



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 08:47 PM EST

PDB ID : 5JRD  
Title : E. coli Hydrogenase-1 variant P508A  
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Islam, S.T.A.  
Deposited on : 2016-05-06  
Resolution : 1.20 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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

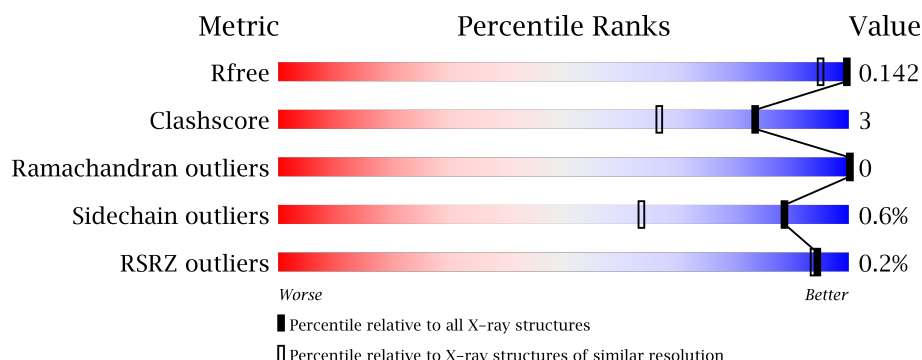
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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))
$R_{free}$	100719	1131 (1.24-1.16)
Clashscore	112137	1201 (1.24-1.16)
Ramachandran outliers	110173	1148 (1.24-1.16)
Sidechain outliers	110143	1147 (1.24-1.16)
RSRZ outliers	101464	1132 (1.24-1.16)

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	<div> <div></div> <div>73% 5% 21%</div> </div>
1	T	335	<div> <div></div> <div>74% . . 21%</div> </div>
2	L	582	<div> <div></div> <div>95% 5%</div> </div>
2	M	582	<div> <div></div> <div>94% 5%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	L	604	-	-	-	X
10	SO4	M	604	-	X	-	-
2	CSO	L	79	-	-	X	-
2	CSO	M	79	-	-	X	-
6	CL	T	405	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15068 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	264	Total	C	N	O	S	0	14	0
			2116	1353	357	385	21			
1	T	264	Total	C	N	O	S	0	13	0
			2112	1349	359	383	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	328	ARG	-	expression tag	UNP P69740
S	329	SER	-	expression tag	UNP P69740
S	330	HIS	-	expression tag	UNP P69740
S	331	HIS	-	expression tag	UNP P69740
S	332	HIS	-	expression tag	UNP P69740
S	333	HIS	-	expression tag	UNP P69740
S	334	HIS	-	expression tag	UNP P69740
S	335	HIS	-	expression tag	UNP P69740
T	328	ARG	-	expression tag	UNP P69740
T	329	SER	-	expression tag	UNP P69740
T	330	HIS	-	expression tag	UNP P69740
T	331	HIS	-	expression tag	UNP P69740
T	332	HIS	-	expression tag	UNP P69740
T	333	HIS	-	expression tag	UNP P69740
T	334	HIS	-	expression tag	UNP P69740
T	335	HIS	-	expression tag	UNP P69740

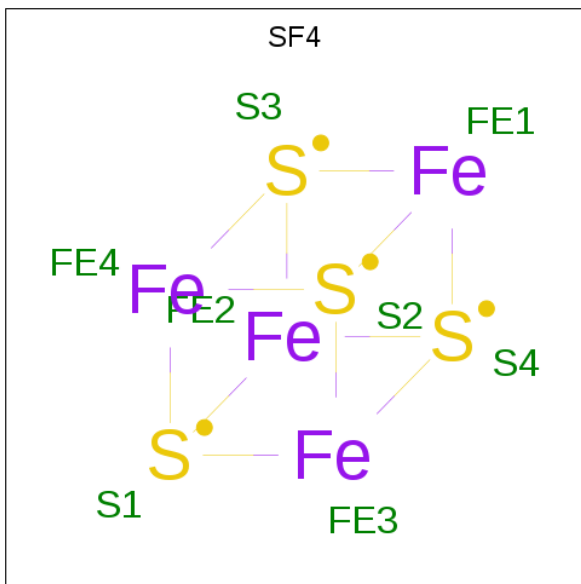
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	29	0
			4701	2989	819	862	31			
2	M	581	Total	C	N	O	S	0	27	0
			4685	2987	808	859	31			

