



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:17 PM UTC

PDB ID : 1HFE / pdb_00001hfe
Title : 1.6 Å RESOLUTION STRUCTURE OF THE FE-ONLY HYDROGENASE
FROM DESULFOVIBRIO DESULFURICANS
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Deposited on : 1998-11-11
Resolution : 1.60 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

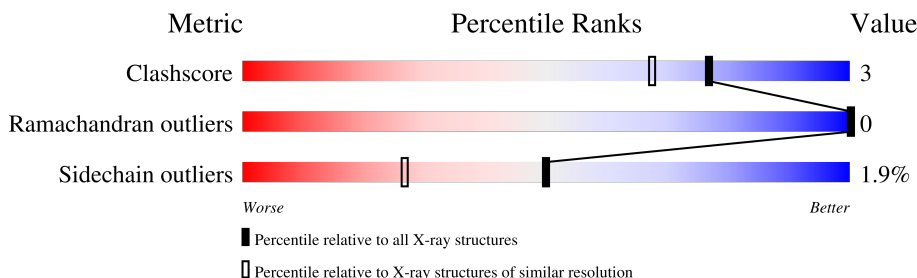
1 Overall quality at a glance

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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	-
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			

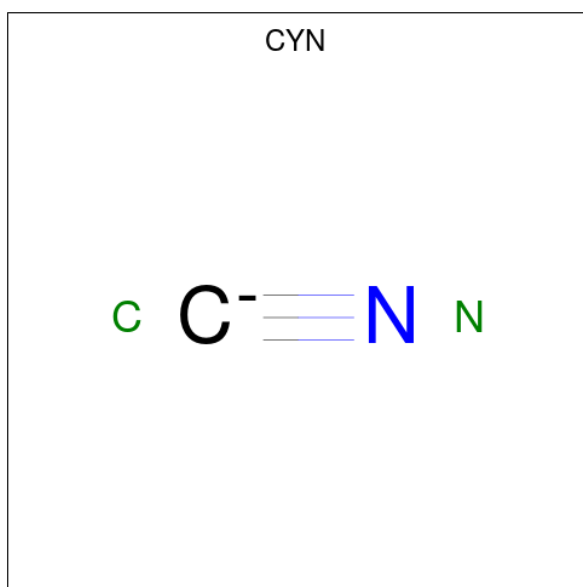
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

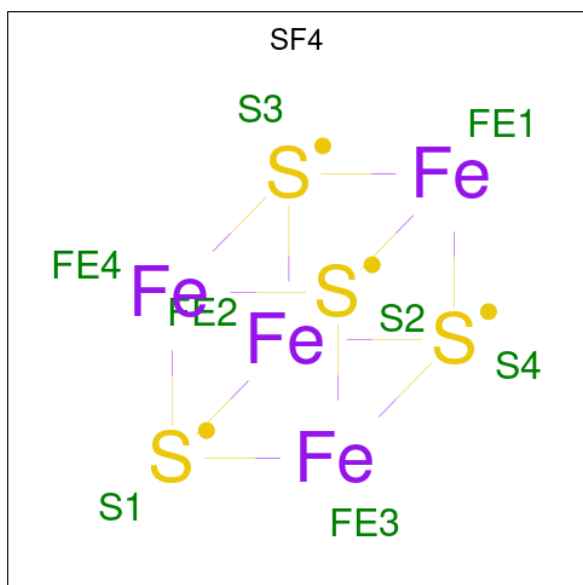
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	2	Total	Fe	0	0
			2	2		
4	M	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CYANIDE ION (CCD ID: CYN) (formula: CN).



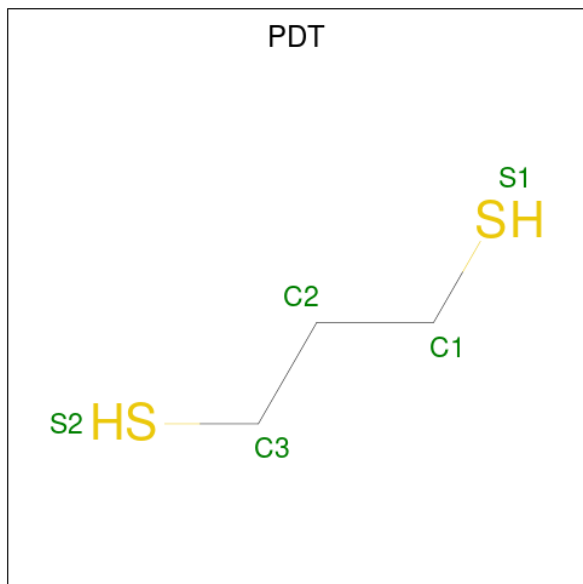
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	N	0	0
			2	1	1		
5	L	1	Total	C	N	0	0
			2	1	1		
5	M	1	Total	C	N	0	0
			2	1	1		
5	M	1	Total	C	N	0	0
			2	1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



