



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:04 pm BST

PDB ID : 1HFE  
Title : 1.6 Å RESOLUTION STRUCTURE OF THE FE-ONLY HYDROGENASE  
FROM DESULFOVIBRIO DESULFURICANS  
Authors : Nicolet, Y.; Piras, C.; Legrand, P.; Hatchikian, E.C.; Fontecilla-Camps, J.C.  
Deposited on : 1998-11-11  
Resolution : 1.60 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

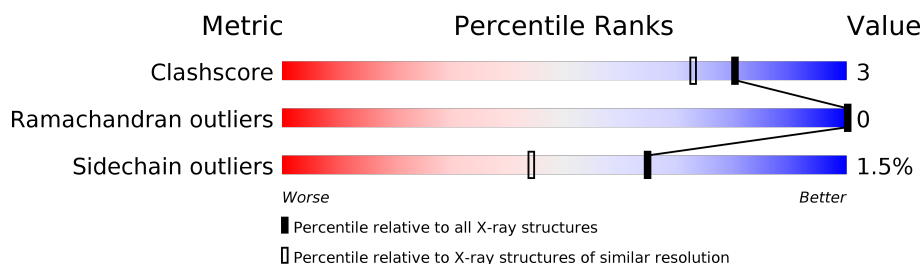
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	123	
1	T	123	
2	L	421	
2	M	421	

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
6	SF4	L	424	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SF4	M	424	-	-	X	-
7	PDT	L	425	-	X	-	-
7	PDT	M	425	-	X	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9079 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 PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (SMALLER SUBUNIT)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	88	Total	C	N	O	S	15	6	0
			761	491	131	138	1			
1	T	88	Total	C	N	O	S	16	6	0
			761	489	132	139	1			

- Molecule 2 is a protein called PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (LARGER SUBUNIT)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	397	Total	C	N	O	S	65	16	1
			3136	1993	519	586	38			
2	M	397	Total	C	N	O	S	65	14	1
			3117	1977	517	584	39			

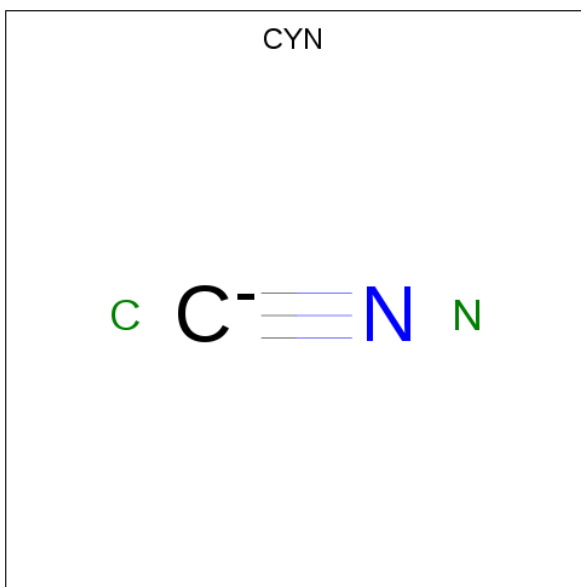
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	1	Total	Zn	0	0
			1	1		

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

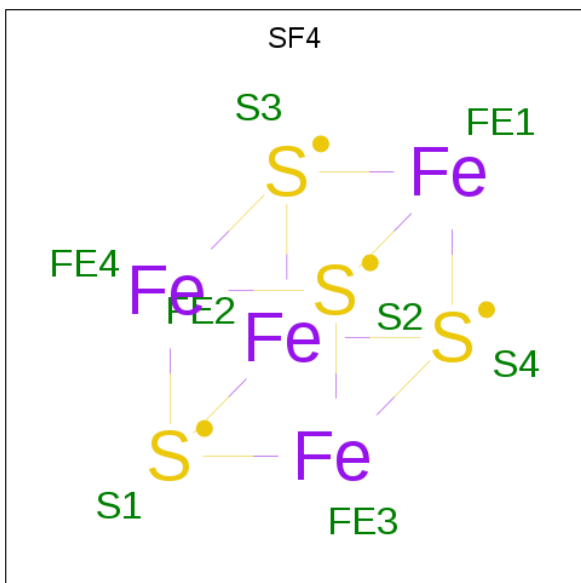
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	2	Total	Fe	0	0
			2	2		
4	M	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN).