There are 2 discrepancies between the modelled and reference sequences:

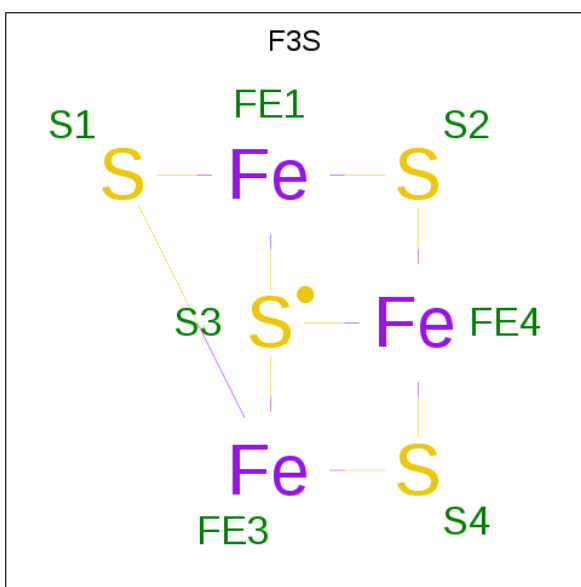
Chain	Residue	Modelled	Actual	Comment	Reference
L	508	ALA	PRO	conflict	UNP P0ACD8
M	508	ALA	PRO	conflict	UNP P0ACD8

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



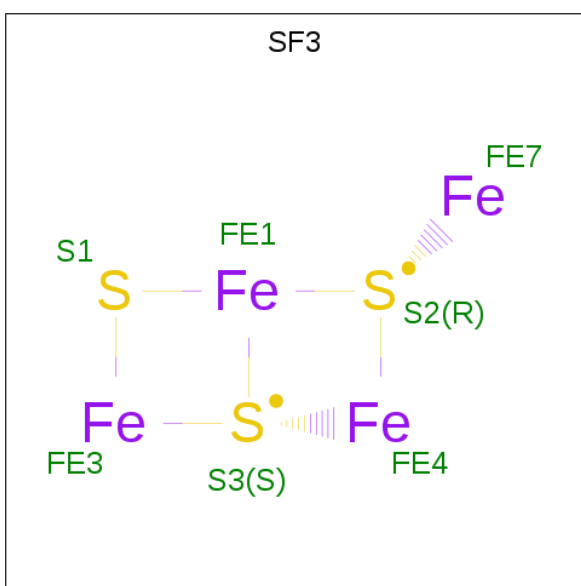
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

- 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 FE4-S3 CLUSTER (three-letter code: SF3) (formula:  $\text{Fe}_4\text{S}_3$ ).

