



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:48 AM BST

PDB ID : 6Z8J  
Title : Structure of [NiFeSe] hydrogenase from *Desulfovibrio vulgaris hildenborough* pressurized with Oxygen gas - structure wtO2  
Authors : Zacarias, S.; Temporao, A.; Carpentier, P.; van der Linden, P.; Pereira, I.A.C.; Matias, P.M.  
Deposited on : 2020-06-02  
Resolution : 1.09 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) : 1.13  
EDS : 2.14.6  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

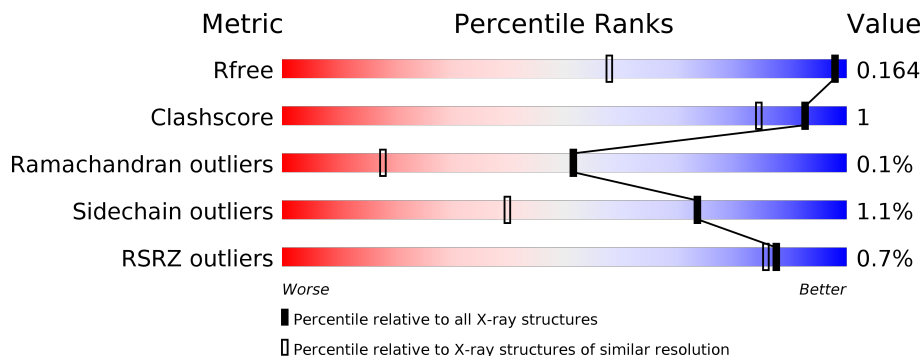
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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  $\leq 5\%$ . 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	A	283	 94%
1	C	283	 96%
2	B	484	 96%
2	D	484	 95% 5%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 24806 atoms, of which 11823 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.

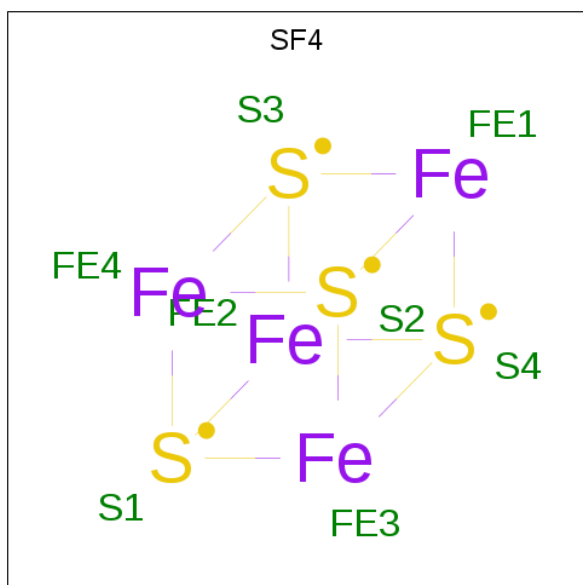
- Molecule 1 is a protein called Periplasmic [NiFeSe] hydrogenase, small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	279	Total 4208	C 1360	H 2081	N 351	O 395	S 21	0	6	0
1	C	279	Total 4203	C 1359	H 2077	N 351	O 395	S 21	0	6	0

- Molecule 2 is a protein called Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing.

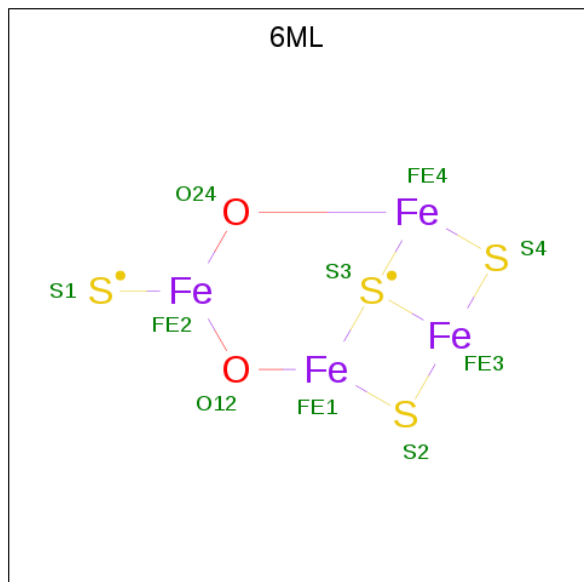
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
2	B	484	Total 7639	C 2433	H 3828	N 663	O 693	S 19	Se 3	0	11	0
2	D	481	Total 7584	C 2413	H 3805	N 657	O 687	S 19	Se 3	0	8	0