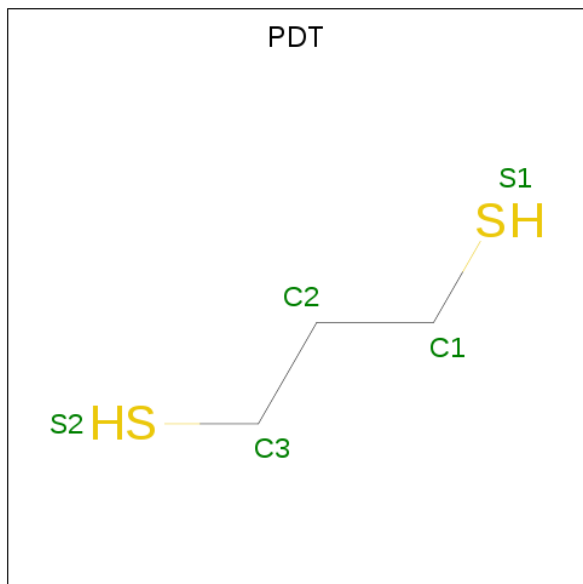
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	N	0	0
			2	1	1		
5	L	1	Total	C	N	0	0
			2	1	1		
5	M	1	Total	C	N	0	0
			2	1	1		
5	M	1	Total	C	N	0	0
			2	1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



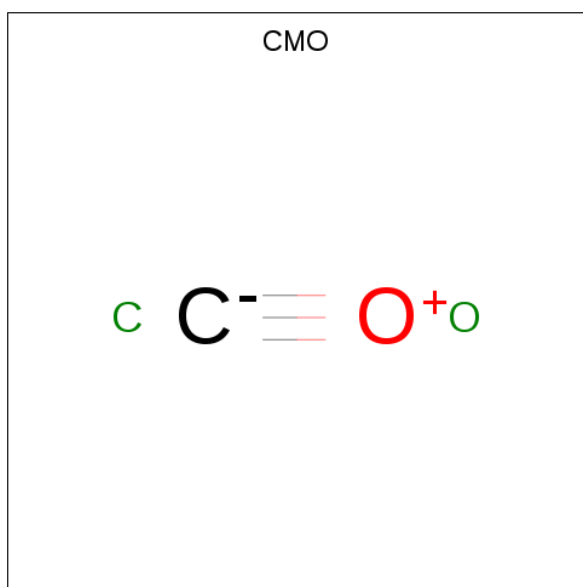
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	Fe	S	0	0
			8	4	4		
6	L	1	Total	Fe	S	0	0
			8	4	4		
6	L	1	Total	Fe	S	0	0
			8	4	4		
6	M	1	Total	Fe	S	0	0
			8	4	4		
6	M	1	Total	Fe	S	0	0
			8	4	4		
6	M	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is 1,3-PROPANEDITHIOL (three-letter code: PDT) (formula:  $C_3H_8S_2$ ).