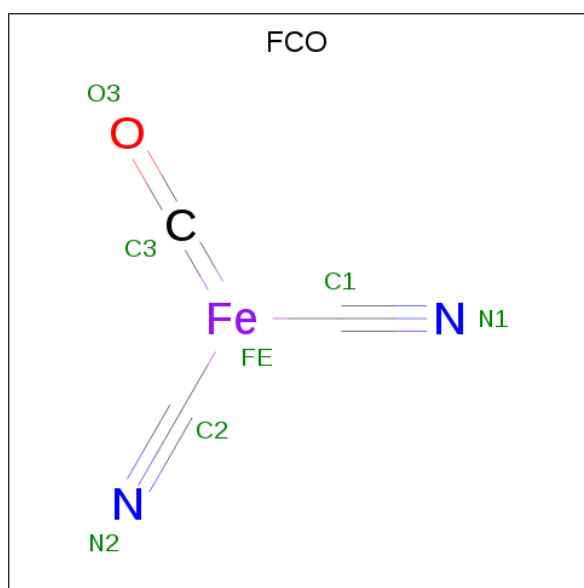


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	1
			8	5	3		
5	T	1	Total	Fe	S	0	1
			8	5	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	2	Total	Cl	0	0
			2	2		
6	S	2	Total	Cl	0	0
			2	2		

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C<sub>3</sub>FeN<sub>2</sub>O).



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

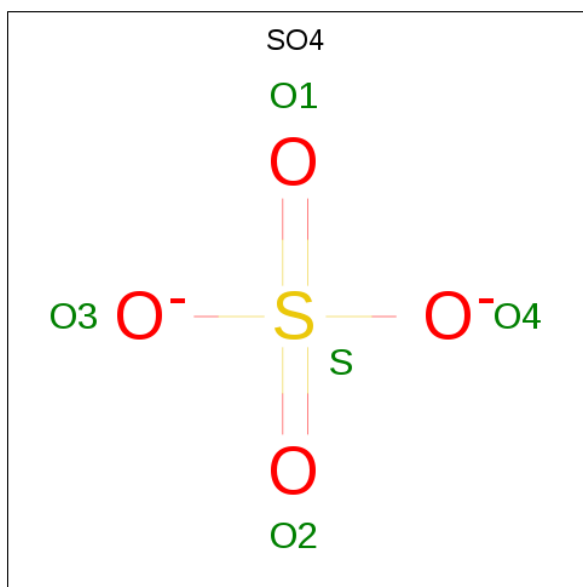
- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total O S 5 4 1	0	0
10	L	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0

- Molecule 11 is water.

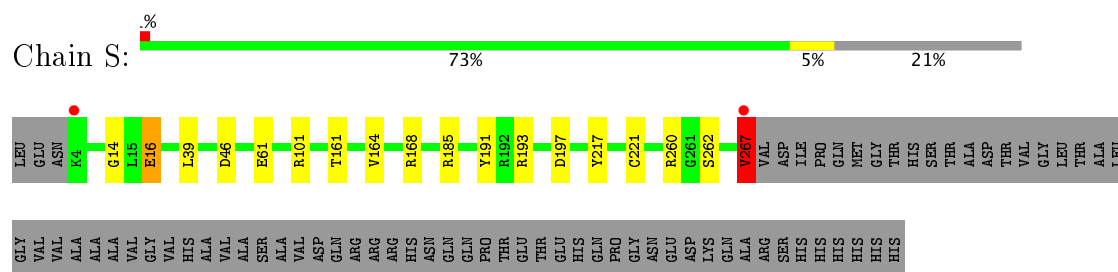
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	S	207	Total O 207 207	0	0
11	L	474	Total O 474 474	0	0
11	T	195	Total O 195 195	0	0
11	M	495	Total O 495 495	0	0



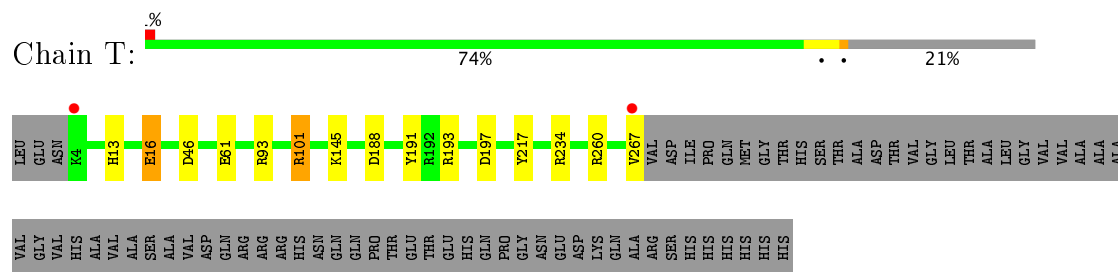
### 3 Residue-property plots [i](#)

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.