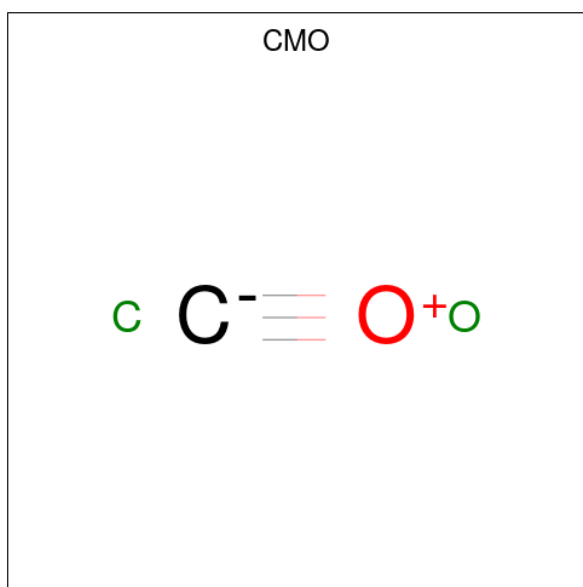
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	Fe	S	0	0
			8	4	4		
6	L	1	Total	Fe	S	0	0
			8	4	4		
6	L	1	Total	Fe	S	0	0
			8	4	4		
6	M	1	Total	Fe	S	0	0
			8	4	4		
6	M	1	Total	Fe	S	0	0
			8	4	4		
6	M	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is 1,3-PROPANEDITHIOL (CCD ID: PDT) (formula: $C_3H_8S_2$).



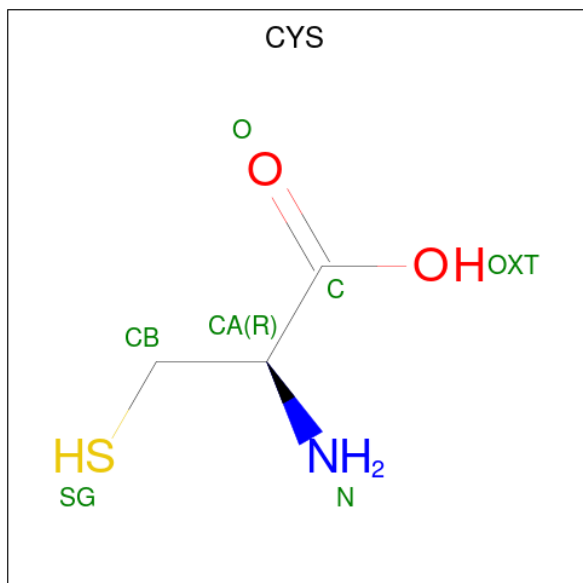
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	S	0	0
			5	3	2		
7	M	1	Total	C	S	0	0
			5	3	2		

- Molecule 8 is CARBON MONOXIDE (CCD ID: 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 (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



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		

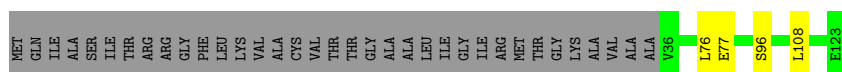
3 Residue-property plots

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. 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.

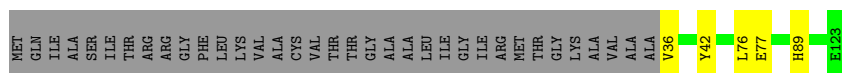
- Molecule 1: PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (SMALLER SUBUNIT))

Chain S: 



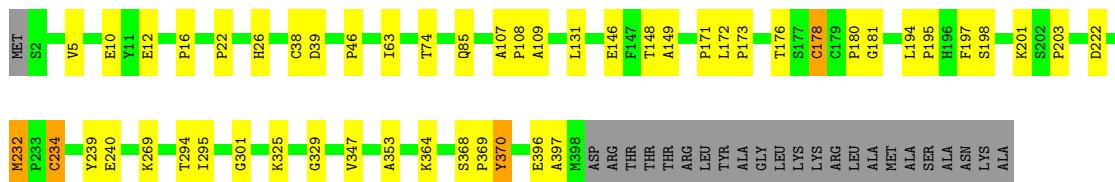
- Molecule 1: PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (SMALLER SUBUNIT))

Chain T: 



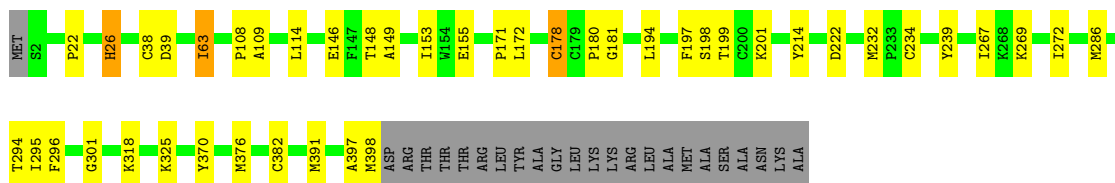
- Molecule 2: PROTEIN (FE-ONLY HYDROGENASE (E.C.1.18.99.1) (LARGER SUBUNIT))

