



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 02:03 am GMT

PDB ID : 6EN9  
Title : E. coli Hydrogenase-2 (hydrogen reduced form)  
Authors : Carr, S.B.; Beaton, S.E.; Evans, R.M.; Armstrong, F.A.  
Deposited on : 2017-10-04  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 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

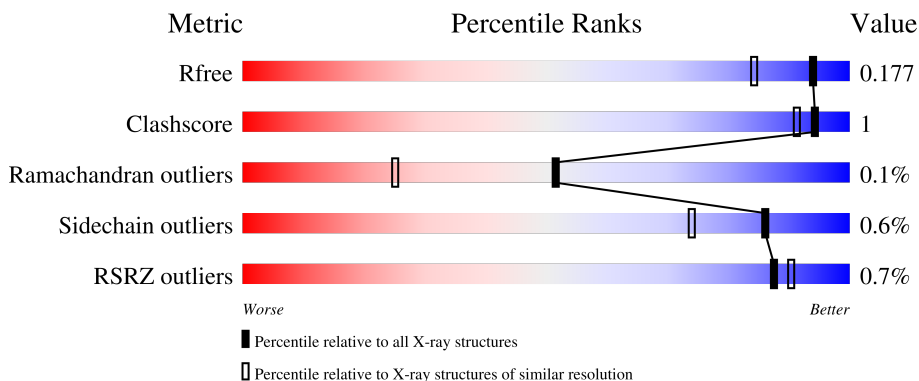
# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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  $\geq 3$ , 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	298	88% 10%
1	T	298	86% 10%
2	L	567	91% 6%
2	M	567	91% 6%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13927 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
			Total	C	N	O	S			
1	S	267	2059	1304	364	378	13	0	4	0
1	T	267	2059	1306	362	378	13	0	5	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	294	HIS	ASN	conflict	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
T	294	HIS	ASN	conflict	UNP P69741
T	295	HIS	-	expression tag	UNP P69741
T	296	HIS	-	expression tag	UNP P69741
T	297	HIS	-	expression tag	UNP P69741
T	298	HIS	-	expression tag	UNP P69741
T	299	HIS	-	expression tag	UNP P69741

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

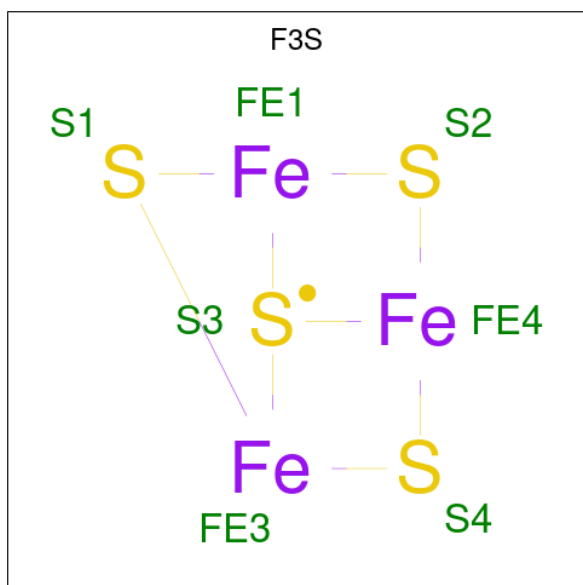
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	551	4319	2748	741	812	18	0	6	0
2	M	551	4303	2738	740	807	18	0	3	0

- 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>).



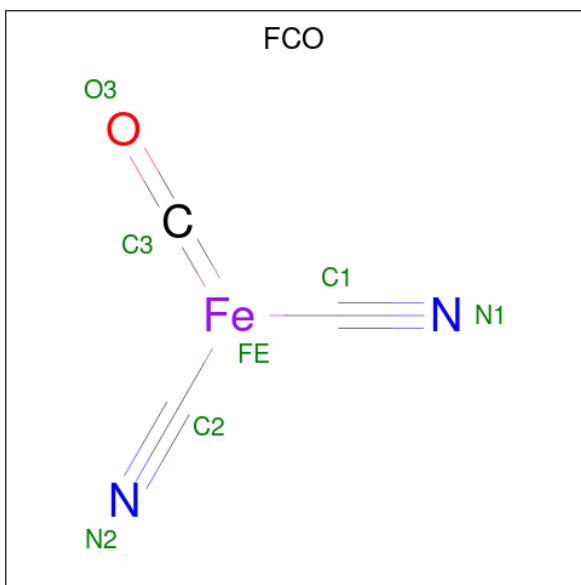
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total Fe S 7 3 4	0	0
4	T	1	Total Fe S 7 3 4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C<sub>3</sub>FeN<sub>2</sub>O).