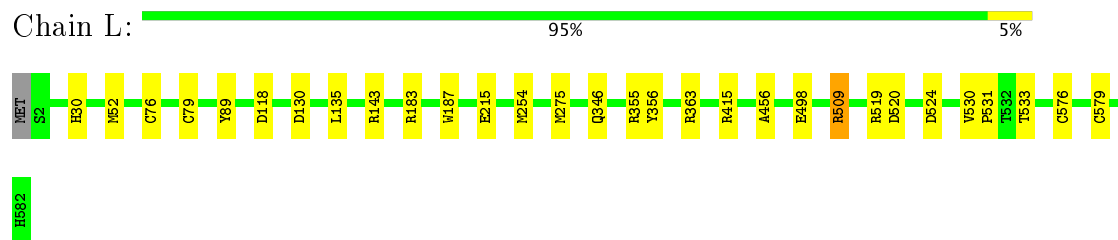
- Molecule 1: Hydrogenase-1 small chain



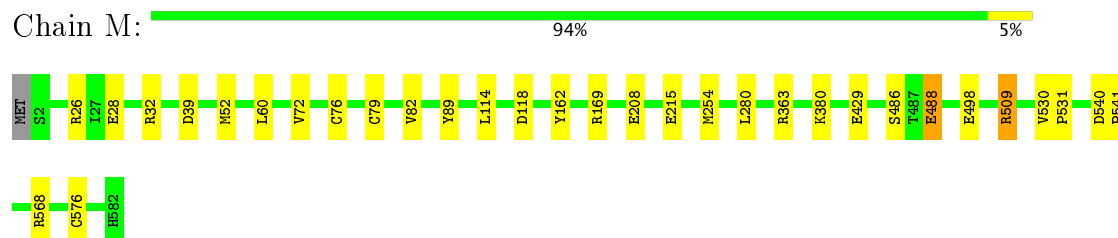
- Molecule 1: Hydrogenase-1 small chain



- Molecule 2: Hydrogenase-1 large chain



- Molecule 2: Hydrogenase-1 large chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.69 Å 98.59 Å 185.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.69 – 1.20 92.69 – 1.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.69-1.20) 100.0 (92.69-1.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.20 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.121 , 0.141 0.122 , 0.142	Depositor DCC
$R_{free}$ test set	26714 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	15068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CSO, CL, SF4, MG, SF3, F3S, SO4, 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	0.93	3/2207 (0.1%)	0.96	10/2996 (0.3%)
1	T	0.93	2/2203 (0.1%)	0.93	10/2990 (0.3%)
2	L	0.87	1/4899 (0.0%)	0.85	10/6660 (0.2%)
2	M	0.89	3/4879 (0.1%)	0.87	10/6630 (0.2%)
All	All	0.90	9/14188 (0.1%)	0.89	40/19276 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	498	GLU	CD-OE2	-10.59	1.14	1.25
2	L	498	GLU	CD-OE2	-8.85	1.16	1.25
1	S	217	TYR	CZ-OH	-6.16	1.27	1.37
1	T	260	ARG	CZ-NH1	6.05	1.41	1.33
2	M	28	GLU	CD-OE2	6.03	1.32	1.25
1	T	188	ASP	CB-CG	5.92	1.64	1.51
1	S	260	ARG	CZ-NH1	5.83	1.40	1.33
2	M	39	ASP	CB-CG	-5.69	1.39	1.51
1	S	262	SER	CB-OG	5.24	1.49	1.42

