



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:43 PM GMT

PDB ID : 3UQY  
Title : H2-reduced structure of E. coli hydrogenase-1  
Authors : Volbeda, A.; Fontecilla-Camps, J.C.; Darnault, C.  
Deposited on : 2011-11-21  
Resolution : 1.47 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

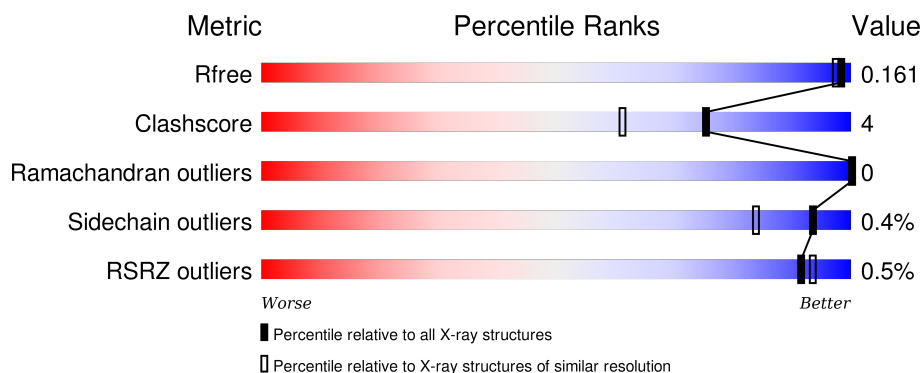
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.47 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))
$R_{free}$	91344	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (1.50-1.46)

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. 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	335	 74% 5% 21%
1	T	335	 74% 5% 21%
2	L	582	 93% 7%
2	M	582	 93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	GOL	L	605	-	-	-	X
12	GOL	L	606	-	-	-	X
6	LMT	S	404	-	-	-	X
6	LMT	T	404	-	-	-	X
8	SO4	T	407	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 15535 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-1 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	265	Total	C	N	O	S	0	16	0
			2136	1363	367	385	21			
1	T	265	Total	C	N	O	S	0	18	0
			2150	1374	370	385	21			

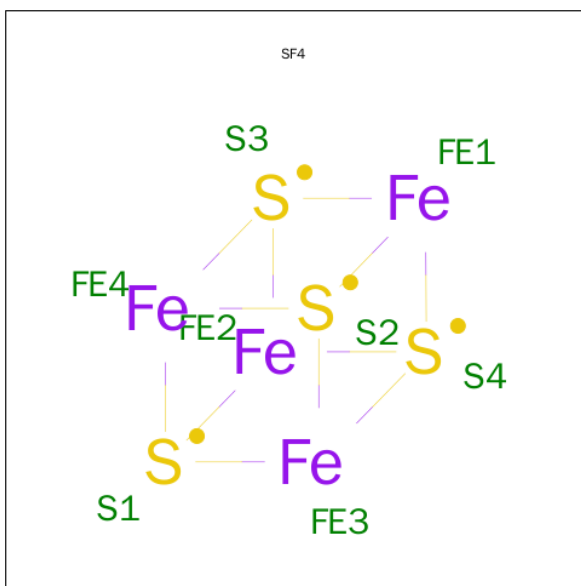
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	328	ARG	-	EXPRESSION TAG	UNP P69739
S	329	SER	-	EXPRESSION TAG	UNP P69739
S	330	HIS	-	EXPRESSION TAG	UNP P69739
S	331	HIS	-	EXPRESSION TAG	UNP P69739
S	332	HIS	-	EXPRESSION TAG	UNP P69739
S	333	HIS	-	EXPRESSION TAG	UNP P69739
S	334	HIS	-	EXPRESSION TAG	UNP P69739
S	335	HIS	-	EXPRESSION TAG	UNP P69739
T	328	ARG	-	EXPRESSION TAG	UNP P69739
T	329	SER	-	EXPRESSION TAG	UNP P69739
T	330	HIS	-	EXPRESSION TAG	UNP P69739
T	331	HIS	-	EXPRESSION TAG	UNP P69739
T	332	HIS	-	EXPRESSION TAG	UNP P69739
T	333	HIS	-	EXPRESSION TAG	UNP P69739
T	334	HIS	-	EXPRESSION TAG	UNP P69739
T	335	HIS	-	EXPRESSION TAG	UNP P69739

- Molecule 2 is a protein called Hydrogenase-1 large chain.