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



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

- Molecule 4 is oxygen-damaged SF<sub>4</sub> (three-letter code: 6ML) (formula: Fe<sub>4</sub>O<sub>2</sub>S<sub>4</sub>).



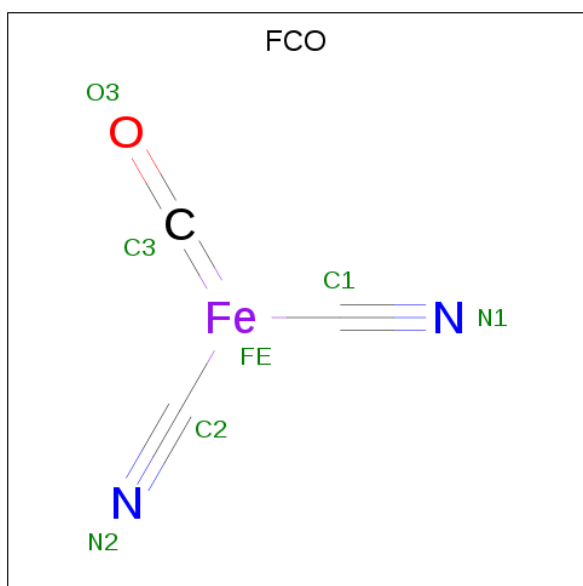
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	O	S	0	1
			10	4	2	4		
4	C	1	Total	Fe	O	S	0	1
			10	4	2	4		

- Molecule 5 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
			Total	C	H	O		
5	A	1	Total 14	C 3	H 8	O 3	0	0
5	B	1	Total 14	C 3	H 8	O 3	0	0
5	B	1	Total 14	C 3	H 8	O 3	0	0
5	C	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula:  $C_3FeN_2O$ ).



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

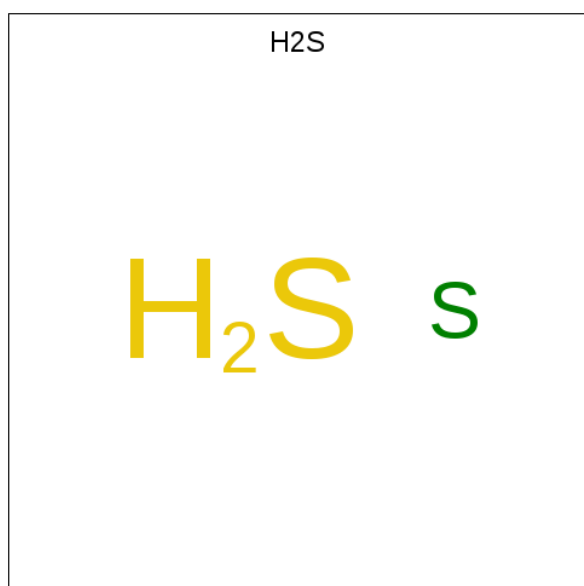
- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ni	0	0
			1	1		
7	D	1	Total	Ni	0	0
			1	1		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Fe	0	0
			1	1		
8	D	1	Total	Fe	0	0
			1	1		