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

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	Mg	0	0
			1	1		
8	M	1	Total	Mg	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	189	Total	O	0	0
			189	189		

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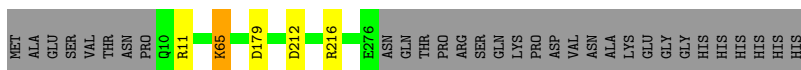
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
9	L	408	Total 408	O 408	0	0
9	T	163	Total 163	O 163	0	0
9	M	353	Total 353	O 353	0	0

### 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

Chain S:  88% 10%

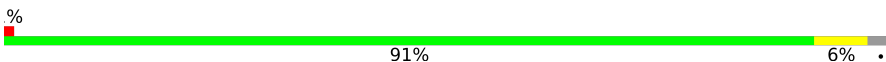


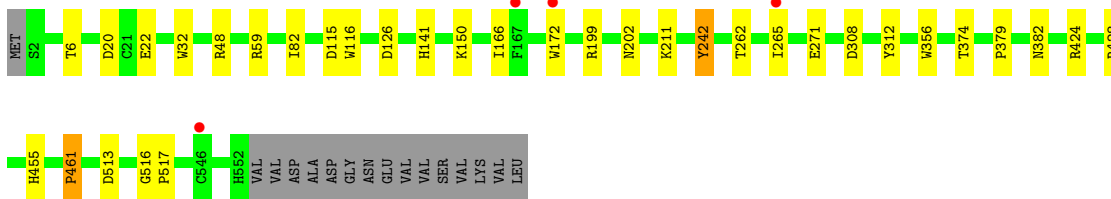
- Molecule 1: Hydrogenase-2 small chain

Chain T:  86% 10%

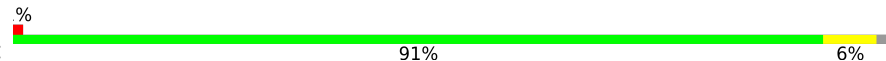


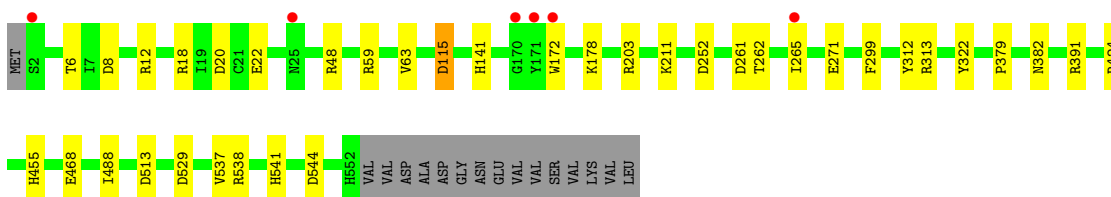
- Molecule 2: Hydrogenase-2 large chain

Chain L:  91% 6%



- Molecule 2: Hydrogenase-2 large chain

Chain M:  91% 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.60Å 100.54Å 168.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.35 – 1.50 86.35 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (86.35-1.50) 99.1 (86.35-1.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.152 , 0.175 0.155 , 0.177	Depositor DCC
$R_{free}$ test set	13461 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: FCO, MG, NI, F3S, SF4, SO4