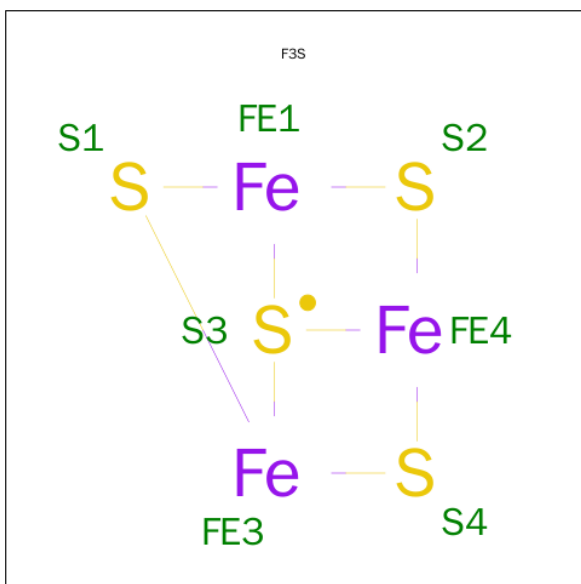
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	43	0
			4794	3053	832	880	29			
2	M	581	Total	C	N	O	S	0	29	0
			4712	3001	819	863	29			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	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:  $\text{Fe}_3\text{S}_4$ ).



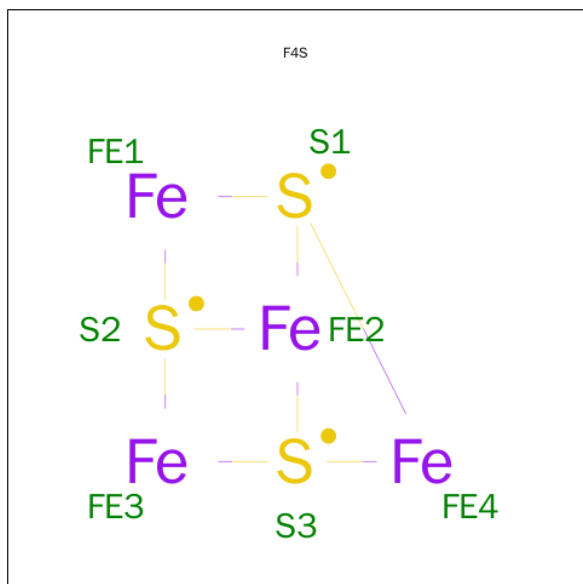
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

*Continued on next page...*

*Continued from previous page...*

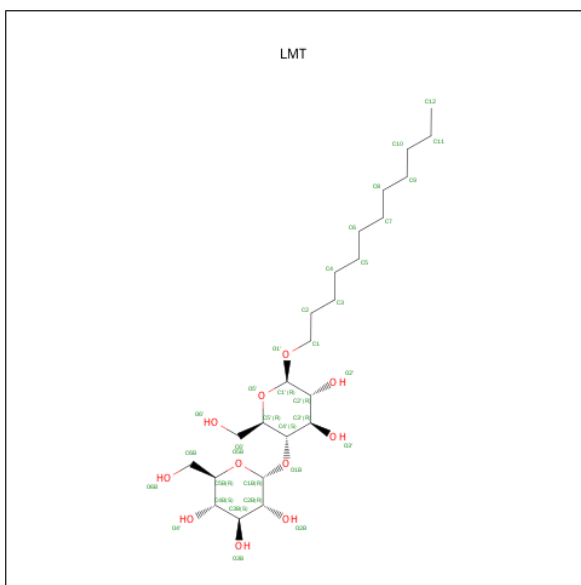
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	T	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: F4S) (formula:  $\text{Fe}_4\text{S}_3$ ).



