wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 01:29 AM EST

PDB ID	:	1Z01
Title	:	2-Oxoquinoline 8-Monooxygenase Component: Active site Modulation by Rieske-[2fe-2S] Center Oxidation/Reduction
Authors	:	Martins, B.M.; Svetlitchnaia, T.; Dobbek, H.
Deposited on	:	2005-03-01
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

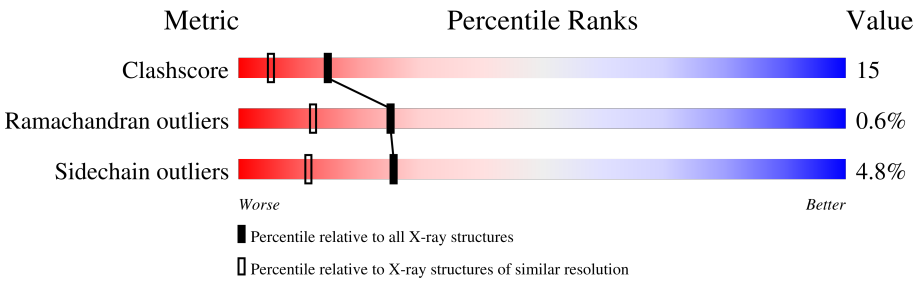
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 of 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	75% 18% • •
1	B	446	72% 21% • •
1	C	446	72% 22% • •
1	D	446	74% 20% • •
1	E	446	69% 24% • •
1	F	446	71% 23% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24517 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.

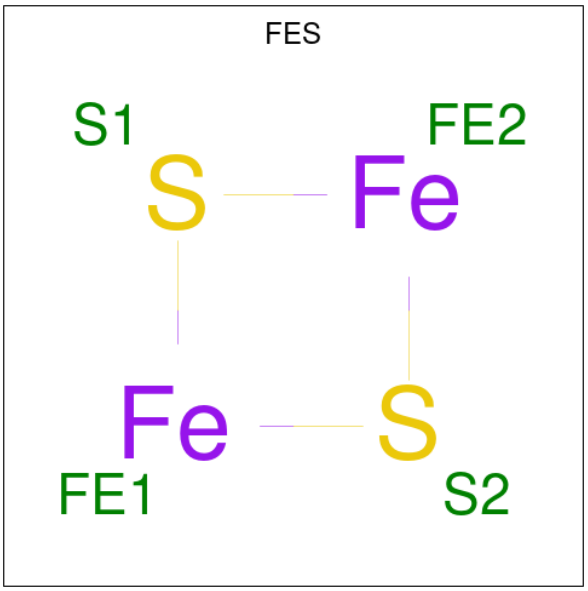
- Molecule 1 is a protein called 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3454	2211	592	635	16	0	0	0
1	B	427	3454	2211	592	635	16	0	0	0
1	C	427	3454	2211	592	635	16	0	0	0
1	D	427	3454	2211	592	635	16	0	0	0
1	E	427	3454	2211	592	635	16	0	0	0
1	F	427	3454	2211	592	635	16	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	F	1	4	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	668	668	668	0	0
4	B	620	620	620	0	0
4	C	603	603	603	0	0
4	D	663	663	663	0	0
4	E	590	590	590	0	0
4	F	619	619	619	0	0

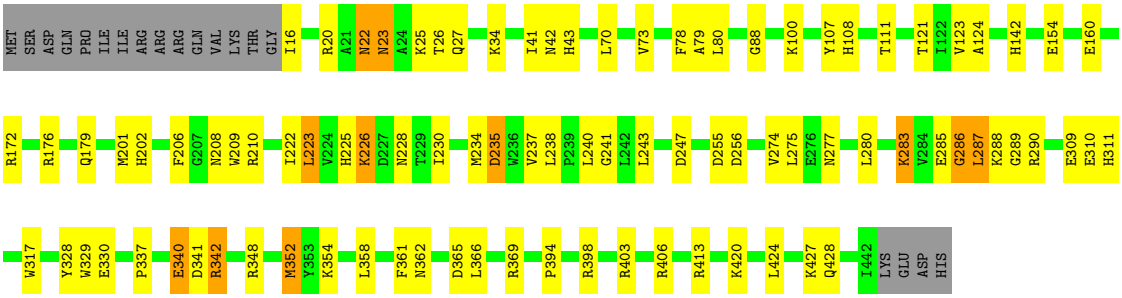
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