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	0.84	0/2122	0.92	7/2888 (0.2%)
1	T	0.89	0/2131	0.96	9/2900 (0.3%)
2	L	0.88	4/4441 (0.1%)	0.93	11/6054 (0.2%)
2	M	0.88	1/4419 (0.0%)	0.97	18/6024 (0.3%)
All	All	0.87	5/13113 (0.0%)	0.95	45/17866 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	271	GLU	CD-OE1	-10.46	1.14	1.25
2	M	172	TRP	CB-CG	8.27	1.65	1.50
2	L	271	GLU	CD-OE2	-5.28	1.19	1.25
2	L	172	TRP	CB-CG	5.20	1.59	1.50
2	L	172	TRP	CE3-CZ3	5.08	1.47	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	59	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	S	179	ASP	CB-CG-OD1	7.72	125.25	118.30
2	M	59	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	M	59	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	M	424	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	M	48	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	M	203	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	M	115	ASP	CB-CG-OD1	6.82	124.43	118.30
1	S	179	ASP	CB-CG-OD2	-6.81	112.17	118.30
2	M	424	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	T	102	ASP	CB-CG-OD1	6.73	124.36	118.30
2	M	299	PHE	CB-CG-CD1	6.72	125.50	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	202	ASP	CB-CG-OD1	6.32	123.98	118.30
1	S	65	LYS	CD-CE-NZ	6.29	126.16	111.70
1	T	81	ASP	CB-CG-OD1	6.29	123.96	118.30
2	M	12	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	M	299	PHE	CB-CG-CD2	-6.25	116.43	120.80
2	L	513	ASP	CB-CG-OD1	6.17	123.86	118.30
1	S	11	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	L	308	ASP	CB-CG-OD2	-6.01	112.89	118.30
2	M	8	ASP	CB-CG-OD1	5.92	123.62	118.30
2	L	115	ASP	CB-CG-OD2	-5.88	113.01	118.30
2	M	529	ASP	CB-CG-OD1	5.80	123.52	118.30
2	L	115	ASP	CB-CG-OD1	5.75	123.47	118.30
2	M	203	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	L	199	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	T	216[A]	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	T	216[B]	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	L	242	TYR	CB-CG-CD1	5.44	124.26	121.00
1	S	216[A]	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	S	216[B]	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	L	424	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	M	252	ASP	CB-CG-OD1	5.34	123.11	118.30
2	M	18	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	L	428	ARG	CD-NE-CZ	5.31	131.03	123.60
1	T	212	ASP	CB-CG-OD1	5.25	123.03	118.30
1	T	198	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	S	212	ASP	CB-CG-OD1	5.22	123.00	118.30
2	M	544	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	L	48	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	T	102	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	M	391	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	L	126	ASP	CB-CG-OD1	5.04	122.83	118.30
2	M	513	ASP	CB-CG-OD1	5.04	122.83	118.30
1	T	11	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2059	0	1987	1	0
1	T	2059	0	1995	3	0
2	L	4319	0	4263	18	0
2	M	4303	0	4246	13	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	S	5	0	0	0	0
5	T	5	0	0	0	0
6	L	7	0	0	0	0
6	M	7	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
9	L	408	0	0	6	1
9	M	353	0	0	6	0
9	S	189	0	0	2	0
9	T	163	0	0	0	0
All	All	13927	0	12491	34	1

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.

All (34) 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)
2:M:6:THR:HB	9:M:983:HOH:O	1.67	0.93
2:L:356:TRP:HH2	9:L:1016:HOH:O	1.71	0.72
2:L:22:GLU:OE1	9:L:701:HOH:O	2.10	0.70
2:M:455:HIS:HD2	9:M:984:HOH:O	1.78	0.66
2:M:22:GLU:HG3	9:M:1017:HOH:O	2.03	0.59
2:M:6:THR:HG23	2:M:20:ASP:OD1	2.03	0.58
2:L:150:LYS:HD3	9:M:1037:HOH:O	2.04	0.58
2:L:455:HIS:HD2	9:L:1050:HOH:O	1.89	0.55
2:M:261:ASP:O	2:M:265:ILE:HG23	2.08	0.53
2:L:262:THR:O	2:L:265:ILE:HG22	2.07	0.53
2:L:150:LYS:HE2	9:M:1037:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:379:PRO:HB2	9:M:772:HOH:O	2.09	0.52
9:S:548:HOH:O	2:L:166:ILE:HG22	2.11	0.50
2:M:313:ARG:HD3	2:M:322:TYR:CE2	2.47	0.50
1:T:87:LYS:HE3	1:T:133:PRO:O	2.11	0.50
2:L:379:PRO:HB2	9:L:921:HOH:O	2.10	0.50
1:S:65:LYS:HE2	9:S:402:HOH:O	2.13	0.49
2:L:6[A]:THR:HG23	2:L:20:ASP:OD1	2.13	0.48
2:M:178:LYS:HE2	2:M:271:GLU:OE2	2.13	0.48
2:L:116:TRP:CG	2:L:265:ILE:HD11	2.49	0.47
2:L:374[B]:THR:HG21	2:L:516:GLY:HA2	1.96	0.47
2:L:356:TRP:CH2	9:L:1016:HOH:O	2.54	0.47
1:T:15[B]:ILE:CD1	1:T:69:LEU:HD23	2.44	0.47
2:L:6[A]:THR:HG21	9:L:852:HOH:O	2.17	0.44
2:L:374[B]:THR:CG2	2:L:517:PRO:HD3	2.47	0.44
2:M:537:VAL:CG1	2:M:541:HIS:CE1	3.01	0.43
2:M:115:ASP:HB3	2:M:538:ARG:HG2	2.02	0.41
2:L:82:ILE:HD11	2:L:461:PRO:HB3	2.02	0.41
2:L:150:LYS:HB3	2:L:150:LYS:HE3	1.91	0.41
1:T:23:THR:HB	2:M:63:VAL:HG23	2.03	0.41
2:M:262:THR:O	2:M:265:ILE:HG12	2.21	0.41
2:L:22:GLU:HG3	2:L:32:TRP:CZ3	2.56	0.40
2:L:202:ASN:HD22	2:L:202:ASN:HA	1.74	0.40
2:M:468:GLU:HA	2:M:488:ILE:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:704:HOH:O	9:L:769:HOH:O[3_755]	1.13	1.07