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, α , β , γ	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 ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, PDT, CYN, CMO, SF4, ZN

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	0.54	0/783	0.92	1/1058 (0.1%)
1	T	0.52	0/784	0.91	0/1057
2	L	0.57	1/3212 (0.0%)	0.96	16/4347 (0.4%)
2	M	0.57	1/3193 (0.0%)	0.95	13/4320 (0.3%)
All	All	0.56	2/7972 (0.0%)	0.95	30/10782 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	397	ALA	C-N	-5.60	1.25	1.33
2	L	397	ALA	C-N	-5.46	1.25	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	178	CYS	N-CA-C	8.17	121.30	111.82
2	L	171	PRO	N-CA-C	7.91	123.23	111.38
2	M	171	PRO	N-CA-C	6.79	122.17	111.38
2	L	370	TYR	N-CA-C	6.60	120.25	110.48
2	L	325	LYS	N-CA-C	6.45	120.25	112.38

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	761	0	754	1	0
1	T	761	0	749	4	0
2	L	3136	0	3089	20	0
2	M	3117	0	3065	20	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
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	2	0
8	L	4	0	0	1	0
8	M	4	0	0	0	0
9	L	7	0	4	1	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	44	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.

The worst 5 of 44 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

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	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%)	43	19
1	T	82/100 (82%)	81 (99%)	1 (1%)	63	43
2	L	337/340 (99%)	327 (97%)	10 (3%)	36	13
2	M	335/340 (98%)	326 (97%)	9 (3%)	39	16
All	All	836/880 (95%)	814 (97%)	22 (3%)	50	17

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	63[A]	ILE
2	M	114[B]	LEU
2	M	114[A]	LEU

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Mol	Chain	Res	Type
2	M	148[A]	THR
2	L	269	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	174	GLN
2	M	358	GLN
2	L	183	GLN
1	T	89	HIS
2	M	29	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 oligosaccharides 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	$\# Z > 2$
8	CMO	L	430	-	0,1,1	-	-	-		
8	CMO	M	430	-	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SF4	L	423	2	0,12,12	-	-	-		
5	CYN	M	429	-	1,1,1	0.18	0	-		
5	CYN	M	428	-	1,1,1	0.24	0	-		
6	SF4	L	422	2	0,12,12	-	-	-		
5	CYN	L	429	-	1,1,1	0.17	0	-		
8	CMO	L	431	-	0,1,1	-	-	-		
8	CMO	M	431	-	0,1,1	-	-	-		
9	CYS	M	433	-	5,6,6	1.80	1 (20%)	3,7,7	1.22	0
6	SF4	M	422	2	0,12,12	-	-	-		
6	SF4	M	423	2	0,12,12	-	-	-		
6	SF4	M	424	2	0,12,12	-	-	-		
6	SF4	L	424	2	0,12,12	-	-	-		
7	PDT	L	425	4	4,4,4	0.47	0	3,3,3	2.57	2 (66%)
7	PDT	M	425	4	4,4,4	0.36	0	3,3,3	4.05	3 (100%)
9	CYS	L	432	-	5,6,6	1.79	1 (20%)	3,7,7	1.66	1 (33%)
5	CYN	L	428	-	1,1,1	0.23	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
6	SF4	L	423	2	-	-	0/6/5/5
6	SF4	L	422	2	-	-	0/6/5/5
9	CYS	M	433	-	-	2/6/6/6	-
6	SF4	M	422	2	-	-	0/6/5/5
7	PDT	L	425	4	-	2/2/2/2	-
6	SF4	M	423	2	-	-	0/6/5/5
6	SF4	L	424	2	-	-	0/6/5/5
6	SF4	M	424	2	-	-	0/6/5/5
7	PDT	M	425	4	-	2/2/2/2	-
9	CYS	L	432	-	-	1/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	433	CYS	CB-SG	-3.40	1.74	1.81
9	L	432	CYS	CB-SG	-3.29	1.74	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	425	PDT	C2-C1-S1	-4.63	98.94	113.10
7	M	425	PDT	C2-C3-S2	-4.55	99.19	113.10
7	L	425	PDT	C2-C3-S2	-3.33	102.92	113.10
7	L	425	PDT	C2-C1-S1	-2.79	104.57	113.10
7	M	425	PDT	C3-C2-C1	-2.65	102.91	113.07

There are no chirality outliers.

5 of 7 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
7	M	425	PDT	C1-C2-C3-S2
9	L	432	CYS	C-CA-CB-SG

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	428	CYN	1	0
8	L	431	CMO	1	0
6	M	424	SF4	2	0
6	L	424	SF4	2	0
7	L	425	PDT	1	0
7	M	425	PDT	2	0
9	L	432	CYS	1	0
5	L	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.