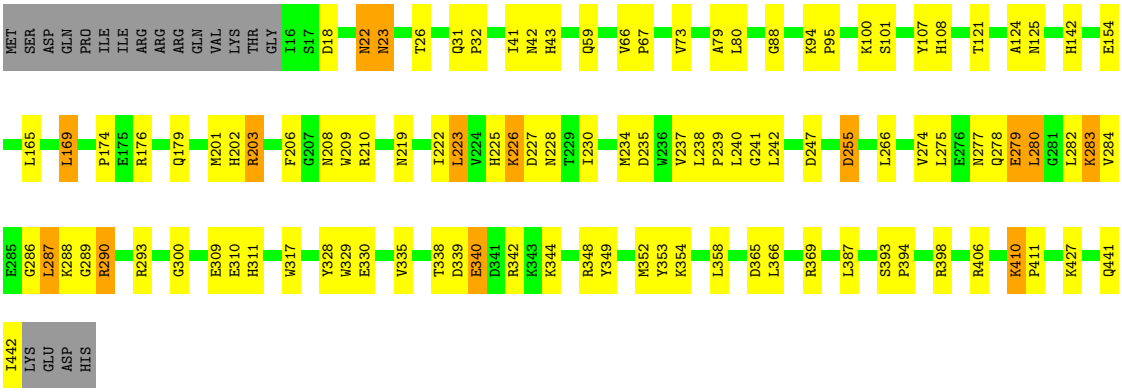
• Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain A:



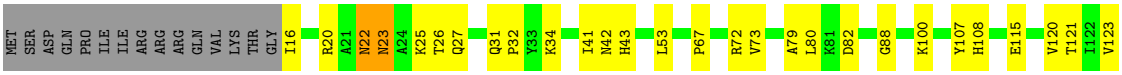
• Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain B:



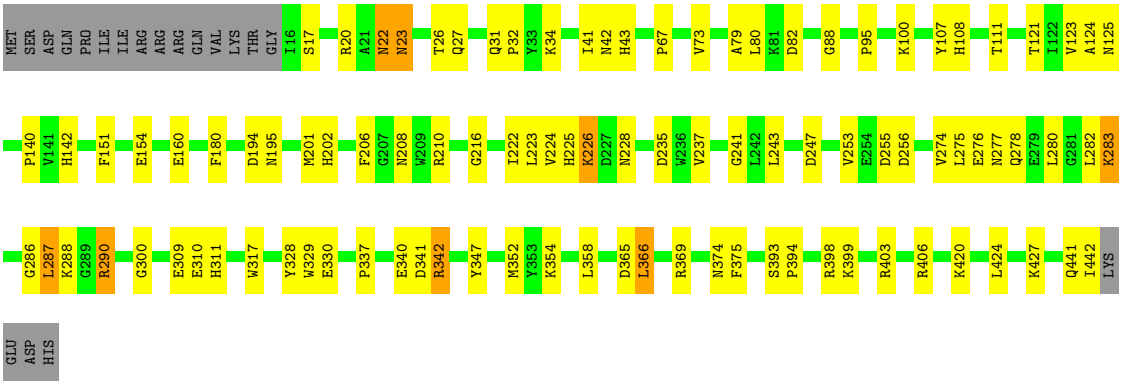
• Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain C:



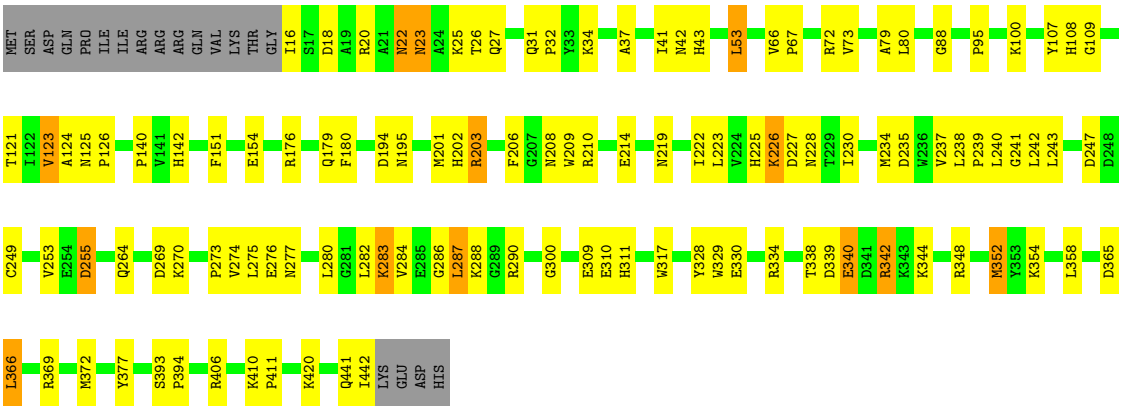
• Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain D:



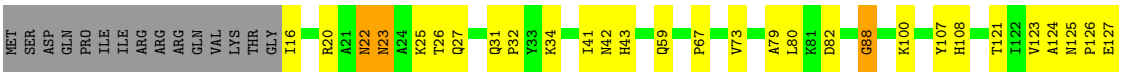
• Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain E:



• Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain F:



L130
P140
V141
H142
F151
V152
R153
E154
E160
R176
Q179
F180
P186
D194
N195
M201
H202
R203
N208
W209
R210
G216
N219
I222
L223
V224
H225
K226
D227
N228
T229
I230
M234
D235
W236
V237
L238
G241
L242
L243
D247
D248
C249
V253
E254
D255
D256
K260
Q264
W265
L266
D269
K270
V274
L275
E276
N277
L280
K283
G286
L287
K288
G289
R290
R293
G300
E310
H311
W317
Y328
W329
E330
E340
D341
R342
M352
Y353
K354
L358
D365
L366
R369
M372
L387
S393
P394
R398
R406
K410
P411
G412
R413
K427
Q428
I442
LYS
GLU
ASP
HIS

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.46Å 166.96Å 173.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	98.7 (20.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24517	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

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: FE, FES

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	0.36	0/3560	0.66	2/4853 (0.0%)
1	B	0.35	0/3560	0.65	1/4853 (0.0%)
1	C	0.35	0/3560	0.65	1/4853 (0.0%)
1	D	0.35	0/3560	0.66	3/4853 (0.1%)
1	E	0.35	0/3560	0.65	1/4853 (0.0%)
1	F	0.36	0/3560	0.65	1/4853 (0.0%)
All	All	0.35	0/21360	0.65	9/29118 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	342	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	342	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	88	GLY	N-CA-C	5.44	126.70	113.10
1	D	88	GLY	N-CA-C	5.30	126.35	113.10
1	E	88	GLY	N-CA-C	5.29	126.33	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3454	0	3307	97	0
1	B	3454	0	3307	130	0
1	C	3454	0	3307	97	0
1	D	3454	0	3307	95	0
1	E	3454	0	3307	130	0
1	F	3454	0	3307	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	4	0	0	1	0
3	E	4	0	0	1	0
3	F	4	0	0	1	0
4	A	668	0	0	24	0
4	B	620	0	0	39	0
4	C	603	0	0	20	0
4	D	663	0	0	18	0
4	E	590	0	0	34	0
4	F	619	0	0	19	0
All	All	24517	0	19842	620	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 15.

The worst 5 of 620 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:174:PRO:HB3	1:F:127:GLU:OE2	1.51	1.10
1:A:287:LEU:H	1:A:287:LEU:HD23	0.96	1.09
1:E:222:ILE:HG21	4:E:980:HOH:O	1.61	0.98
1:A:287:LEU:HD23	1:A:287:LEU:N	1.80	0.96
1:C:287:LEU:H	1:C:287:LEU:HD23	1.31	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	425/446 (95%)	398 (94%)	25 (6%)	2 (0%)	29	15
1	B	425/446 (95%)	399 (94%)	23 (5%)	3 (1%)	22	10
1	C	425/446 (95%)	395 (93%)	26 (6%)	4 (1%)	17	6
1	D	425/446 (95%)	401 (94%)	22 (5%)	2 (0%)	29	15
1	E	425/446 (95%)	400 (94%)	23 (5%)	2 (0%)	29	15
1	F	425/446 (95%)	400 (94%)	23 (5%)	2 (0%)	29	15
All	All	2550/2676 (95%)	2393 (94%)	142 (6%)	15 (1%)	25	12

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	GLU
1	C	235	ASP
1	A	123	VAL
1	C	123	VAL
1	D	123	VAL

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	373/392 (95%)	358 (96%)	15 (4%)	31	16
1	B	373/392 (95%)	355 (95%)	18 (5%)	25	11
1	C	373/392 (95%)	353 (95%)	20 (5%)	22	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	373/392 (95%)	358 (96%)	15 (4%)	31 16
1	E	373/392 (95%)	354 (95%)	19 (5%)	24 10
1	F	373/392 (95%)	353 (95%)	20 (5%)	22 9
All	All	2238/2352 (95%)	2131 (95%)	107 (5%)	25 11

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	223	LEU
1	E	53	LEU
1	F	255	ASP
1	D	235	ASP
1	D	340	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	27	GLN
1	D	374	ASN
1	F	195	ASN
1	D	43	HIS
1	D	228	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	FES	F	500	1	0,4,4	-	-	-		
3	FES	C	500	1	0,4,4	-	-	-		
3	FES	E	500	1	0,4,4	-	-	-		
3	FES	B	500	1	0,4,4	-	-	-		
3	FES	D	500	1	0,4,4	-	-	-		
3	FES	A	500	1	0,4,4	-	-	-		

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	FES	F	500	1	-	-	0/1/1/1
3	FES	C	500	1	-	-	0/1/1/1
3	FES	E	500	1	-	-	0/1/1/1
3	FES	B	500	1	-	-	0/1/1/1
3	FES	D	500	1	-	-	0/1/1/1
3	FES	A	500	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	500	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	500	FES	1	0
3	E	500	FES	1	0
3	B	500	FES	1	0
3	D	500	FES	1	0
3	A	500	FES	1	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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.