- Molecule 9 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	S	0	1
			2	2		

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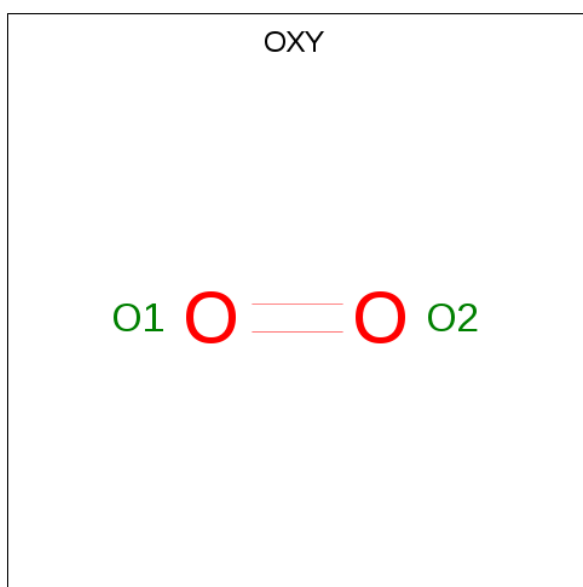
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total S 2 2	0	1

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

- Molecule 11 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total O 2 2	0	0
11	D	1	Total O 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	187	Total O 189 189	0	2
12	B	309	Total O 312 312	0	4

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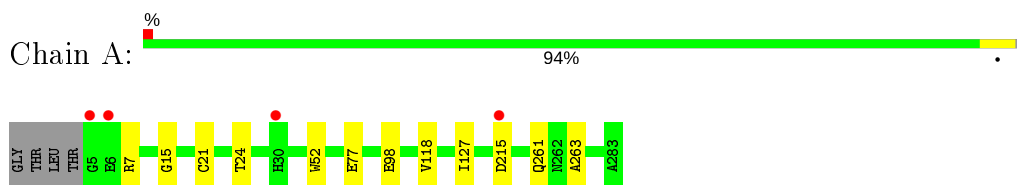
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
12	C	219	Total 221	O 221	0	2
12	D	298	Total 298	O 298	0	0



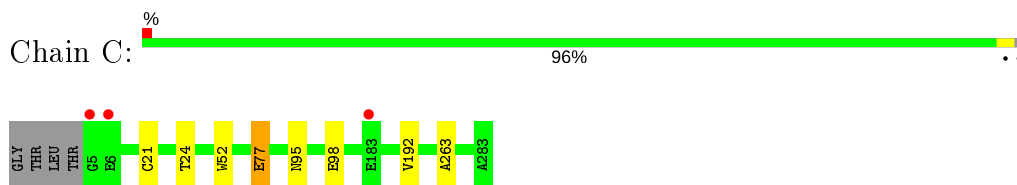
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

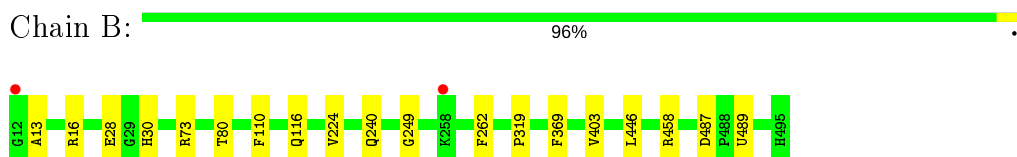
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit



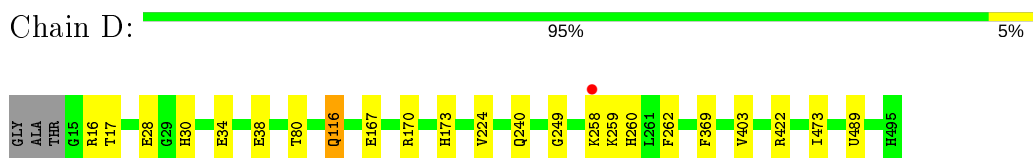
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit



- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing



- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.86Å 93.99Å 98.61Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	42.41 – 1.09 98.46 – 1.09	Depositor EDS
% Data completeness (in resolution range)	50.3 (42.41-1.09) 62.8 (98.46-1.09)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 1.09Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.140 , 0.164 0.140 , 0.164	Depositor DCC
$R_{free}$ test set	17823 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.0	Xtrriage
Anisotropy	0.068	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	24806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3076e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 6ML, OXY, GOL, CSD, SF4, CL, H2S, SEC, FE2, 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	A	0.42	0/2197	0.63	0/2984
1	C	0.41	1/2196 (0.0%)	0.62	0/2983
2	B	0.41	0/3892	0.68	5/5259 (0.1%)
2	D	0.40	0/3857	0.65	0/5213
All	All	0.41	1/12142 (0.0%)	0.65	5/16439 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	77	GLU	CG-CD	5.30	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	458	ARG	NE-CZ-NH2	-7.19	116.71	120.30
2	B	487	ASP	CB-CG-OD1	5.75	123.47	118.30
2	B	458	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	B	110	PHE	CB-CG-CD1	5.19	124.43	120.80
2	B	487	ASP	CB-CG-OD2	-5.11	113.70	118.30

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	A	2127	2081	2080	8	0
1	C	2126	2077	2078	5	0
2	B	3811	3828	3828	9	0
2	D	3779	3805	3793	15	0
3	A	24	0	0	0	0
3	C	24	0	0	0	0
4	A	10	0	0	0	0
4	C	10	0	0	0	0
5	A	6	8	8	1	0
5	B	12	16	16	0	0
5	C	6	8	8	0	0
6	B	7	0	0	1	0
6	D	7	0	0	1	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	2	0	0	0	0
9	D	2	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
12	A	189	0	0	2	0
12	B	312	0	0	0	0
12	C	221	0	0	3	0
12	D	298	0	0	3	0
All	All	12983	11823	11811	35	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 1.

All (35) 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:A:21[B]:CYS:SG	1:A:118:VAL:HG12	2.14	0.87
1:A:7:ARG:NH2	12:A:401:HOH:O	2.16	0.78
1:C:95:ASN:ND2	12:C:401:HOH:O	2.20	0.74
2:D:16:ARG:NH1	12:D:601:HOH:O	2.17	0.73
2:B:489[A]:SEC:SE	6:B:501:FCO:C1	2.87	0.72
2:D:489[A]:SEC:SE	6:D:501:FCO:C1	2.91	0.68
2:D:167:GLU:OE1	2:D:170:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ALA:HB3	2:B:16[B]:ARG:HD3	1.84	0.58
2:D:16:ARG:NE	2:D:38:GLU:OE2	2.35	0.56
1:C:21[B]:CYS:HB2	1:C:77:GLU:OE2	2.11	0.51
2:B:28:GLU:HB3	2:B:489[A]:SEC:CB	2.41	0.51
2:D:260:HIS:HE1	12:D:866:HOH:O	1.94	0.51
2:D:34:GLU:OE2	12:D:602:HOH:O	2.19	0.50
1:A:98:GLU:HG2	5:A:305:GOL:H11	1.92	0.50
2:D:28:GLU:HB3	2:D:489[A]:SEC:CB	2.43	0.49
1:C:21[B]:CYS:HB2	1:C:77:GLU:CD	2.36	0.46
1:C:98[B]:GLU:HG2	12:C:488:HOH:O	2.16	0.46
1:A:21[B]:CYS:HB2	1:A:77:GLU:CD	2.35	0.46
1:C:21[B]:CYS:O	1:C:24:THR:HG22	2.16	0.46
1:A:127:ILE:HD12	2:B:73:ARG:HG2	1.97	0.45
1:A:21[B]:CYS:HB2	1:A:77:GLU:OE2	2.16	0.45
1:A:21[B]:CYS:O	1:A:24:THR:HG22	2.17	0.44
2:D:240:GLN:HA	2:D:369:PHE:O	2.18	0.44
2:D:17:THR:HG21	2:D:473[B]:ILE:HG21	1.98	0.44
2:B:240:GLN:HA	2:B:369:PHE:O	2.16	0.44
2:D:249:GLY:HA2	2:D:262:PHE:O	2.18	0.44
12:C:577:HOH:O	2:D:30:HIS:HD2	1.99	0.44
2:B:249:GLY:HA2	2:B:262:PHE:O	2.17	0.43
2:B:319:PRO:HG3	2:B:446:LEU:HG	2.02	0.42
2:D:258:LYS:HG3	2:D:259:LYS:H	1.84	0.42
2:D:422:ARG:CD	2:D:489[A]:SEC:SE	3.18	0.41
1:A:15:GLY:O	2:B:30:HIS:HE1	2.03	0.41
12:A:558:HOH:O	2:B:30:HIS:HD2	2.04	0.40
2:D:116:GLN:HG3	2:D:173:HIS:CD2	2.57	0.40
2:D:258:LYS:HG3	2:D:259:LYS:N	2.37	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	A	283/283 (100%)	275 (97%)	7 (2%)	1 (0%)	34	10
1	C	283/283 (100%)	276 (98%)	6 (2%)	1 (0%)	34	10
2	B	488/484 (101%)	477 (98%)	11 (2%)	0	100	100
2	D	483/484 (100%)	472 (98%)	11 (2%)	0	100	100
All	All	1537/1534 (100%)	1500 (98%)	35 (2%)	2 (0%)	51	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ALA
1	C	263	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/226 (101%)	226 (99%)	3 (1%)	69	32
1	C	229/226 (101%)	227 (99%)	2 (1%)	78	48
2	B	399/391 (102%)	395 (99%)	4 (1%)	76	44
2	D	396/391 (101%)	392 (99%)	4 (1%)	76	44
All	All	1253/1234 (102%)	1240 (99%)	13 (1%)	73	44

