



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:38 PM GMT

PDB ID : 1XRB  
Title : S-adenosylmethionine synthetase (MAT, ATP: L-methionine S-adenosyltransferase, E.C.2.5.1.6) in which MET residues are replaced with selenomethionine residues (MSE)  
Authors : Takusagawa, F.; Kamitori, S.; Misaki, S.; Markham, G.D.  
Deposited on : 1995-10-26  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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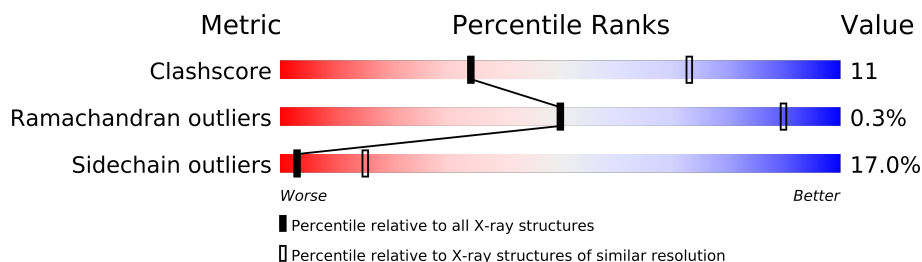
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	

## 2 Entry composition i

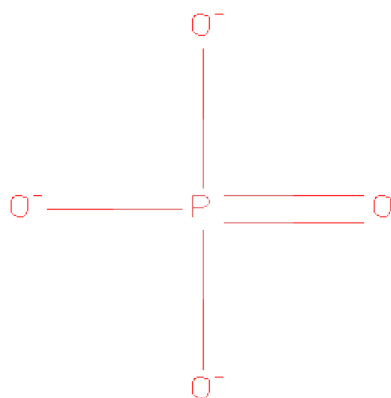
There are 4 unique types of molecules in this entry. The entry contains 3544 atoms, of which 632 are hydrogens and 0 are deuterium.

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 S-ADENOSYLMETHIONINE SYNTHETASE.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	377	Total	C	H	N	O	S	Se	632	0	0
			3530	1830	632	495	560	4	9			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

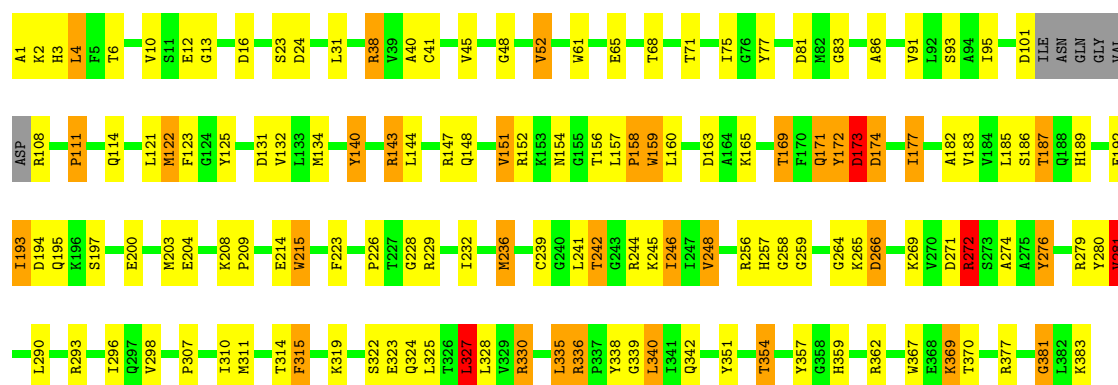
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: S-ADENOSYLMETHIONINE SYNTHETASE

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.90Å 128.90Å 139.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	97.7 (10.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.188 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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: PO4, MG, K

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	0.91	0/2947	1.67	49/3978 (1.2%)

