



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 02:13 am BST

PDB ID : 6G7M  
Title : Four-site variant (Y222C, C197S, C432S, C433S) of E. coli hydrogenase-2  
Authors : Carr, S.B.; Armstrong, F.A.; Zhang, L.; Beaton, S.E.  
Deposited on : 2018-04-06  
Resolution : 1.71 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](mailto: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 ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

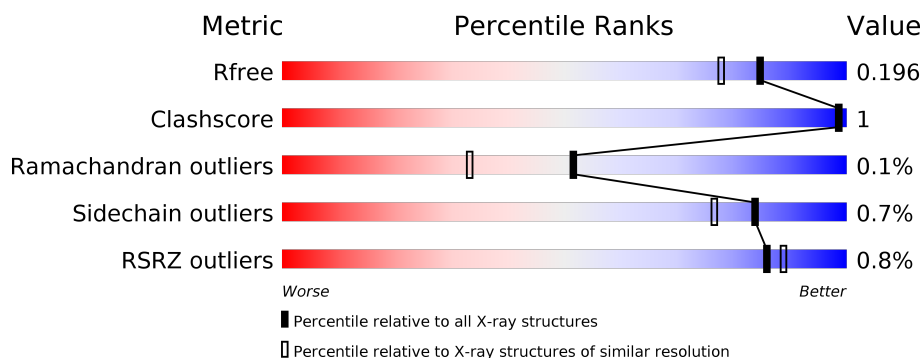
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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))
$R_{free}$	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	S	304	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	T	304	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> </div> </div>
2	L	567	<div> <div></div> <div>94%</div> <div></div> </div>
2	M	567	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13667 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 Hydrogenase-2 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	268	Total	C	N	O	S	0	1	0
			2038	1288	361	375	14			
1	T	268	Total	C	N	O	S	0	1	0
			2035	1287	360	374	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	222	CYS	TYR	conflict	UNP P69741
S	297	ARG	-	expression tag	UNP P69741
S	298	SER	-	expression tag	UNP P69741
S	299	HIS	-	expression tag	UNP P69741
S	300	HIS	-	expression tag	UNP P69741
S	301	HIS	-	expression tag	UNP P69741
S	302	HIS	-	expression tag	UNP P69741
S	303	HIS	-	expression tag	UNP P69741
S	304	HIS	-	expression tag	UNP P69741
T	222	CYS	TYR	conflict	UNP P69741
T	297	ARG	-	expression tag	UNP P69741
T	298	SER	-	expression tag	UNP P69741
T	299	HIS	-	expression tag	UNP P69741
T	300	HIS	-	expression tag	UNP P69741
T	301	HIS	-	expression tag	UNP P69741
T	302	HIS	-	expression tag	UNP P69741
T	303	HIS	-	expression tag	UNP P69741
T	304	HIS	-	expression tag	UNP P69741

- Molecule 2 is a protein called Hydrogenase-2 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	551	Total	C	N	O	S	0	2	0
			4300	2735	740	810	15			

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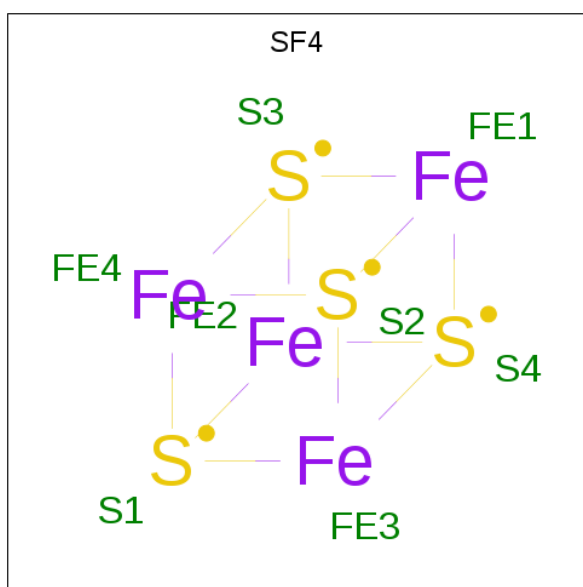
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	551	Total	C	N	O	S	0	1	0
			4296	2732	740	809	15			

There are 6 discrepancies between the modelled and reference sequences:

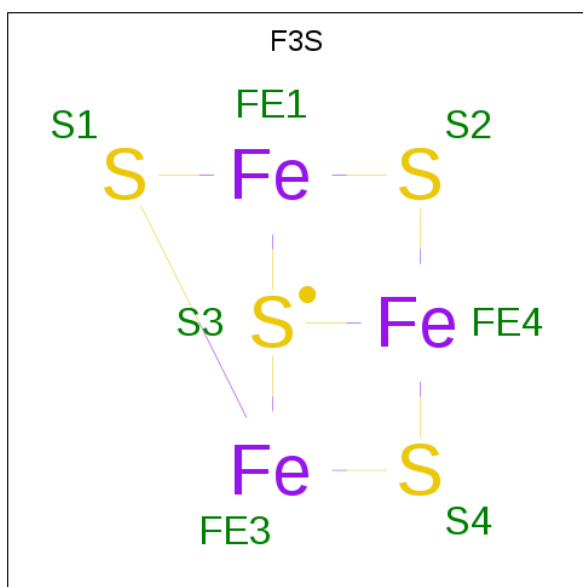
Chain	Residue	Modelled	Actual	Comment	Reference
L	197	SER	CYS	engineered mutation	UNP P0ACE0
L	432	SER	CYS	engineered mutation	UNP P0ACE0
L	433	SER	CYS	engineered mutation	UNP P0ACE0
M	197	SER	CYS	engineered mutation	UNP P0ACE0
M	432	SER	CYS	engineered mutation	UNP P0ACE0
M	433	SER	CYS	engineered mutation	UNP P0ACE0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



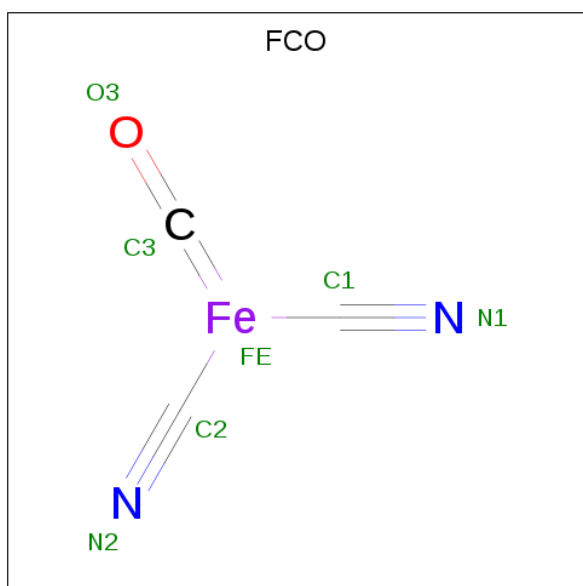
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		
4	T	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula:  $\text{C}_3\text{FeN}_2\text{O}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	Ni	0	0
			1	1		
6	M	1	Total	Ni	0	0
			1	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	2	Total	Mg	0	0
			2	2		
7	M	2	Total	Mg	0	0
			2	2		

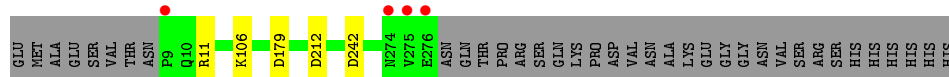
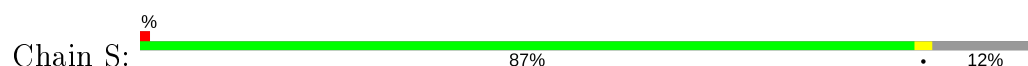
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	S	150	Total	O	0	0
			150	150		
8	L	347	Total	O	0	0
			347	347		
8	T	130	Total	O	0	0
			130	130		
8	M	305	Total	O	0	0
			305	305		

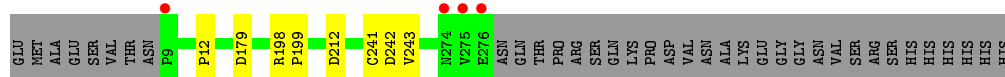
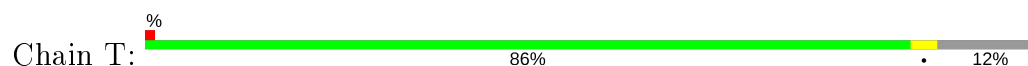
### 3 Residue-property plots [i](#)

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

- Molecule 1: Hydrogenase-2 small chain



- Molecule 1: Hydrogenase-2 small chain



- Molecule 2: Hydrogenase-2 large chain



- Molecule 2: Hydrogenase-2 large chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.24Å 100.99Å 169.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.75 – 1.71 86.27 – 1.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.75-1.71) 100.0 (86.27-1.71)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.157 , 0.190 0.166 , 0.196	Depositor DCC
$R_{free}$ test set	8958 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NI, MG, F3S, SF4, FCO

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	S	0.79	0/2095	0.83	4/2852 (0.1%)
1	T	0.76	0/2095	0.80	3/2852 (0.1%)
2	L	0.79	0/4410	0.84	6/6011 (0.1%)
2	M	0.76	1/4403 (0.0%)	0.83	6/6002 (0.1%)
All	All	0.77	1/13003 (0.0%)	0.83	19/17717 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	172	TRP	CB-CG	5.01	1.59	1.50

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	428	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	M	424	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	L	513	ASP	CB-CG-OD1	7.57	125.11	118.30
2	M	424	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	S	179	ASP	CB-CG-OD1	6.76	124.39	118.30

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	S	2038	0	1962	0	0
1	T	2035	0	1963	3	0
2	L	4300	0	4237	7	0
2	M	4296	0	4230	3	0
3	S	16	0	0	0	0
3	T	16	0	0	0	0
4	S	7	0	0	0	0
4	T	7	0	0	0	0
5	L	7	0	0	0	0
5	M	7	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
7	L	2	0	0	0	0
7	M	2	0	0	0	0
8	L	347	0	0	3	0
8	M	305	0	0	1	0
8	S	150	0	0	0	0
8	T	130	0	0	2	0
All	All	13667	0	12392	13	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 1.