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

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $\text{C}_{24}\text{H}_{46}\text{O}_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	S	1	Total 14	C 13	O 1	0	0
6	T	1	Total 14	C 13	O 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	1	Total Cl 1 1	0	0
7	L	1	Total Cl 1 1	0	0
7	S	2	Total Cl 2 2	0	0
7	M	1	Total Cl 1 1	0	0

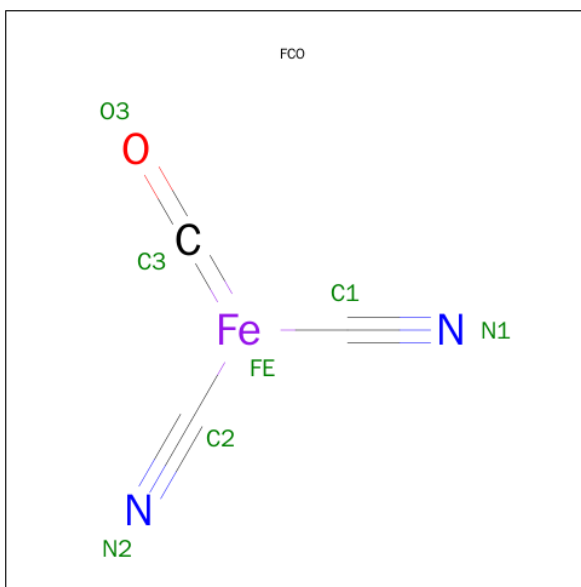
- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula:  $\text{C}_3\text{FeN}_2\text{O}$ ).





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

- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			6	3	3		
12	L	1	Total	C	O	0	0
			6	3	3		

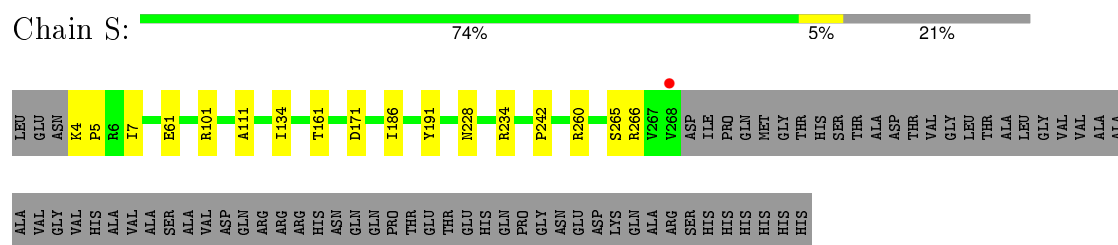
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	S	249	Total	O	0	2
			251	251		
13	L	539	Total	O	0	2
			541	541		
13	T	239	Total	O	0	1
			240	240		
13	M	579	Total	O	0	0
			579	579		

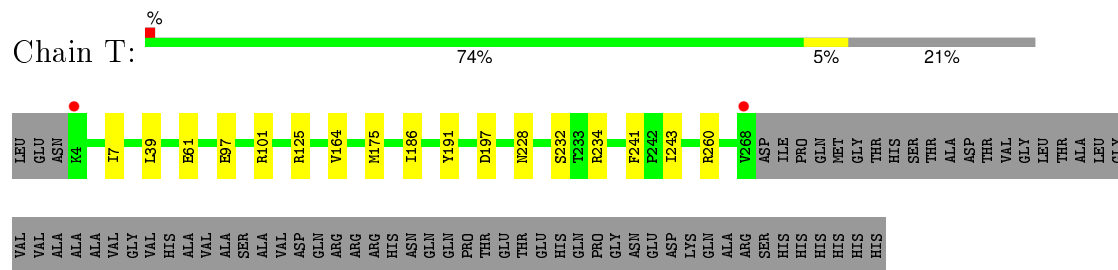
### 3 Residue-property plots [i](#)