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	363	ARG	NE-CZ-NH2	10.72	125.66	120.30
2	M	39	ASP	CB-CG-OD1	-9.83	109.45	118.30
1	T	260	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	T	197	ASP	CB-CG-OD1	9.42	126.77	118.30
1	S	260	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	S	197	ASP	CB-CG-OD1	9.02	126.42	118.30
2	L	143	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	S	260	ARG	NE-CZ-NH1	7.88	124.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	93	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	S	193	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	T	260	ARG	NE-CZ-NH1	7.25	123.92	120.30
2	L	89	TYR	CB-CG-CD1	7.17	125.30	121.00
1	S	267	VAL	CA-CB-CG1	7.11	121.56	110.90
1	S	185	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	T	234	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	M	26	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	T	193	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	M	89	TYR	CB-CG-CD1	6.49	124.89	121.00
2	M	32	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	S	168	ARG	NE-CZ-NH2	-6.45	117.07	120.30
2	L	415	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	L	363[A]	ARG	NE-CZ-NH1	-6.17	117.21	120.30
2	L	363[B]	ARG	NE-CZ-NH1	-6.17	117.21	120.30
2	M	568	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	S	168	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	L	89	TYR	CB-CG-CD2	-6.11	117.34	121.00
2	M	39	ASP	CB-CG-OD2	6.08	123.78	118.30
1	T	46	ASP	CB-CG-OD1	6.08	123.77	118.30
2	L	509	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	M	509	ARG	NE-CZ-NH2	-5.99	117.30	120.30
2	M	215	GLU	OE1-CD-OE2	-5.87	116.26	123.30
1	T	234	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	S	193	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	L	215	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	T	188	ASP	CB-CG-OD1	5.52	123.27	118.30
1	T	101	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	M	169	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	S	46	ASP	CB-CG-OD1	5.18	122.96	118.30
2	L	130	ASP	CB-CG-OD2	-5.15	113.66	118.30
2	L	356	TYR	CB-CG-CD1	5.06	124.03	121.00

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	2116	0	2097	12	0
1	T	2112	0	2093	9	0
2	L	4701	0	4644	27	0
2	M	4685	0	4646	26	0
3	S	8	0	0	0	0
3	T	8	0	0	0	0
4	S	7	0	0	0	0
4	T	7	0	0	0	0
5	S	8	0	0	0	0
5	T	8	0	0	0	0
6	S	2	0	0	0	0
6	T	2	0	0	0	0
7	L	7	0	0	0	0
7	M	7	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
10	L	10	0	0	0	0
10	M	5	0	0	0	0
11	L	474	0	0	7	0
11	M	495	0	0	5	0
11	S	207	0	0	6	0
11	T	195	0	0	4	0
All	All	15068	0	13480	73	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 3.