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	13

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	MSE	CA-CB-CG	-11.19	94.28	113.30
1	A	61	TRP	CD1-CG-CD2	9.04	113.53	106.30
1	A	215	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	A	362	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	159	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	A	276	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	A	271	ASP	CB-CG-OD1	8.07	125.56	118.30
1	A	336	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	61	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	A	159	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	A	354	THR	N-CA-CB	-7.67	95.73	110.30
1	A	367	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	A	256	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	272	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	38	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	246	ILE	CA-CB-CG2	7.06	125.03	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	TRP	CG-CD2-CE3	6.86	140.08	133.90
1	A	314	THR	N-CA-C	-6.84	92.53	111.00
1	A	159	TRP	CB-CG-CD1	-6.82	118.13	127.00
1	A	367	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	362	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	215	TRP	CE2-CD2-CG	-6.54	102.06	107.30
1	A	187	THR	CA-CB-OG1	-6.50	95.34	109.00
1	A	143	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	163	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	279	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	24	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	215	TRP	CG-CD1-NE1	-5.98	104.12	110.10
1	A	77	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	61	TRP	CB-CG-CD1	-5.78	119.48	127.00
1	A	61	TRP	CG-CD2-CE3	5.78	139.10	133.90
1	A	61	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	A	108	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	86	ALA	CB-CA-C	-5.58	101.72	110.10
1	A	41	CYS	N-CA-CB	-5.54	100.62	110.60
1	A	367	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	271	ASP	OD1-CG-OD2	-5.54	112.78	123.30
1	A	200	GLU	N-CA-CB	5.43	120.37	110.60
1	A	159	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	A	281	VAL	CA-CB-CG2	5.32	118.87	110.90
1	A	369	LYS	CA-CB-CG	5.29	125.04	113.40
1	A	327	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	354	THR	CA-CB-CG2	5.17	119.64	112.40
1	A	272	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	71	THR	CA-CB-OG1	-5.08	98.33	109.00
1	A	140	TYR	CA-CB-CG	-5.06	103.79	113.40
1	A	200	GLU	CA-CB-CG	5.04	124.49	113.40
1	A	173	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	172	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	PHE	Sidechain
1	A	125	TYR	Sidechain
1	A	13	GLY	Peptide
1	A	140	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	173	ASP	Peptide
1	A	194	ASP	Peptide
1	A	228	GLY	Peptide
1	A	244	ARG	Sidechain
1	A	259	GLY	Peptide
1	A	280	TYR	Sidechain
1	A	293	ARG	Sidechain
1	A	336	ARG	Sidechain
1	A	48	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2898	632	2234	56	0
2	A	10	0	0	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
All	All	2912	632	2234	56	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (56) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:351:TYR:O	1:A:354:THR:HB	1.78	0.82
1:A:354:THR:HG23	1:A:359:HIS:NE2	2.03	0.73
1:A:354:THR:HG23	1:A:359:HIS:CD2	2.23	0.73
1:A:122:MSE:HG2	1:A:274:ALA:HB3	1.73	0.68
1:A:83:GLY:HA2	1:A:236:MSE:HG3	1.78	0.64
1:A:223:PHE:HB3	1:A:226:PRO:HG3	1.80	0.63
1:A:23:SER:OG	1:A:242:THR:HG21	1.99	0.63
1:A:290:LEU:HD23	1:A:325:LEU:HD21	1.85	0.59
1:A:83:GLY:CA	1:A:236:MSE:HG3	2.33	0.58
1:A:189:HIS:HE1	1:A:229:ARG:O	1.87	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:324:GLN:O	1:A:328:LEU:HD12	2.04	0.57
1:A:189:HIS:CE1	1:A:229:ARG:O	2.59	0.56
1:A:339:GLY:O	1:A:342:GLN:HB3	2.05	0.56
1:A:257:HIS:CD2	1:A:258:GLY:O	2.62	0.53
1:A:6:THR:OG1	1:A:169:THR:HB	2.09	0.52
1:A:265:LYS:HB3	1:A:269:LYS:HG3	1.90	0.51
1:A:10:VAL:HG12	1:A:165:LYS:HD2	1.93	0.50
1:A:132:VAL:HG23	1:A:134:MSE:HB2	1.94	0.49
1:A:232:ILE:HG12	1:A:236:MSE:HE3	1.95	0.49
1:A:189:HIS:HD2	1:A:193:ILE:CG2	2.26	0.49
1:A:257:HIS:HD2	1:A:258:GLY:O	1.96	0.49
1:A:246:ILE:HG23	1:A:257:HIS:NE2	2.28	0.49
1:A:52:VAL:O	1:A:93:SER:HA	2.13	0.48
1:A:151:VAL:HA	1:A:154:ASN:OD1	2.14	0.48
1:A:169:THR:HG23	1:A:182:ALA:HB3	1.94	0.48
1:A:266:ASP:OD2	1:A:269:LYS:NZ	2.47	0.48
1:A:281:VAL:HG22	1:A:296:ILE:HG13	1.97	0.47
1:A:381:GLY:O	1:A:383:LYS:NZ	2.48	0.46
1:A:298:VAL:HG12	1:A:310:ILE:HG12	1.97	0.46
1:A:245:LYS:HB3	1:A:248:VAL:HG13	1.96	0.46
1:A:2:LYS:NZ	1:A:173:ASP:OD2	2.49	0.45
1:A:68:THR:HG21	1:A:91:VAL:HG13	1.99	0.45
1:A:327:LEU:HA	1:A:330:ARG:NH1	2.32	0.45
1:A:4:LEU:HD23	1:A:171:GLN:HB2	1.98	0.45
1:A:156:THR:O	1:A:158:PRO:HD3	2.17	0.45
1:A:204:GLU:O	1:A:209:PRO:HD3	2.17	0.45
1:A:12:GLU:HG2	1:A:357:TYR:OH	2.17	0.45
1:A:246:ILE:HG23	1:A:257:HIS:CE1	2.52	0.44
1:A:203:MSE:O	1:A:208:LYS:HB2	2.17	0.44
1:A:1:ALA:N	1:A:174:ASP:OD2	2.51	0.44
1:A:185:LEU:HD13	1:A:186:SER:N	2.33	0.43
1:A:338:TYR:N	1:A:338:TYR:CD1	2.85	0.43
1:A:335:LEU:HA	1:A:340:LEU:CD1	2.49	0.43
1:A:177:ILE:HG13	1:A:215:TRP:CZ2	2.54	0.43
1:A:377:ARG:CZ	1:A:383:LYS:HG3	2.50	0.42
1:A:40:ALA:HA	1:A:264:GLY:O	2.19	0.42
1:A:157:LEU:HD22	1:A:159:TRP:CZ2	2.54	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.76	0.41
1:A:276:TYR:OH	1:A:359:HIS:HD2	2.03	0.41
1:A:75:ILE:O	1:A:152:ARG:NH2	2.53	0.41
1:A:324:GLN:O	1:A:327:LEU:HB3	2.21	0.41
1:A:272:ARG:HD2	1:A:276:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:381:GLY:O	1:A:383:LYS:HG2	2.21	0.40
1:A:2:LYS:HA	1:A:172:TYR:O	2.21	0.40
1:A:315:PHE:N	1:A:315:PHE:CD1	2.88	0.40
1:A:111:PRO:O	1:A:114:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	373/383 (97%)	342 (92%)	30 (8%)	1 (0%)	50	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	GLY

