78	0	9,10,12	0.98	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	13P	B	3002	1	8,8,9	0.78	0	9,10,12	0.98	1 (11%)
2	13P	C	3003	1	8,8,9	0.83	0	9,10,12	1.00	1 (11%)
2	13P	D	3004	1	8,8,9	0.82	0	9,10,12	1.04	1 (11%)

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	13P	A	3001	1	-	0/6/6/8	0/0/0/0
2	13P	B	3002	1	-	0/6/6/8	0/0/0/0
2	13P	C	3003	1	-	0/6/6/8	0/0/0/0
2	13P	D	3004	1	-	0/6/6/8	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3002	13P	C1-C2-C3	2.69	120.39	113.71
2	A	3001	13P	C1-C2-C3	2.70	120.41	113.71
2	C	3003	13P	C1-C2-C3	2.76	120.56	113.71
2	D	3004	13P	C1-C2-C3	2.91	120.93	113.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	13P	1	0
2	C	3003	13P	1	0
2	D	3004	13P	3	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	349/363 (96%)	-0.31	2 (0%)	90	91	9, 17, 37, 69	1 (0%)
1	B	351/363 (96%)	-0.14	10 (2%)	56	60	9, 18, 43, 79	3 (0%)
1	C	353/363 (97%)	0.18	16 (4%)	37	41	10, 20, 47, 83	5 (1%)
1	D	363/363 (100%)	0.06	16 (4%)	38	42	10, 20, 48, 79	4 (1%)
All	All	1416/1452 (97%)	-0.05	44 (3%)	52	56	9, 19, 44, 83	13 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	346	GLY	18.2
1	B	345	SER	13.9
1	B	358	ILE	12.3
1	C	348	ALA	10.5
1	C	347	GLN	8.1

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
2	13P	C	3003	9/10	0.96	0.12	1.12	19,23,26,27	0
2	13P	D	3004	9/10	0.98	0.10	-0.33	19,20,26,26	0
2	13P	A	3001	9/10	0.97	0.07	-0.57	18,19,22,23	0
2	13P	B	3002	9/10	0.97	0.08	-1.19	21,23,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.