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

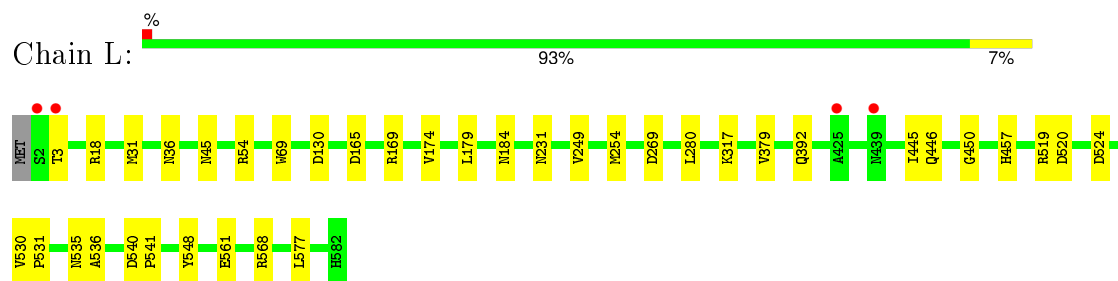
- Molecule 1: Hydrogenase-1 small chain



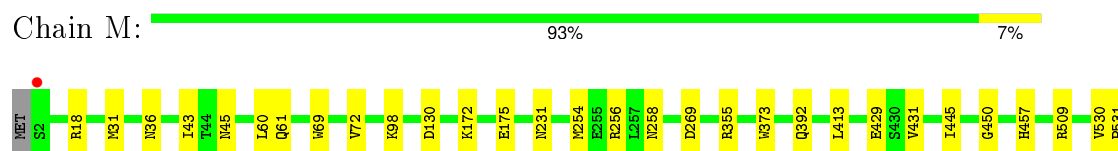
- Molecule 1: Hydrogenase-1 small chain



- Molecule 2: Hydrogenase-1 large chain



- Molecule 2: Hydrogenase-1 large chain



M535	A536	D540	P541	Y548	T555	R568	C576	L577	H582
------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.71Å 97.40Å 183.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.47 29.57 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-1.47) 99.8 (29.57-1.47)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.122 , 0.160 0.123 , 0.161	Depositor DCC
$R_{free}$ test set	14104 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	8.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.0	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 283897 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, CL, SF4, LMT, F4S, F3S, SO4, NI, 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	0.50	0/2239	0.61	0/3037
1	T	0.50	0/2259	0.61	0/3065
2	L	0.46	0/5028	0.59	1/6832 (0.0%)
2	M	0.46	0/4913	0.60	0/6677
All	All	0.47	0/14439	0.60	1/19611 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	54	ARG	NE-CZ-NH2	-5.45	117.57	120.30

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	2136	0	2130	15	0
1	T	2150	0	2157	23	0
2	L	4794	0	4764	35	0
2	M	4712	0	4663	36	0
3	S	8	0	0	0	0
3	T	8	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	7	0	0	0	0
4	T	7	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
6	S	14	0	25	1	0
6	T	14	0	25	1	0
7	L	1	0	0	0	0
7	M	1	0	0	1	0
7	S	2	0	0	1	0
7	T	1	0	0	0	0
8	L	5	0	0	0	0
8	S	10	0	0	1	0
8	T	10	0	0	0	0
9	L	7	0	0	0	0
9	M	7	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
12	L	12	0	16	3	0
13	L	541	0	0	20	0
13	M	579	0	0	16	0
13	S	251	0	0	6	0
13	T	240	0	0	15	0
All	All	15535	0	13780	109	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 4.

All (109) 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:97[B]:GLU:OE1	13:T:683:HOH:O	1.53	1.23
2:M:457[A]:HIS:CD2	13:M:1195:HOH:O	1.87	1.23
13:L:1171:HOH:O	1:T:39[A]:LEU:HD11	1.06	1.19
1:T:61[B]:GLU:HG2	13:T:652:HOH:O	1.39	1.16
1:T:175[A]:MET:HE3	13:T:736:HOH:O	1.41	1.15
1:T:61[A]:GLU:OE1	13:T:690:HOH:O	1.61	1.15
2:L:269[A]:ASP:OD1	13:L:1096:HOH:O	1.64	1.14
2:M:175[B]:GLU:HG3	13:M:1149:HOH:O	0.97	1.11
13:L:1171:HOH:O	1:T:39[A]:LEU:CD1	1.68	1.09