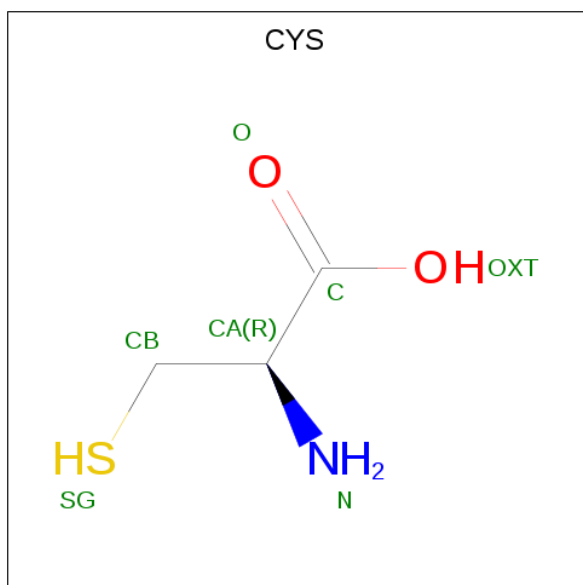
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	S	0	0
			5	3	2		
7	M	1	Total	C	S	0	0
			5	3	2		

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			2	1	1		
8	L	1	Total	C	O	0	0
			2	1	1		
8	M	1	Total	C	O	0	0
			2	1	1		
8	M	1	Total	C	O	0	0
			2	1	1		

- Molecule 9 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	S	146	Total	O	0	8
			154	154		
10	L	437	Total	O	0	14
			451	451		
10	T	159	Total	O	0	3
			162	162		
10	M	437	Total	O	0	7
			444	444		



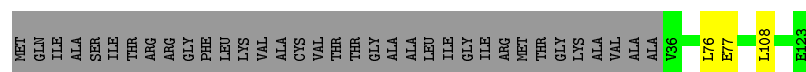
### 3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

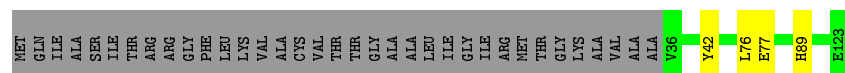
- Molecule 1: PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (SMALLER SUBUNIT))

Chain S: 




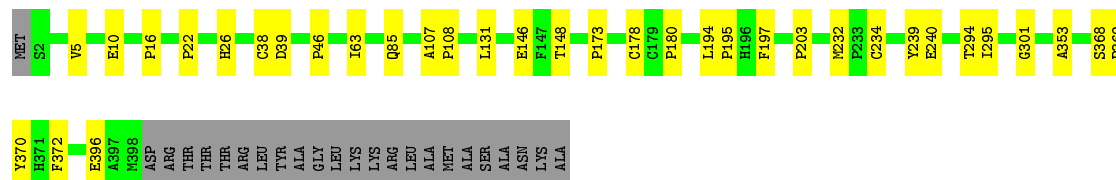
- Molecule 1: PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (SMALLER SUBUNIT))

Chain T: 



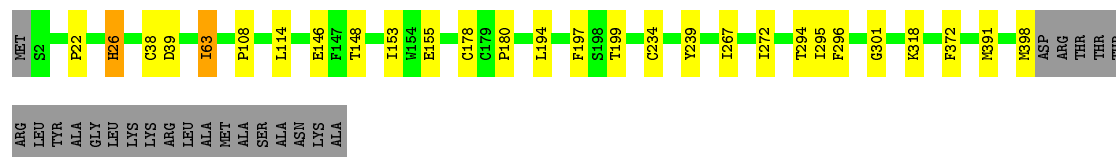
- Molecule 2: PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (LARGER SUBUNIT))

Chain L: 



- Molecule 2: PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (LARGER SUBUNIT))

Chain M: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.97Å 123.07Å 65.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.60	Depositor
% Data completeness (in resolution range)	98.3 (7.00-1.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.158 , 0.182	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 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: CMO, ZN, SF4, PDT, FE2, CYN

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	0.51	0/783	0.69	0/1058
1	T	0.49	0/784	0.67	0/1057
2	L	0.50	0/3212	0.72	0/4347
2	M	0.50	0/3193	0.71	0/4320
All	All	0.50	0/7972	0.71	0/10782

There are no bond length outliers.

There are no bond angle outliers.

