

wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 12:05 am GMT

PDB ID : 6EHS

Title : E. coli Hydrogenase-2 chemically reduced structure Authors : Carr, S.B.; Evans, R.M.; Beaton, S.E.; Armstrong, F.A.

Deposited on : 2017-09-15

Resolution : 1.50 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

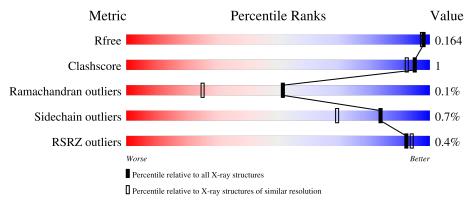
Validation Pipeline (wwPDB-VP) : 2.36

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 1.50 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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% 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	300	87%	• 11%
1	Т	300	87%	11%
2	L	552	95%	•
2	M	552	95%	5%



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13761 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.

	\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
	1 S	267	Total	С	N	О	S	0	1	0		
			201	2037	1289	360	375	13	Ü	1		
	1	Т	268	Total C	N	Ο	S	0	1	0		
	1	1	200	2041	1293	360	375	13	0	1	0	

There are 14 discrepancies between the modelled and reference sequences:

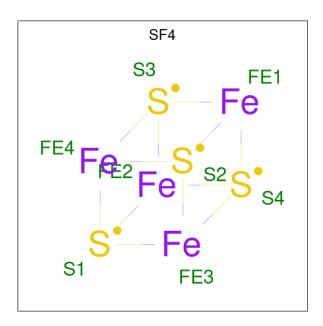
Chain	Residue	Modelled	Actual	Comment	Reference
S	0	MET	-	initiating methionine	UNP P69741
S	294	HIS	-	expression tag	UNP P69741
S	295	HIS	-	expression tag	UNP P69741
S	296	HIS	-	expression tag	UNP P69741
S	297	HIS	-	expression tag	UNP P69741
S	298	HIS	-	expression tag	UNP P69741
S	299	HIS	-	expression tag	UNP P69741
Т	0	MET	-	initiating methionine	UNP P69741
Т	294	HIS	-	expression tag	UNP P69741
Т	295	HIS	-	expression tag	UNP P69741
Т	296	HIS	-	expression tag	UNP P69741
Т	297	HIS	-	expression tag	UNP P69741
Т	298	HIS	-	expression tag	UNP P69741
Т	299	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	- '	0	S	0	3	0
			4306	2738	740	810	18			
2	M	551	Total	\mathbf{C}	N	O	\mathbf{S}	0	0	0
	IVI	991	4290	2728	738	806	18			

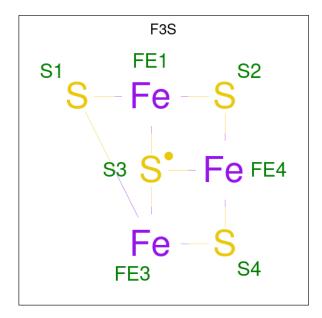
• Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	Q	1	Total Fe S	0	0	
9	Ъ	1	8 4 4	0	0	
3	C	1	Total Fe S	0	0	
)	b	1	8 4 4			
3	Т	1	Total Fe S	0	0	
)	1	1	8 4 4	0		
3	Т	1	Total Fe S	0	0	
3	1	1	8 4 4	U		

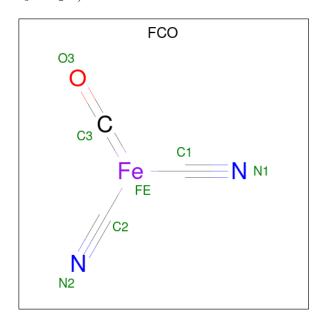
 \bullet Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe $_3$ S $_4$).





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

• Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
5	L	1	Total				O	0	0
	_	_	7	3	1	2	1		
5	М	1	Total	\mathbf{C}	Fe	Ν	Ο	0	0
9	1V1	1	7	3	1	2	1	0	

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total Mg 1 1	0	0

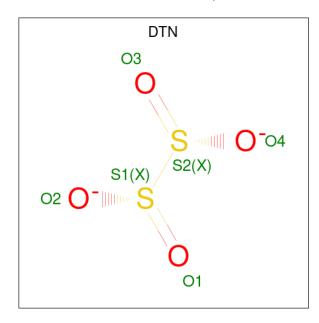
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total Mg 1 1	0	0

 \bullet Molecule 8 is DITHIONITE (three-letter code: DTN) (formula: $\mathrm{O_4S_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	T.	1	Total O S	0	0
	נו	1	6 4 2	O	U
8	т	1	Total O S	0	0
0	П		6 4 2		U
8	M	1	Total O S	0	0
0	1V1	1	6 4 2		
0	М	1	Total O S	0	0
0	M	$M \mid I \mid$	6 4 2	U	

• Molecule 9 is water.

