wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 03:22 PM UTC

PDB ID	:	6Z8M / pdb_00006z8m
Title	:	Structure of [NiFeSe] hydrogenase G491S variant from Desulfovibrio vulgaris Hildenborough pressurized with Oxygen gas - structure G491S-O2
Authors	:	Zacarias, S.; Temporao, A.; Carpentier, P.; van der Linden, P.; Pereira, I.A.C.; Matias, P.M.
Deposited on	:	2020-06-02
Resolution	:	1.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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 (i) 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 (1)) were used in the production of this report:

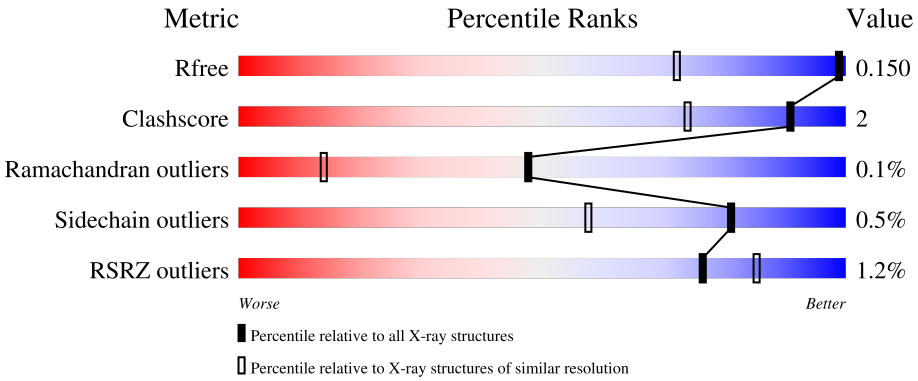
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.02 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}	180053	1726 (1.06-0.98)
Clashscore	190562	1007 (1.04-1.00)
Ramachandran outliers	187476	1715 (1.06-0.98)
Sidechain outliers	187428	1716 (1.06-0.98)
RSRZ outliers	180081	1723 (1.06-0.98)

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 <=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	2% 97% .
2	B	485	95% 5%

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
9	H2S	B	504[B]	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 12865 atoms, of which 6071 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	283	4378	1411	2179	359	408	21	0	17	0

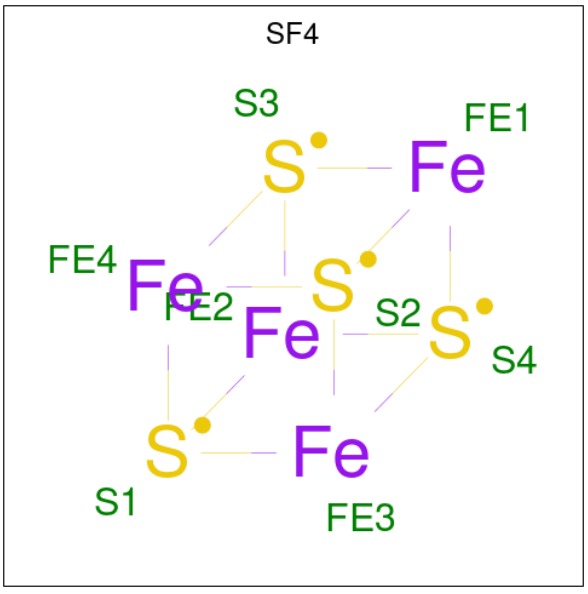
- Molecule 2 is a protein called Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
2	B	483	7679	2440	3860	661	696	19	3	0	14	0

There is a discrepancy between the modelled and reference sequences:

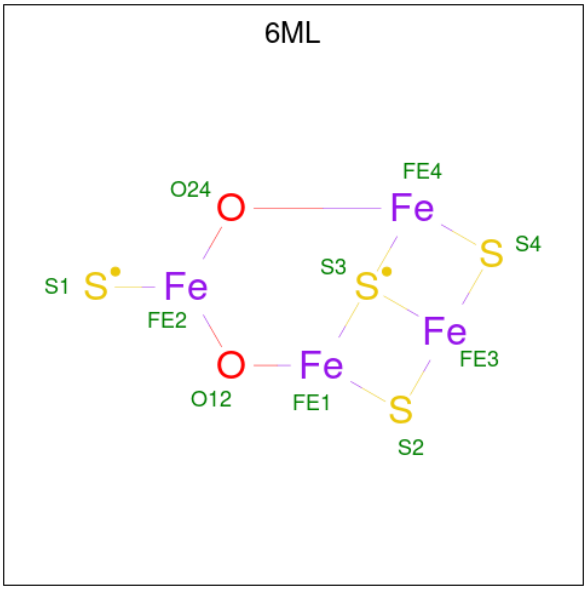
Chain	Residue	Modelled	Actual	Comment	Reference
B	491	SER	GLY	engineered mutation	UNP Q72AS3

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



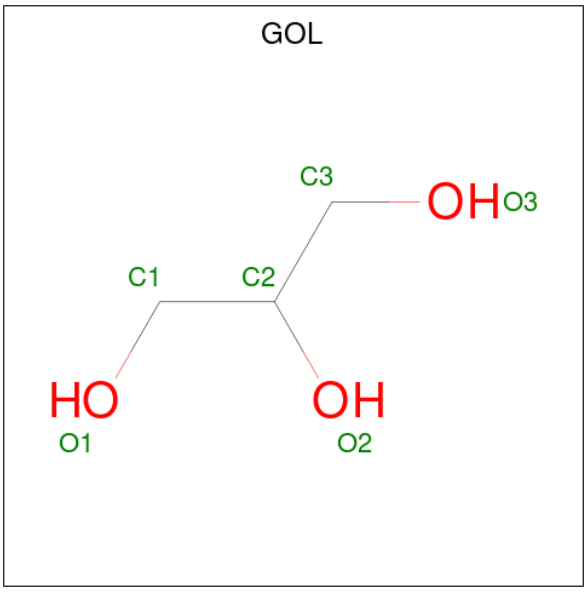
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	1

- Molecule 4 is oxygen-damaged SF4 (CCD ID: 6ML) (formula: $Fe_4O_2S_4$).



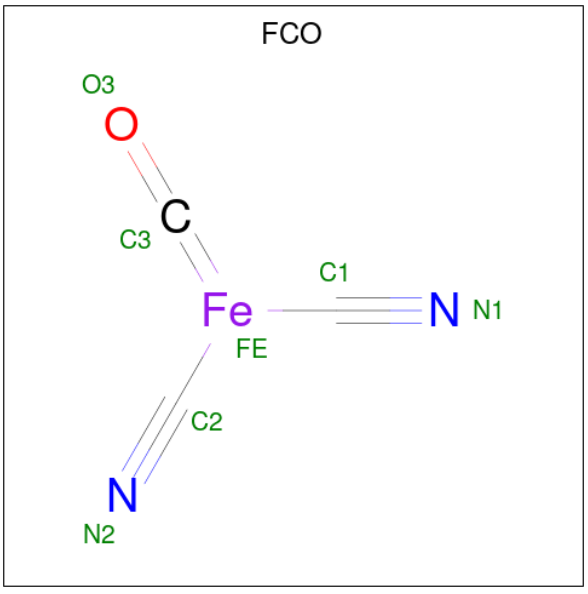
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe O S 10 4 2 4	0	1

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 28 6 16 6	0	1
5	B	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: 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		

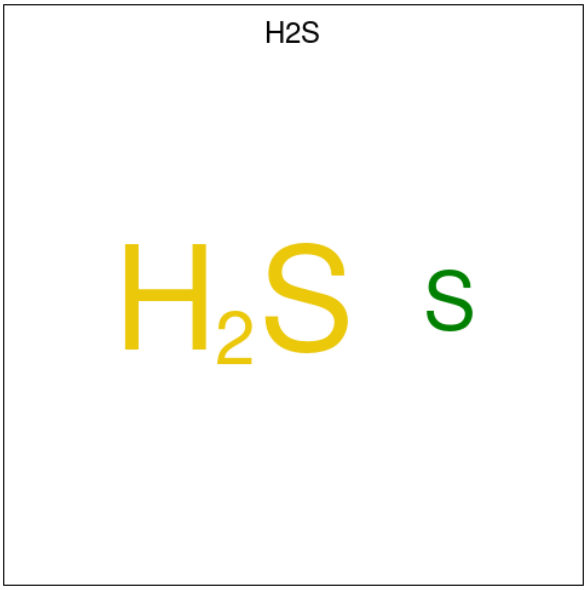
- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ni	0	1
			2	2		