## 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	269/298 (90%)	260 (97%)	9 (3%)	0	100	100
1	T	270/298 (91%)	261 (97%)	9 (3%)	0	100	100
2	L	555/567 (98%)	532 (96%)	22 (4%)	1 (0%)	47	23
2	M	552/567 (97%)	532 (96%)	19 (3%)	1 (0%)	47	23
All	All	1646/1730 (95%)	1585 (96%)	59 (4%)	2 (0%)	51	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	211	LYS
2	M	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	216/239 (90%)	216 (100%)	0	100	100
1	T	217/239 (91%)	217 (100%)	0	100	100
2	L	471/479 (98%)	465 (99%)	6 (1%)	69	44
2	M	468/479 (98%)	464 (99%)	4 (1%)	78	61
All	All	1372/1436 (96%)	1362 (99%)	10 (1%)	86	69

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	141	HIS
2	L	242	TYR
2	L	312	TYR
2	L	382[A]	ASN
2	L	382[B]	ASN
2	L	461	PRO
2	M	141	HIS
2	M	312	TYR
2	M	382[A]	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	382[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	47	ASN
2	L	202	ASN
2	L	411	ASN
2	L	455	HIS
2	L	531	ASN
1	T	75	GLN
2	M	47	ASN
2	M	411	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
6	FCO	M	601	2	0,6,6	-	-	-		
5	SO4	S	304	-	4,4,4	0.58	0	6,6,6	0.57	0
6	FCO	L	601	2	0,6,6	-	-	-		
4	F3S	T	302	1	0,9,9	-	-	-		
3	SF4	S	303	1	0,12,12	-	-	-		
5	SO4	T	304	-	4,4,4	0.53	0	6,6,6	0.14	0
3	SF4	T	303	1	0,12,12	-	-	-		
3	SF4	T	301	1	0,12,12	-	-	-		
4	F3S	S	302	1	0,9,9	-	-	-		
3	SF4	S	301	1	0,12,12	-	-	-		

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
4	F3S	T	302	1	-	-	0/3/3/3
3	SF4	S	303	1	-	-	0/6/5/5
3	SF4	T	303	1	-	-	0/6/5/5
3	SF4	T	301	1	-	-	0/6/5/5
4	F3S	S	302	1	-	-	0/3/3/3
3	SF4	S	301	1	-	-	0/6/5/5

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	267/298 (89%)	-0.17	0 <a href="#">100</a> <a href="#">100</a>	12, 16, 28, 43	0
1	T	267/298 (89%)	-0.11	1 (0%) <a href="#">92</a> <a href="#">94</a>	12, 19, 34, 47	0
2	L	551/567 (97%)	-0.17	4 (0%) <a href="#">87</a> <a href="#">90</a>	11, 16, 30, 41	0
2	M	551/567 (97%)	-0.09	6 (1%) <a href="#">80</a> <a href="#">84</a>	12, 19, 35, 56	0
All	All	1636/1730 (94%)	-0.13	11 (0%) <a href="#">87</a> <a href="#">90</a>	11, 17, 33, 56	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	172	TRP	4.7
2	M	2	SER	3.0
2	L	546	CYS	2.7
2	M	172	TRP	2.6
2	M	265	ILE	2.5
2	M	171	TYR	2.4
1	T	276	GLU	2.4
2	M	170	GLY	2.3
2	L	167	PHE	2.2
2	M	25	ASN	2.1
2	L	265	ILE	2.0

### 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 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<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(Å <sup>2</sup> )	Q<0.9
5	SO4	T	304	5/5	0.88	0.21	64,71,72,75	0
5	SO4	S	304	5/5	0.95	0.25	41,44,45,48	0
3	SF4	T	301	8/8	0.99	0.07	14,15,15,15	0
3	SF4	T	303	8/8	0.99	0.08	14,14,14,14	0
4	F3S	T	302	7/7	0.99	0.08	13,13,13,14	0
3	SF4	S	301	8/8	0.99	0.09	14,14,14,14	0
3	SF4	S	303	8/8	0.99	0.09	11,12,12,12	0
6	FCO	M	601	7/7	0.99	0.09	12,13,15,15	0
7	NI	M	602	1/1	0.99	0.07	15,15,15,15	0
8	MG	M	603	1/1	0.99	0.10	12,12,12,12	0
7	NI	L	602	1/1	1.00	0.08	13,13,13,13	0
6	FCO	L	601	7/7	1.00	0.09	11,12,12,13	0
8	MG	L	603	1/1	1.00	0.11	9,9,9,9	0
4	F3S	S	302	7/7	1.00	0.08	12,12,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.