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	TRP
1	A	215	ASP
1	A	261	GLN
2	B	80	THR
2	B	116	GLN
2	B	224	VAL
2	B	403	VAL
1	C	52	TRP
1	C	192	VAL

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Mol	Chain	Res	Type
2	D	80	THR
2	D	116	GLN
2	D	224	VAL
2	D	403	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	30	HIS
2	B	39	ASN
2	B	260	HIS
2	D	30	HIS
2	D	260	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 4 are modelled with single atom and 6 are monoatomic - leaving 16 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
3	SF4	C	302	1	0,12,12	0.00	-	-		
4	6ML	C	304[B]	1	0,12,12	0.00	-	-		
3	SF4	A	303[A]	1	0,12,12	0.00	-	-		
5	GOL	B	507	-	5,5,5	0.92	0	5,5,5	0.78	0
3	SF4	C	303[A]	1	0,12,12	0.00	-	-		
6	FCO	D	501	2	0,6,6	0.00	-	-		
4	6ML	A	304[B]	1	0,12,12	0.00	-	-		
6	FCO	B	501	2	0,6,6	0.00	-	-		
5	GOL	C	305	-	5,5,5	1.02	0	5,5,5	0.92	0
5	GOL	A	305	-	5,5,5	0.88	0	5,5,5	0.78	0
3	SF4	A	301	1	0,12,12	0.00	-	-		
3	SF4	C	301	1	0,12,12	0.00	-	-		
11	OXY	B	508	-	1,1,1	0.13	0	-		
5	GOL	B	506	-	5,5,5	1.19	0	5,5,5	0.71	0
11	OXY	D	506	-	1,1,1	0.13	0	-		
3	SF4	A	302	1	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
3	SF4	C	302	1	-	-	0/6/5/5
4	6ML	C	304[B]	1	-	-	0/2/3/3
3	SF4	A	303[A]	1	-	-	0/6/5/5
5	GOL	B	507	-	-	0/4/4/4	-
3	SF4	C	303[A]	1	-	-	0/6/5/5
4	6ML	A	304[B]	1	-	-	0/2/3/3
5	GOL	C	305	-	-	0/4/4/4	-
5	GOL	A	305	-	-	0/4/4/4	-
3	SF4	A	301	1	-	-	0/6/5/5
3	SF4	C	301	1	-	-	0/6/5/5
5	GOL	B	506	-	-	0/4/4/4	-
3	SF4	A	302	1	-	-	0/6/5/5