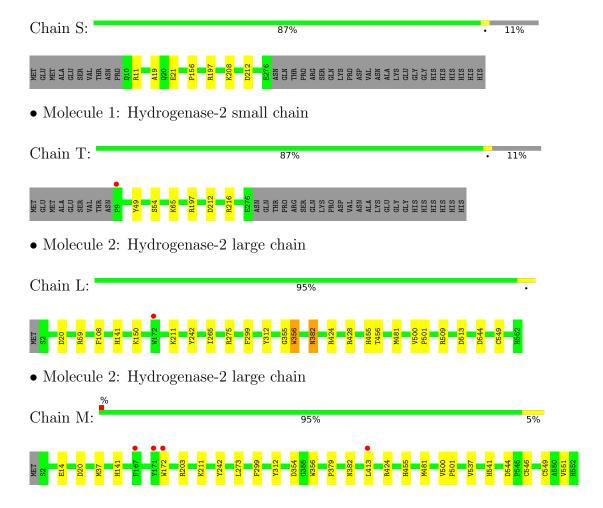
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	S	167	Total O 167 167	0	0
9	L	367	Total O 367 367	0	0
9	Т	140	Total O 140 140	0	0
9	M	325	Total O 325 325	0	0



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 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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	99.89Å 100.06Å 168.80Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.08 - 1.50	Depositor
Resolution (A)	65.21 - 1.50	EDS
% Data completeness	100.0 (86.08-1.50)	Depositor
(in resolution range)	$100.0 \ (65.21 \text{-} 1.50)$	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.77 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.124 , 0.163	Depositor
it, it free	0.125 , 0.164	DCC
R_{free} test set	13573 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 45.9	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13761	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: SF4, FCO, MG, DTN, CSO, F3S, NI

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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	S	0.71	0/2094	0.83	3/2851 (0.1%)
1	Т	0.72	0/2102	0.79	3/2862 (0.1%)
2	L	0.76	1/4411 (0.0%)	0.85	10/6010 (0.2%)
2	M	0.72	$2/4389 \ (0.0\%)$	0.82	6/5980 (0.1%)
All	All	0.73	$3/12996 \ (0.0\%)$	0.83	$22/17703 \ (0.1\%)$

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
2	L	356	TRP	CE3-CZ3	-6.74	1.26	1.38
2	M	172	TRP	CB-CG	6.47	1.61	1.50
2	M	356	TRP	CE3-CZ3	-5.12	1.29	1.38

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	L	59	ARG	NE-CZ-NH2	-8.54	116.03	120.30
2	L	509	ARG	NE-CZ-NH1	8.08	124.34	120.30
2	L	275	ARG	NE-CZ-NH1	6.76	123.68	120.30
2	L	513	ASP	CB-CG-OD1	6.48	124.13	118.30
2	M	299	PHE	CB-CG-CD2	-6.22	116.44	120.80

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	2037	0	1958	5	0
1	Т	2041	0	1967	2	0
2	L	4306	0	4244	13	0
2	M	4290	0	4225	9	0
3	S	16	0	0	0	0
3	Т	16	0	0	0	0
4	S	7	0	0	0	0
4	Т	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	1	0	0	0	0
7	M	1	0	0	0	0
8	L	12	0	0	0	0
8	M	12	0	0	0	0
9	L	367	0	0	9	0
9	M	325	0	0	3	0
9	S	167	0	0	4	0
9	Т	140	0	0	1	0
All	All	13761	0	12394	29	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 29 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \AA) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:L:356:TRP:HH2	9:L:976:HOH:O	1.71	0.71
1:S:208:LYS:CE	9:S:499:HOH:O	2.45	0.64
2:M:455:HIS:HD2	9:M:968:HOH:O	1.84	0.60
2:L:150:LYS:HD3	9:L:707:HOH:O	2.02	0.58
2:L:356:TRP:CH2	9:L:976:HOH:O	2.53	0.56

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	Perce	$_{ m ntiles}$
1	S	266/300 (89%)	257 (97%)	9 (3%)	0	100	100
1	Т	267/300 (89%)	258 (97%)	9 (3%)	0	100	100
2	L	551/552 (100%)	530 (96%)	20 (4%)	1 (0%)	47	23
2	M	548/552~(99%)	525 (96%)	22 (4%)	1 (0%)	47	23
All	All	1632/1704~(96%)	1570 (96%)	60 (4%)	2 (0%)	51	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	211	LYS
2	L	211	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	S	213/241 (88%)	213 (100%)	0	100 100
1	Т	214/241 (89%)	214 (100%)	0	100 100
2	L	467/465 (100%)	462 (99%)	5 (1%)	73 53
2	M	464/465 (100%)	459 (99%)	5 (1%)	73 53
All	All	1358/1412 (96%)	1348 (99%)	10 (1%)	84 69