The worst 5 of 13 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:T:241:CYS:HB3	8:T:503:HOH:O	1.64	0.95
1:T:243:VAL:HG13	8:T:503:HOH:O	2.08	0.54
2:M:455:HIS:HD2	8:M:881:HOH:O	1.93	0.51
2:M:313:ARG:HD3	2:M:322:TYR:CE2	2.47	0.50
2:L:455:HIS:HD2	8:L:1001:HOH:O	1.95	0.49

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	S	267/304 (88%)	258 (97%)	9 (3%)	0	100	100
1	T	267/304 (88%)	258 (97%)	9 (3%)	0	100	100
2	L	551/567 (97%)	529 (96%)	21 (4%)	1 (0%)	47	30
2	M	550/567 (97%)	529 (96%)	20 (4%)	1 (0%)	47	30
All	All	1635/1742 (94%)	1574 (96%)	59 (4%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	211	LYS
2	L	211	LYS

### 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	S	214/245 (87%)	213 (100%)	1 (0%)	88	83
1	T	214/245 (87%)	213 (100%)	1 (0%)	88	83
2	L	467/479 (98%)	463 (99%)	4 (1%)	78	69
2	M	466/479 (97%)	462 (99%)	4 (1%)	78	69
All	All	1361/1448 (94%)	1351 (99%)	10 (1%)	84	76

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	382	ASN
1	T	12	PRO
2	M	242	TYR
2	L	312	TYR
2	M	141	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	202	ASN
2	L	455	HIS
1	T	89	ASN
2	M	47	ASN
2	M	455	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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z  > 2$
5	FCO	M	601	8,2	0,6,6	0.00	-	-		
3	SF4	S	401	1	0,12,12	0.00	-	-		
4	F3S	T	402	1	0,9,9	0.00	-	-		
3	SF4	S	403	1	0,12,12	0.00	-	-		
3	SF4	T	403	1,8	0,12,12	0.00	-	-		
3	SF4	T	401	1	0,12,12	0.00	-	-		
5	FCO	L	601	8,2	0,6,6	0.00	-	-		
4	F3S	S	402	1	0,9,9	0.00	-	-		

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	SF4	S	401	1	-	-	0/6/5/5
4	F3S	T	402	1	-	-	0/3/3/3
3	SF4	S	403	1	-	-	0/6/5/5
3	SF4	T	403	1,8	-	-	0/6/5/5
3	SF4	T	401	1	-	-	0/6/5/5
4	F3S	S	402	1	-	-	0/3/3/3

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.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	S	268/304 (88%)	-0.12	4 (1%) 73 78	11, 16, 29, 73	0
1	T	268/304 (88%)	-0.08	4 (1%) 73 78	12, 18, 34, 78	0
2	L	551/567 (97%)	-0.22	1 (0%) 95 95	10, 15, 28, 40	0
2	M	551/567 (97%)	-0.17	4 (0%) 87 90	11, 17, 34, 46	0
All	All	1638/1742 (94%)	-0.17	13 (0%) 86 89	10, 16, 31, 78	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	276	GLU	8.4
1	S	275	VAL	8.4
1	T	275	VAL	6.1
1	S	276	GLU	4.3
1	S	9	PRO	3.7

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	L	604	1/1	0.85	0.13	47,47,47,47	0
7	MG	M	604	1/1	0.94	0.13	39,39,39,39	0
3	SF4	S	403	8/8	0.97	0.08	12,15,24,26	0
3	SF4	T	403	8/8	0.97	0.07	15,16,23,29	0
5	FCO	M	601	7/7	0.99	0.09	11,11,12,12	0
3	SF4	S	401	8/8	0.99	0.08	14,15,15,16	0
6	NI	L	602	1/1	0.99	0.07	14,14,14,14	0
6	NI	M	602	1/1	0.99	0.06	16,16,16,16	0
3	SF4	T	401	8/8	0.99	0.07	14,15,15,16	0
4	F3S	T	402	7/7	0.99	0.07	13,13,13,13	0
5	FCO	L	601	7/7	0.99	0.09	9,11,11,12	0
4	F3S	S	402	7/7	0.99	0.07	12,12,12,13	0
7	MG	L	603	1/1	1.00	0.11	7,7,7,7	0
7	MG	M	603	1/1	1.00	0.13	9,9,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.