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:457[A]:HIS:NE2	13:M:1208:HOH:O	1.87	1.07
2:L:317[A]:LYS:HD3	13:L:1154:HOH:O	1.55	1.06
7:S:406:CL:CL	13:S:658:HOH:O	2.07	1.05
2:M:457[A]:HIS:CE1	13:M:1208:HOH:O	2.07	1.04
1:S:61[B]:GLU:HG2	13:S:621:HOH:O	1.57	1.03
1:S:101[B]:ARG:HG3	1:S:101[B]:ARG:HH11	1.24	0.97
1:S:101[B]:ARG:CG	1:S:101[B]:ARG:HH11	1.87	0.88
2:M:254[A]:MET:HE1	13:M:916:HOH:O	1.75	0.85
2:L:269[B]:ASP:OD1	13:L:1081:HOH:O	1.94	0.83
2:M:254[A]:MET:CE	13:M:916:HOH:O	2.27	0.83
13:L:1171:HOH:O	1:T:39[A]:LEU:CG	2.10	0.81
1:S:171[A]:ASP:OD1	13:S:699:HOH:O	2.00	0.80
2:L:280[A]:LEU:HG	13:L:908:HOH:O	1.80	0.80
7:M:604:CL:CL	13:M:1115:HOH:O	2.38	0.78
2:M:175[B]:GLU:CG	13:M:1149:HOH:O	1.73	0.78
2:M:269[A]:ASP:OD1	13:M:1132:HOH:O	2.03	0.76
2:L:169[B]:ARG:NH1	13:L:1186:HOH:O	2.19	0.76
2:L:457[A]:HIS:CD2	13:L:1235:HOH:O	2.40	0.75
1:T:125[B]:ARG:NH2	13:T:696:HOH:O	2.19	0.75
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.67	0.74
2:L:457[A]:HIS:NE2	13:L:1235:HOH:O	2.20	0.74
2:M:18:ARG:HH11	2:M:36:ASN:HD21	1.35	0.73
2:L:165[B]:ASP:OD1	13:L:823:HOH:O	2.06	0.73
2:M:431:VAL:HG13	2:M:445[B]:ILE:HD11	1.71	0.72
1:T:61[B]:GLU:OE2	13:T:668:HOH:O	2.08	0.72
2:M:392[B]:GLN:NE2	13:M:1002:HOH:O	2.21	0.72
2:L:446:GLN:HE22	12:L:605:GOL:H12	1.53	0.72
2:L:18:ARG:HH11	2:L:36:ASN:HD21	1.37	0.72
1:T:197[B]:ASP:OD2	13:T:688:HOH:O	2.11	0.69
2:L:269[A]:ASP:CG	13:L:1096:HOH:O	2.17	0.67
1:S:4:LYS:HB3	1:S:5:PRO:HD3	1.77	0.67
2:L:457[B]:HIS:CE1	13:L:908:HOH:O	2.47	0.66
2:M:98[B]:LYS:HD3	13:M:1137:HOH:O	1.97	0.64
2:L:457[B]:HIS:HE1	13:L:908:HOH:O	1.82	0.62
2:L:36:ASN:HD22	2:L:45:ASN:HD22	1.47	0.62
2:L:379[A]:VAL:O	13:L:1191:HOH:O	2.16	0.61
2:M:36:ASN:HD22	2:M:45:ASN:HD22	1.48	0.60
1:S:161[A]:THR:HG21	2:M:258:ASN:HD21	1.66	0.60
2:M:429[B]:GLU:HG3	13:M:943:HOH:O	2.01	0.60
2:M:256[B]:ARG:NH1	13:M:828:HOH:O	0.76	0.60
1:T:61[A]:GLU:CG	13:T:690:HOH:O	2.52	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:175[A]:MET:CE	13:T:736:HOH:O	2.19	0.56
1:T:234[B]:ARG:NE	13:T:686:HOH:O	2.38	0.56
2:M:457[B]:HIS:HE1	13:M:1206:HOH:O	1.88	0.56
2:M:457[B]:HIS:CE1	13:M:1206:HOH:O	2.59	0.55
2:M:60:LEU:HD11	2:M:72:VAL:CG1	2.36	0.55
2:L:3[A]:THR:HG23	13:L:1234:HOH:O	2.07	0.55
1:T:186:ILE:HD11	1:T:228:ASN:HB3	1.89	0.55
2:L:446:GLN:NE2	12:L:605:GOL:H12	2.21	0.55