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	761	0	754	1	0
1	T	761	0	749	4	0
2	L	3136	0	3089	19	0
2	M	3117	0	3065	18	0
3	S	1	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
5	L	4	0	0	1	0
5	M	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	24	0	0	2	0
6	M	24	0	0	2	0
7	L	5	0	6	1	0
7	M	5	0	6	1	0
8	L	4	0	0	1	0
8	M	4	0	0	0	0
9	L	7	0	4	0	0
9	M	7	0	4	0	0
10	L	451	0	0	2	0
10	M	444	0	0	3	0
10	S	154	0	0	0	0
10	T	162	0	0	0	0
All	All	9079	0	7677	41	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 (41) 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:153[A]:ILE:HD11	2:M:296:PHE:HE1	1.60	0.67
5:M:428:CYN:C	10:M:434:HOH:O	2.47	0.62
2:M:153[A]:ILE:HD11	2:M:296:PHE:CE1	2.34	0.62
1:T:89:HIS:HE1	2:M:155:GLU:OE1	1.87	0.57
2:L:63[B]:ILE:HG12	10:L:830:HOH:O	2.05	0.56
2:M:178:CYS:SG	7:M:425:PDT:H22	2.45	0.56
2:L:178:CYS:SG	7:L:425:PDT:H22	2.48	0.54
2:M:295:ILE:O	2:M:301:GLY:HA3	2.10	0.52
2:L:108:PRO:HG3	2:L:146:GLU:HG3	1.92	0.51
2:L:180:PRO:HD2	6:L:424:SF4:S3	2.51	0.50
5:L:428:CYN:C	10:L:433:HOH:O	2.58	0.50
2:L:26:HIS:CE1	2:L:63[A]:ILE:HG23	2.47	0.50
2:M:234:CYS:HB2	6:M:424:SF4:S1	2.51	0.50
1:T:89:HIS:HD2	2:M:199:THR:OG1	1.95	0.50
2:L:295:ILE:O	2:L:301:GLY:HA3	2.12	0.48
2:M:38:CYS:O	2:M:39:ASP:HB2	2.13	0.48
2:L:368:SER:HA	2:L:369:PRO:HD3	1.79	0.47
2:M:108:PRO:HG3	2:M:146:GLU:HG3	1.96	0.47
2:M:398:MET:N	10:M:870:HOH:O	2.48	0.46
2:M:26:HIS:CE1	2:M:63[B]:ILE:HG23	2.51	0.46
2:L:234:CYS:HB2	6:L:424:SF4:S1	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:180:PRO:HD2	6:M:424:SF4:S3	2.57	0.45
1:S:76:LEU:O	1:S:77:GLU:HB2	2.17	0.44
2:L:180:PRO:HB3	2:L:240:GLU:HB2	2.00	0.44
2:L:107:ALA:HB2	2:L:232:MET:SD	2.58	0.44
2:M:22:PRO:HB2	2:M:239:TYR:CD2	2.52	0.44
2:L:173:PRO:HB3	2:L:370:TYR:O	2.17	0.44
2:L:22:PRO:HB2	2:L:239:TYR:CD2	2.54	0.42
2:L:203:PRO:HG2	8:L:431:CMO:C	2.49	0.42
1:T:42:TYR:HB3	2:M:391[A]:MET:SD	2.58	0.42
1:T:76:LEU:O	1:T:77:GLU:HB2	2.20	0.42
2:L:38:CYS:O	2:L:39:ASP:HB2	2.20	0.41
2:L:16:PRO:HG3	2:L:85:GLN:OE1	2.20	0.41
2:M:194:LEU:O	2:M:197:PHE:HB2	2.21	0.41
2:M:63[A]:ILE:HD13	10:M:505:HOH:O	2.19	0.41
2:L:194:LEU:N	2:L:195[A]:PRO:HD2	2.35	0.41
2:M:318:LYS:HE3	2:M:318:LYS:HB3	1.85	0.41
2:M:267:ILE:HG23	2:M:272:ILE:HB	2.03	0.40
2:L:194:LEU:O	2:L:197:PHE:HB2	2.22	0.40
2:L:46:PRO:HB3	2:L:353:ALA:HB3	2.03	0.40
2:L:5:VAL:HG22	2:L:10[B]:GLU:HG2	2.03	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	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
1	T	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
2	L	411/421 (98%)	402 (98%)	9 (2%)	0	100	100
2	M	409/421 (97%)	400 (98%)	9 (2%)	0	100	100
All	All	1004/1088 (92%)	982 (98%)	22 (2%)	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	82/100 (82%)	80 (98%)	2 (2%)	49	24
1	T	82/100 (82%)	82 (100%)	0	100	100
2	L	337/340 (99%)	330 (98%)	7 (2%)	53	29
2	M	335/340 (98%)	326 (97%)	9 (3%)	44	20
All	All	836/880 (95%)	818 (98%)	18 (2%)	65	27