All (73) 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:L:79:CSO:SG	2:L:79:CSO:OD	1.95	1.24
2:M:79:CSO:OD	2:M:79:CSO:SG	1.94	1.23
1:S:61[B]:GLU:OE2	1:S:101[B]:ARG:NH1	1.76	1.18
2:L:183[B]:ARG:NH1	11:L:702:HOH:O	1.78	1.16
2:L:509:ARG:NE	2:L:576[B]:CYS:SG	2.28	1.07
2:M:509:ARG:NE	2:M:576[B]:CYS:SG	2.31	1.04
2:L:76[B]:CYS:SG	2:L:79:CSO:OD	2.15	1.02
2:L:509:ARG:CD	2:L:576[B]:CYS:SG	2.56	0.93
2:M:486[A]:SER:OG	2:M:488[A]:GLU:OE1	1.84	0.92
2:M:76[B]:CYS:SG	2:M:79:CSO:OD	2.28	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:509:ARG:CD	2:M:576[B]:CYS:SG	2.59	0.89
1:S:267:VAL:HG23	11:S:560:HOH:O	1.76	0.84
2:L:346[A]:GLN:OE1	11:L:704:HOH:O	1.97	0.82
2:M:82[B]:VAL:HG13	2:M:114[B]:LEU:CD2	2.08	0.82
2:M:82[B]:VAL:HG13	2:M:114[B]:LEU:HD23	1.62	0.79
1:S:267:VAL:CG2	11:S:560:HOH:O	2.31	0.77
1:T:217:TYR:CE1	1:T:267:VAL:HG12	2.25	0.72
2:L:355[B]:ARG:NH1	11:L:703:HOH:O	1.88	0.69
1:T:217:TYR:HE1	1:T:267:VAL:HG12	1.59	0.68
2:M:118[B]:ASP:OD1	11:M:701:HOH:O	2.12	0.68
2:L:76[A]:CYS:HB3	2:L:79:CSO:OD	1.93	0.67
1:T:61[B]:GLU:HG2	11:T:591:HOH:O	1.94	0.65
2:M:76[A]:CYS:HB3	2:M:79:CSO:OD	1.98	0.63
2:M:76[B]:CYS:HB2	2:M:79:CSO:OD	1.98	0.63
2:L:509:ARG:CZ	2:L:576[B]:CYS:SG	2.86	0.63
2:L:76[B]:CYS:CB	2:L:79:CSO:OD	2.43	0.62
2:M:509:ARG:CZ	2:M:576[B]:CYS:SG	2.87	0.62
1:S:61[B]:GLU:HG2	11:S:636:HOH:O	2.00	0.61
2:M:76[B]:CYS:CB	2:M:79:CSO:OD	2.47	0.61
2:L:118[B]:ASP:OD1	11:L:705:HOH:O	2.16	0.61
2:L:76[B]:CYS:HB2	2:L:79:CSO:OD	2.01	0.60
2:M:82[B]:VAL:CG1	2:M:114[B]:LEU:HD23	2.29	0.60
1:S:221:CYS:O	1:S:267:VAL:CG2	2.49	0.60
2:L:183[B]:ARG:CZ	11:L:702:HOH:O	2.32	0.58
2:M:576[B]:CYS:SG	11:M:918:HOH:O	2.13	0.58
1:S:161[B]:THR:HG23	11:S:679:HOH:O	2.03	0.58
2:L:576[B]:CYS:SG	11:L:949:HOH:O	2.19	0.58
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.86	0.58
2:L:509:ARG:HD3	2:L:576[B]:CYS:SG	2.46	0.56
2:L:275[B]:MET:HE1	2:L:456:ALA:HA	1.88	0.55
2:M:429[B]:GLU:HG3	11:M:916:HOH:O	2.07	0.55
1:T:145[A]:LYS:NZ	11:T:501:HOH:O	2.38	0.55
2:L:530[B]:VAL:HG21	2:L:579:CYS:O	2.08	0.54
2:M:280[A]:LEU:HG	11:M:1100:HOH:O	2.08	0.54
2:L:52:MET:HG2	11:L:964:HOH:O	2.09	0.53
1:T:16[B]:GLU:HG2	11:T:602:HOH:O	2.09	0.53
2:L:519[B]:ARG:HG2	2:L:520:ASP:OD2	2.09	0.52
2:L:135:LEU:HD22	2:L:187:TRP:CD1	2.45	0.52
1:S:16[B]:GLU:HG2	11:S:624:HOH:O	2.09	0.51
2:M:60[B]:LEU:HD11	2:M:72:VAL:CG1	2.40	0.51
1:T:217:TYR:HE1	1:T:267:VAL:CG1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:79:CSO:OD	2:M:79:CSO:N	2.44	0.50
2:M:254[B]:MET:HE2	2:M:254[B]:MET:HA	1.95	0.49
2:M:509:ARG:HD2	2:M:576[B]:CYS:SG	2.50	0.48
1:T:101:ARG:HH11	1:T:101:ARG:HG3	1.78	0.48
2:L:530[B]:VAL:HG21	2:L:579:CYS:C	2.34	0.47
1:S:221:CYS:O	1:S:267:VAL:HG22	2.13	0.47
2:M:488[A]:GLU:CD	2:M:488[A]:GLU:H	2.18	0.47
2:M:52:MET:HG2	11:M:893:HOH:O	2.15	0.47
2:L:79:CSO:N	2:L:79:CSO:OD	2.49	0.46
2:L:509:ARG:HD2	2:L:576[B]:CYS:SG	2.50	0.46
1:S:221:CYS:O	1:S:267:VAL:HG21	2.15	0.46
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.47	0.45
1:S:14:GLY:O	2:L:30[B]:HIS:HE1	2.01	0.43
2:L:530[B]:VAL:HG22	2:L:533:THR:OG1	2.19	0.43
1:T:61[B]:GLU:OE1	1:T:101:ARG:NH2	2.43	0.42
1:T:13:HIS:HD2	11:T:570:HOH:O	2.02	0.42
1:S:39[B]:LEU:HG	1:S:164:VAL:HG21	2.01	0.42
2:L:530[A]:VAL:CG1	2:L:531:PRO:HD2	2.50	0.42
2:M:509:ARG:HD3	2:M:576[B]:CYS:SG	2.52	0.42
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.50	0.41
1:S:267:VAL:HG22	11:S:560:HOH:O	2.11	0.41
2:M:162:TYR:OH	2:M:208[B]:GLU:OE2	2.31	0.40