1:S:101[B]:ARG:NH1	1:S:101[B]:ARG:CG	2.55	0.54
2:M:413:LEU:HD13	2:M:445[B]:ILE:HG22	1.90	0.54
2:L:392[A]:GLN:NE2	13:L:1234:HOH:O	2.40	0.54
1:S:234[B]:ARG:NH2	13:T:686:HOH:O	2.41	0.54
1:S:266:ARG:NH2	8:S:408:SO4:O3	2.40	0.53
2:L:69:TRP:HH2	2:L:231:ASN:HD22	1.57	0.51
2:L:530:VAL:CG1	2:L:531:PRO:HD2	2.40	0.51
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.40	0.51
2:L:31:MET:HB2	2:L:577:LEU:HG	1.92	0.51
1:T:234[A]:ARG:NH1	13:T:583:HOH:O	2.37	0.50
2:L:535:ASN:HB3	2:L:548:TYR:CE1	2.47	0.50
1:S:111:ALA:HB2	1:S:134[B]:ILE:HD11	1.92	0.50
2:M:36:ASN:ND2	2:M:45:ASN:HD22	2.09	0.49
1:T:39[B]:LEU:HD11	13:T:735:HOH:O	2.12	0.49
2:L:317[A]:LYS:CD	13:L:1154:HOH:O	2.34	0.49
2:M:69:TRP:HH2	2:M:231:ASN:HD22	1.60	0.49
2:L:174[A]:VAL:HG13	2:L:179:LEU:HD11	1.95	0.49
2:L:184:ASN:H	12:L:606:GOL:C1	2.25	0.48
1:T:260[B]:ARG:HG3	13:T:670:HOH:O	2.12	0.48
2:L:540:ASP:HB2	2:L:541:PRO:CD	2.43	0.48
2:M:31:MET:HB2	2:M:577:LEU:HG	1.94	0.48
2:L:36:ASN:ND2	2:L:45:ASN:HD22	2.10	0.48
2:M:43:ILE:HD12	2:M:555:THR:HB	1.95	0.48
13:L:1171:HOH:O	1:T:39[A]:LEU:HG	1.95	0.47
2:L:317[A]:LYS:NZ	13:L:1154:HOH:O	2.47	0.47
2:M:535:ASN:HB3	2:M:548:TYR:CE1	2.50	0.47
2:M:431:VAL:HG13	2:M:445[B]:ILE:CD1	2.43	0.47
2:L:536:ALA:HB2	2:L:548:TYR:CE2	2.49	0.47
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.44	0.47
1:S:265[B]:SER:OG	13:S:585:HOH:O	2.20	0.46
1:S:186:ILE:HD11	1:S:228:ASN:HB3	1.98	0.46
2:M:530:VAL:HG13	2:M:531:PRO:HD2	1.97	0.46
2:L:561[A]:GLU:CD	2:L:561[A]:GLU:H	2.18	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:130:ASP:HB3	2:M:568:ARG:HG2	1.97	0.45
2:L:445:ILE:O	2:L:450:GLY:HA3	2.16	0.45
1:S:260:ARG:HG3	13:S:724:HOH:O	2.17	0.43
1:S:171[A]:ASP:OD1	13:S:679:HOH:O	2.21	0.43
1:T:260[A]:ARG:HG3	13:T:670:HOH:O	2.19	0.43
2:L:519[A]:ARG:HG2	2:L:520:ASP:OD2	2.18	0.43
1:T:241:PHE:CE2	1:T:243:ILE:HB	2.54	0.43
2:M:172:LYS:O	2:M:175[A]:GLU:HG2	2.19	0.42
1:S:7[B]:ILE:HD12	6:S:404:LMT:H42	2.01	0.42
2:M:457[A]:HIS:HD2	13:M:1195:HOH:O	1.56	0.42
2:M:355:ARG:HG3	2:M:373:TRP:HB2	2.02	0.42
2:L:249:VAL:HB	1:T:232[B]:SER:OG	2.20	0.41
1:T:39[B]:LEU:HG	1:T:164:VAL:HG21	2.02	0.41
1:T:7[A]:ILE:HG21	6:T:404:LMT:H61	2.02	0.41
2:M:536:ALA:HB2	2:M:548:TYR:CE2	2.56	0.41
2:M:509:ARG:CD	2:M:576:CYS:HB2	2.51	0.41
2:L:130:ASP:HB3	2:L:568:ARG:HG2	2.03	0.41