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	108[A]	LEU
1	S	108[B]	LEU
2	L	131[A]	LEU
2	L	131[B]	LEU
2	L	148[A]	THR
2	L	148[B]	THR
2	L	294	THR
2	L	372	PHE
2	L	396	GLU
2	M	26	HIS
2	M	63[A]	ILE
2	M	63[B]	ILE
2	M	114[A]	LEU
2	M	114[B]	LEU
2	M	148[A]	THR
2	M	148[B]	THR
2	M	294	THR
2	M	372	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	26	HIS
2	L	135	GLN
1	T	89	HIS
2	M	26	HIS
2	M	29	GLN
2	M	174	GLN

### 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 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	CYN	L	429	-	0,1,1	0.00	-	-		
6	SF4	M	424	2	0,12,12	0.00	-	-		
8	CMO	L	431	-	0,1,1	0.00	-	-		
6	SF4	L	424	2	0,12,12	0.00	-	-		
7	PDT	M	425	4	4,4,4	0.33	0	3,3,3	3.88	3 (100%)
7	PDT	L	425	4	4,4,4	0.43	0	3,3,3	2.42	2 (66%)
5	CYN	L	428	-	0,1,1	0.00	-	-		
8	CMO	M	430	-	0,1,1	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	CMO	L	430	-	0,1,1	0.00	-	-		
6	SF4	M	423	2	0,12,12	0.00	-	-		
5	CYN	M	429	-	0,1,1	0.00	-	-		
6	SF4	M	422	2	0,12,12	0.00	-	-		
6	SF4	L	423	2	0,12,12	0.00	-	-		
6	SF4	L	422	2	0,12,12	0.00	-	-		
5	CYN	M	428	-	0,1,1	0.00	-	-		
8	CMO	M	431	-	0,1,1	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
6	SF4	L	424	2	-	-	0/6/5/5
7	PDT	M	425	4	-	2/2/2/2	-
7	PDT	L	425	4	-	2/2/2/2	-
6	SF4	M	424	2	-	-	0/6/5/5
6	SF4	M	423	2	-	-	0/6/5/5
6	SF4	M	422	2	-	-	0/6/5/5
6	SF4	L	422	2	-	-	0/6/5/5
6	SF4	L	423	2	-	-	0/6/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	425	PDT	C2-C1-S1	-4.36	98.94	112.96
7	M	425	PDT	C2-C3-S2	-4.29	99.19	112.96
7	L	425	PDT	C2-C3-S2	-3.13	102.92	112.96
7	M	425	PDT	C3-C2-C1	-2.80	102.91	112.99
7	L	425	PDT	C2-C1-S1	-2.61	104.57	112.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	425	PDT	S1-C1-C2-C3
7	L	425	PDT	C1-C2-C3-S2
7	M	425	PDT	S1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	M	425	PDT	C1-C2-C3-S2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	424	SF4	2	0
8	L	431	CMO	1	0
6	L	424	SF4	2	0
7	M	425	PDT	1	0
7	L	425	PDT	1	0
5	L	428	CYN	1	0
5	M	428	CYN	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.