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	276/335 (82%)	264 (96%)	12 (4%)	0	100	100
1	T	275/335 (82%)	262 (95%)	13 (5%)	0	100	100
2	L	607/582 (104%)	591 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	606/582 (104%)	591 (98%)	15 (2%)	0	100	100
All	All	1764/1834 (96%)	1708 (97%)	56 (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	231/274 (84%)	227 (98%)	4 (2%)	66	26
1	T	230/274 (84%)	227 (99%)	3 (1%)	73	35
2	L	507/479 (106%)	506 (100%)	1 (0%)	94	82
2	M	506/479 (106%)	502 (99%)	4 (1%)	85	56
All	All	1474/1506 (98%)	1462 (99%)	12 (1%)	89	56

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	16[A]	GLU
1	S	16[B]	GLU
1	S	191	TYR
1	S	267	VAL
2	L	524	ASP
1	T	16[A]	GLU
1	T	16[B]	GLU
1	T	191	TYR
2	M	380[A]	LYS
2	M	380[B]	LYS
2	M	488[A]	GLU
2	M	488[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	79	8,2,7	4,6,7	1.71	1 (25%)	1,6,8	1.03	0
2	CSO	M	79	8,2,7	4,6,7	1.55	1 (25%)	1,6,8	1.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	L	79	8,2,7	-	0/1/5/7	0/0/0/0
2	CSO	M	79	8,2,7	-	0/1/5/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	79	CSO	CA-C	2.94	1.54	1.50
2	L	79	CSO	CA-C	3.08	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	79	CSO	6	0
2	M	79	CSO	6	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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
7	FCO	L	601	11,2	0,6,6	0.00	-	0,6,6	0.00	-
10	SO4	L	604	-	4,4,4	0.54	0	6,6,6	0.51	0
10	SO4	L	605	-	4,4,4	0.38	0	6,6,6	0.25	0
7	FCO	M	601	11,2	0,6,6	0.00	-	0,6,6	0.00	-
10	SO4	M	604	-	4,4,4	4.49	2 (50%)	6,6,6	1.63	2 (33%)
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	SF3	S	403[B]	1,11	0,8,8	0.00	-	0,12,12	0.00	-
5	SF3	S	403[C]	1,11	0,8,8	0.00	-	0,12,12	0.00	-
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	SF3	T	403[B]	1,11	0,8,8	0.00	-	0,12,12	0.00	-
5	SF3	T	403[C]	1,11	0,8,8	0.00	-	0,12,12	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
7	FCO	L	601	11,2	-	0/0/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SO4	L	604	-	-	0/0/0/0	0/0/0/0
10	SO4	L	605	-	-	0/0/0/0	0/0/0/0
7	FCO	M	601	11,2	-	0/0/6/6	0/0/0/0
10	SO4	M	604	-	-	0/0/0/0	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	SF3	S	403[B]	1,11	-	0/0/17/17	0/2/2/2
5	SF3	S	403[C]	1,11	-	0/0/17/17	0/2/2/2
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	SF3	T	403[B]	1,11	-	0/0/17/17	0/2/2/2
5	SF3	T	403[C]	1,11	-	0/0/17/17	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	604	SO4	O4-S	4.70	1.86	1.47
10	M	604	SO4	O1-S	7.20	1.84	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	604	SO4	O4-S-O1	-2.24	96.89	109.26
10	M	604	SO4	O4-S-O3	3.16	123.18	108.96