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	S	279/335 (83%)	265 (95%)	14 (5%)	0	100	100
1	T	281/335 (84%)	269 (96%)	12 (4%)	0	100	100
2	L	622/582 (107%)	603 (97%)	19 (3%)	0	100	100
2	M	608/582 (104%)	592 (97%)	16 (3%)	0	100	100
All	All	1790/1834 (98%)	1729 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	234/274 (85%)	232 (99%)	2 (1%)	84	64
1	T	236/274 (86%)	234 (99%)	2 (1%)	86	69
2	L	522/481 (108%)	521 (100%)	1 (0%)	95	87
2	M	509/481 (106%)	508 (100%)	1 (0%)	95	87
All	All	1501/1510 (99%)	1495 (100%)	6 (0%)	93	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	191	TYR
1	S	242	PRO
2	L	524	ASP
1	T	101	ARG
1	T	191	TYR
2	M	61	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	130	GLN
1	S	244	GLN
2	L	36	ASN
2	L	108	ASN
2	L	231	ASN
2	L	258	ASN
2	L	332	ASN
2	L	446	GLN
2	L	479	ASN
1	T	244	GLN
2	M	36	ASN
2	M	61	GLN
2	M	108	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	231	ASN
2	M	258	ASN
2	M	328	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 9 are monoatomic - leaving 17 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	$\# Z  > 2$
9	FCO	L	601	2	0,6,6	0.00	-	0,6,6	0.00	-
8	SO4	L	604	-	4,4,4	0.30	0	6,6,6	0.16	0
12	GOL	L	605	-	5,5,5	0.38	0	5,5,5	0.44	0
12	GOL	L	606	-	5,5,5	0.55	0	5,5,5	0.41	0
9	FCO	M	601	2	0,6,6	0.00	-	0,6,6	0.00	-
3	SF4	S	401	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	S	402	1	0,9,9	0.00	-	0,15,15	0.00	-
5	F4S	S	403	1	0,9,9	0.00	-	0,15,15	0.00	-
6	LMT	S	404	-	13,13,36	0.34	0	12,12,47	0.54	0
8	SO4	S	407	-	4,4,4	0.17	0	6,6,6	0.32	0
8	SO4	S	408	-	4,4,4	0.32	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SF4	T	401	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	T	402	1	0,9,9	0.00	-	0,15,15	0.00	-
5	F4S	T	403	1	0,9,9	0.00	-	0,15,15	0.00	-
6	LMT	T	404	-	13,13,36	0.25	0	12,12,47	0.62	0
8	SO4	T	406	-	4,4,4	0.24	0	6,6,6	0.22	0
8	SO4	T	407	-	4,4,4	0.21	0	6,6,6	0.18	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
9	FCO	L	601	2	-	0/0/6/6	0/0/0/0
8	SO4	L	604	-	-	0/0/0/0	0/0/0/0
12	GOL	L	605	-	-	0/4/4/4	0/0/0/0
12	GOL	L	606	-	-	0/4/4/4	0/0/0/0
9	FCO	M	601	2	-	0/0/6/6	0/0/0/0
3	SF4	S	401	1	-	0/0/48/48	0/6/5/5
4	F3S	S	402	1	-	0/0/24/24	0/0/3/3
5	F4S	S	403	1	-	0/0/24/24	0/0/3/3
6	LMT	S	404	-	-	0/11/11/61	0/0/0/2
8	SO4	S	407	-	-	0/0/0/0	0/0/0/0
8	SO4	S	408	-	-	0/0/0/0	0/0/0/0
3	SF4	T	401	1	-	0/0/48/48	0/6/5/5
4	F3S	T	402	1	-	0/0/24/24	0/0/3/3
5	F4S	T	403	1	-	0/0/24/24	0/0/3/3
6	LMT	T	404	-	-	0/11/11/61	0/0/0/2
8	SO4	T	406	-	-	0/0/0/0	0/0/0/0
8	SO4	T	407	-	-	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 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	605	GOL	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	606	GOL	1	0
6	S	404	LMT	1	0
8	S	408	SO4	1	0
6	T	404	LMT	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](#)