### 5.3.2 Protein sidechains ⓘ

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	306/302 (101%)	254 (83%)	52 (17%)	3	15

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	4	LEU
1	A	16	ASP

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Mol	Chain	Res	Type
1	A	31	LEU
1	A	38	ARG
1	A	45	VAL
1	A	52	VAL
1	A	65	GLU
1	A	81	ASP
1	A	95	ILE
1	A	101	ASP
1	A	111	PRO
1	A	121	LEU
1	A	122	MSE
1	A	131	ASP
1	A	143	ARG
1	A	144	LEU
1	A	147	ARG
1	A	148	GLN
1	A	151	VAL
1	A	158	PRO
1	A	160	LEU
1	A	169	THR
1	A	171	GLN
1	A	174	ASP
1	A	177	ILE
1	A	183	VAL
1	A	187	THR
1	A	192	GLU
1	A	193	ILE
1	A	195	GLN
1	A	197	SER
1	A	214	GLU
1	A	239	CYS
1	A	241	LEU
1	A	242	THR
1	A	248	VAL
1	A	266	ASP
1	A	272	ARG
1	A	281	VAL
1	A	307	PRO
1	A	311	MSE
1	A	315	PHE
1	A	319	LYS
1	A	322	SER

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Mol	Chain	Res	Type
1	A	323	GLU
1	A	327	LEU
1	A	330	ARG
1	A	335	LEU
1	A	340	LEU
1	A	369	LYS
1	A	370	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	142	HIS
1	A	189	HIS
1	A	257	HIS
1	A	297	GLN
1	A	359	HIS
1	A	374	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are 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	$\# Z  > 2$
2	PO4	A	384	3	4,4,4	1.31	0	6,6,6	0.32	0
2	PO4	A	385	3	4,4,4	0.95	0	6,6,6	0.33	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	PO4	A	384	3	-	0/0/0/0	0/0/0/0
2	PO4	A	385	3	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.