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



Mol	Chain	Res	Type
2	M	242	TYR
2	M	312	TYR
2	M	382	ASN
2	L	312	TYR
2	L	382	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	Τ	89	ASN
2	M	47	ASN
2	M	411	ASN
2	L	202	ASN
2	L	47	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

2 non-standard protein/DNA/RNA residues 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	CSO	L	546	2,6	3,6,7	0.91	0	0,6,8	-	-
2	CSO	M	546	2,6	3,6,7	1.32	0	0,6,8	-	-

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
ſ	2	CSO	L	546	2,6	-	0/1/5/7	-
	2	CSO	M	546	2,6	=	0/1/5/7	=

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.

1 monomer is involved in 1 short contact:

\mathbf{Mol}	Chain	Res	Type	Clashes	Symm-Clashes
2	M	546	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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).

Mal	Trmo	Chain	Dag	Link	В	ond leng	${ m gths}$	Bond angles		
Mol	Type	Chain	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	Т	303	1	0,12,12	-	-	-		
5	FCO	L	601	2,9	0,6,6	-	-	-		
3	SF4	S	301	1	0,12,12	-	-	-		
8	DTN	M	604	-	0,5,5	-	-	0,6,6	-	-
8	DTN	L	604	-	0,5,5	-	-	0,6,6	-	-
4	F3S	S	302	1	0,9,9	-	-	-		
3	SF4	S	303	1	0,12,12	-	-	-		
3	SF4	Т	301	1	0,12,12	-	-	-		
5	FCO	M	601	2,9	0,6,6	-	=	-		
8	DTN	M	605	-	0,5,5	-	-	0,6,6	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	DTN	L	605	-	0,5,5	-	=	0,6,6	-	-
4	F3S	Т	302	1	0,9,9	-	-	-		_

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	Т	303	1	-	-	0/6/5/5
3	SF4	S	301	1	-	-	0/6/5/5
8	DTN	M	604	-	-	0/0/4/4	-
8	DTN	L	604	-	-	0/0/4/4	-
4	F3S	S	302	1	-	-	0/3/3/3
3	SF4	S	303	1	-	-	0/6/5/5
3	SF4	Т	301	1	-	-	0/6/5/5
8	DTN	M	605	-	-	0/0/4/4	-
8	DTN	L	605	-	-	0/0/4/4	-
4	F3S	Т	302	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^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	S	267/300 (89%)	-0.17	0 100 100	12, 18, 34, 50	0
1	Т	268/300 (89%)	-0.14	1 (0%) 92 94	13, 20, 36, 64	0
2	L	550/552 (99%)	-0.17	1 (0%) 95 95	11, 17, 31, 43	0
2	M	550/552 (99%)	-0.15	4 (0%) 87 90	12, 19, 36, 49	0
All	All	1635/1704 (95%)	-0.16	6 (0%) 92 94	11, 18, 34, 64	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Т	9	PRO	6.1
2	M	172	TRP	4.4
2	L	172	TRP	4.0
2	M	171	TYR	2.7
2	M	167	PHE	2.6

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	CSO	L	546	7/8	0.97	0.10	12,12,22,25	1
2	CSO	M	546	7/8	0.97	0.08	14,14,25,26	1

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
8	DTN	L	604	6/6	0.92	0.12	31,37,37,41	6
8	DTN	L	605	6/6	0.93	0.17	30,39,48,52	6
8	DTN	M	605	6/6	0.93	0.20	27,32,37,41	6
8	DTN	M	604	6/6	0.95	0.14	31,39,41,46	6
4	F3S	S	302	7/7	0.99	0.10	12,13,13,13	0
4	F3S	Т	302	7/7	0.99	0.09	13,14,14,14	0
5	FCO	L	601	7/7	0.99	0.10	10,12,12,14	0
5	FCO	M	601	7/7	0.99	0.09	12,13,14,16	0
3	SF4	S	301	8/8	0.99	0.09	14,14,15,15	0
3	SF4	S	303	8/8	0.99	0.09	13,14,16,17	0
3	SF4	Т	301	8/8	0.99	0.08	14,15,16,16	0
3	SF4	Т	303	8/8	0.99	0.07	15,16,18,19	0
6	NI	L	602	1/1	1.00	0.07	17,17,17,17	0
6	NI	M	602	1/1	1.00	0.05	19,19,19,19	0
7	MG	L	603	1/1	1.00	0.13	9,9,9,9	0
7	MG	M	603	1/1	1.00	0.12	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.