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	265/335 (79%)	-0.51	1 (0%) 93 94	5, 9, 17, 32	2 (0%)
1	T	265/335 (79%)	-0.47	2 (0%) 87 89	5, 10, 18, 34	2 (0%)
2	L	581/582 (99%)	-0.50	4 (0%) 89 91	5, 10, 21, 33	3 (0%)
2	M	581/582 (99%)	-0.54	1 (0%) 95 95	5, 10, 19, 32	1 (0%)
All	All	1692/1834 (92%)	-0.51	8 (0%) 91 93	5, 10, 19, 34	8 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	268	VAL	10.3
1	S	268	VAL	8.9
2	L	2	SER	3.6
2	L	439[A]	ASN	3.1
2	L	3[A]	THR	2.7
2	L	425	ALA	2.3
1	T	4	LYS	2.1
2	M	2	SER	2.1

### 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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
12	GOL	L	605	6/6	0.81	0.29	10.61	28,32,34,36	6
12	GOL	L	606	6/6	0.88	0.20	5.95	14,24,25,25	6
8	SO4	T	407	5/5	0.73	0.34	4.41	24,30,34,35	5
6	LMT	S	404	14/35	0.86	0.19	3.91	16,22,27,28	14
6	LMT	T	404	14/35	0.84	0.15	3.31	23,28,40,41	0
8	SO4	S	407	5/5	0.97	0.12	1.97	13,16,19,19	5
7	CL	S	405	1/1	1.00	0.05	0.68	12,12,12,12	1
9	FCO	L	601	7/7	1.00	0.06	0.03	5,6,8,8	0
4	F3S	T	402	7/7	1.00	0.05	-0.83	6,6,6,7	0
9	FCO	M	601	7/7	1.00	0.05	-0.94	5,6,7,7	0
4	F3S	S	402	7/7	1.00	0.04	-0.99	6,6,6,6	0
11	MG	M	603	1/1	1.00	0.05	-1.01	6,6,6,6	0
3	SF4	T	401	8/8	1.00	0.04	-1.60	6,6,7,7	0
11	MG	L	603	1/1	1.00	0.04	-1.80	6,6,6,6	0
5	F4S	T	403	7/7	1.00	0.03	-1.80	6,7,7,7	0
3	SF4	S	401	8/8	1.00	0.04	-2.08	6,6,7,7	0
7	CL	T	405	1/1	1.00	0.03	-2.21	15,15,15,15	1
5	F4S	S	403	7/7	1.00	0.03	-2.46	5,6,6,6	0
10	NI	L	602	1/1	1.00	0.02	-3.37	8,8,8,8	0
10	NI	M	602	1/1	1.00	0.02	-4.54	9,9,9,9	0
7	CL	S	406	1/1	0.99	0.05	-	22,22,22,22	1
7	CL	M	604	1/1	0.98	0.03	-	22,22,22,22	1
7	CL	L	607	1/1	0.98	0.06	-	21,21,21,21	1
8	SO4	L	604	5/5	0.87	0.15	-	26,27,29,29	5
8	SO4	T	406	5/5	0.92	0.21	-	32,34,35,36	5
8	SO4	S	408	5/5	0.92	0.19	-	32,33,33,34	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.