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	501	FCO	1	0
6	B	501	FCO	1	0
5	A	305	GOL	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	A	279/283 (98%)	-0.41	4 (1%) 75 71	9, 13, 24, 53	5 (1%)
1	C	279/283 (98%)	-0.40	3 (1%) 80 77	8, 13, 26, 58	1 (0%)
2	B	482/484 (99%)	-0.54	2 (0%) 92 90	8, 13, 21, 35	8 (1%)
2	D	479/484 (98%)	-0.53	1 (0%) 95 92	8, 13, 22, 36	7 (1%)
All	All	1519/1534 (99%)	-0.49	10 (0%) 87 86	8, 13, 23, 58	21 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	12.8
1	C	5	GLY	12.5
1	C	6	GLU	7.1
1	A	6	GLU	4.6
2	B	258	LYS	3.3
1	A	215	ASP	3.2
2	D	258	LYS	3.1
2	B	12	GLY	2.7
1	A	30	HIS	2.3
1	C	183	GLU	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSD	B	75[B]	7/9	0.99	0.04	9,10,12,12	1
2	CSD	D	75[B]	7/9	0.99	0.05	8,10,12,12	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CSD	D	75[A]	7/9	0.99	0.05	8,10,12,12	0
2	CSD	B	75[A]	7/9	0.99	0.04	9,10,12,12	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	507	6/6	0.79	0.14	33,40,42,43	0
5	GOL	A	305	6/6	0.83	0.15	29,34,36,37	0
11	OXY	D	506	2/2	0.85	0.12	38,38,38,38	0
5	GOL	C	305	6/6	0.88	0.15	32,39,42,43	0
11	OXY	B	508	2/2	0.94	0.15	37,37,37,37	2
5	GOL	B	506	6/6	0.95	0.14	20,24,27,28	0
8	FE2	B	503	1/1	1.00	0.05	9,9,9,9	0
4	6ML	C	304[B]	10/10	1.00	0.06	7,8,9,10	10
3	SF4	A	303[A]	8/8	1.00	0.06	8,9,9,10	8
9	H2S	D	504[B]	1/1	1.00	0.06	12,12,12,12	1
9	H2S	D	504[A]	1/1	1.00	0.06	9,9,9,9	1
7	NI	B	502	1/1	1.00	0.07	10,10,10,10	1
3	SF4	C	302	8/8	1.00	0.06	9,9,10,10	0
8	FE2	D	503	1/1	1.00	0.08	8,8,8,8	1
3	SF4	C	303[A]	8/8	1.00	0.06	7,8,9,9	8
6	FCO	D	501	7/7	1.00	0.06	9,10,11,13	0
4	6ML	A	304[B]	10/10	1.00	0.06	7,8,9,10	10
6	FCO	B	501	7/7	1.00	0.05	9,10,11,12	0
10	CL	B	505	1/1	1.00	0.07	9,9,9,9	0
3	SF4	A	301	8/8	1.00	0.05	13,14,15,15	0
3	SF4	A	302	8/8	1.00	0.05	10,11,11,11	0
10	CL	D	505	1/1	1.00	0.06	9,9,9,9	0
9	H2S	B	504[A]	1/1	1.00	0.06	9,9,9,9	1
3	SF4	C	301	8/8	1.00	0.05	10,10,10,11	0
9	H2S	B	504[B]	1/1	1.00	0.06	12,12,12,12	1
7	NI	D	502	1/1	1.00	0.07	10,10,10,10	1

## 6.5 Other polymers

There are no such residues in this entry.