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

### 6.1 Protein, DNA and RNA chains

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	264/335 (78%)	-0.60	2 (0%) 86 83	9, 13, 22, 57	0
1	T	264/335 (78%)	-0.55	2 (0%) 86 83	9, 14, 24, 60	0
2	L	580/582 (99%)	-0.65	0 100 100	9, 14, 26, 47	0
2	M	580/582 (99%)	-0.66	0 100 100	9, 14, 23, 39	0
All	All	1688/1834 (92%)	-0.63	4 (0%) 94 94	9, 14, 25, 60	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	267	VAL	4.6
1	S	267	VAL	4.1
1	T	4	LYS	3.8
1	S	4	LYS	2.5

### 6.2 Non-standard residues in protein, DNA, RNA chains

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
2	CSO	M	79	7/8	0.98	0.11	-	12,16,18,20	0
2	CSO	L	79	7/8	0.98	0.10	-	12,16,17,19	0

### 6.3 Carbohydrates ⓘ

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
10	SO4	L	604	5/5	0.98	0.08	3.92	20,21,25,26	5
6	CL	T	405	1/1	0.99	0.09	3.79	26,26,26,26	0
9	MG	L	603	1/1	1.00	0.05	0.65	9,9,9,9	0
9	MG	M	603	1/1	1.00	0.05	0.11	9,9,9,9	0
6	CL	S	405	1/1	1.00	0.06	-0.09	23,23,23,23	0
7	FCO	L	601	7/7	1.00	0.06	-0.43	11,11,12,12	0
7	FCO	M	601	7/7	1.00	0.05	-0.61	10,11,12,12	0
5	SF3	S	403[C]	7/7	0.99	0.04	-0.72	11,13,13,15	1
5	SF3	S	403[B]	7/7	0.99	0.04	-0.72	11,13,13,13	1
5	SF3	T	403[C]	7/7	0.99	0.04	-0.83	11,13,14,17	1
5	SF3	T	403[B]	7/7	0.99	0.04	-0.83	11,13,14,14	1
3	SF4	S	401	8/8	1.00	0.03	-1.31	10,10,11,11	0
3	SF4	T	401	8/8	1.00	0.03	-1.58	10,10,11,11	0
8	NI	L	602	1/1	1.00	0.03	-2.07	19,19,19,19	1
8	NI	M	602	1/1	1.00	0.03	-2.31	21,21,21,21	1
4	F3S	T	402	7/7	1.00	0.03	-2.68	10,10,11,11	0
6	CL	T	404	1/1	1.00	0.03	-2.95	16,16,16,16	0
6	CL	S	404	1/1	1.00	0.03	-3.03	15,15,15,15	0
4	F3S	S	402	7/7	1.00	0.03	-3.27	10,10,11,11	0
10	SO4	L	605	5/5	0.88	0.24	-	51,53,56,65	5
10	SO4	M	604	5/5	0.80	0.23	-	72,76,95,104	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.