- Molecule 8 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 9 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S).

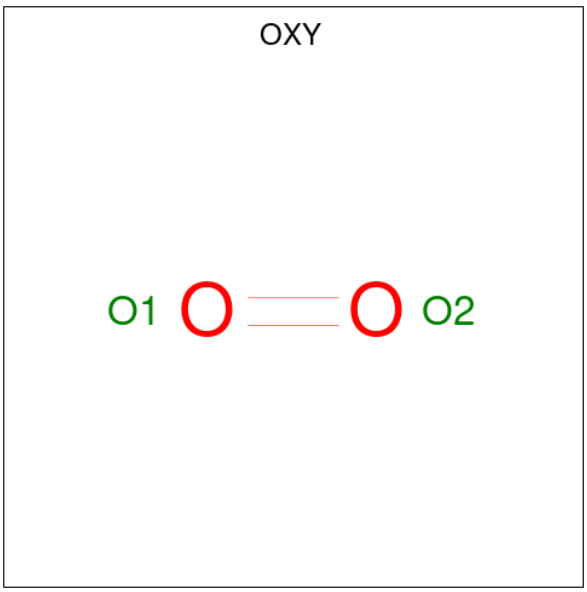


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	S	0	1
			2	2		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 11 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



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

- Molecule 12 is water.

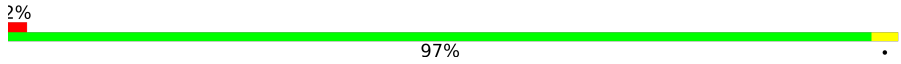
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	274	Total O 283 283	0	15
12	B	410	Total O 418 418	0	12

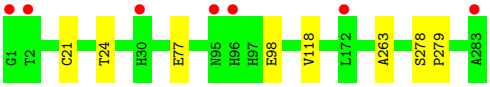
3 Residue-property plots (i)

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

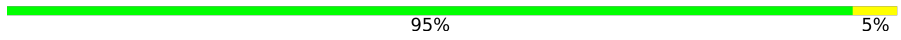
Chain A:

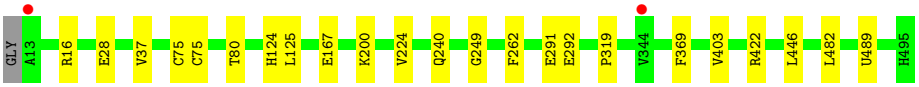




• Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.99Å 62.64Å 110.53Å 90.00° 105.21° 90.00°	Depositor
Resolution (Å)	53.33 – 1.02 53.33 – 1.02	Depositor EDS
% Data completeness (in resolution range)	86.8 (53.33-1.02) 94.5 (53.33-1.02)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.02Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.134 , 0.151 0.134 , 0.150	Depositor DCC
R_{free} test set	16559 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	10.5	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	12865	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SF4, CL, SEC, FE2, GOL, H2S, FCO, NI, CSD, 6ML, OXY

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	0.30	0/2309	0.55	0/3137
2	B	0.30	0/3923	0.59	0/5300
All	All	0.30	0/6232	0.57	0/8437

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

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	2199	2179	2142	5	0
2	B	3819	3860	3832	15	0
3	A	24	0	0	0	0
4	A	10	0	0	0	0
5	A	12	16	16	1	0
5	B	12	16	15	0	0
6	B	7	0	0	1	0
7	B	2	0	0	1	0
8	B	1	0	0	0	0
9	B	2	0	0	2	0
10	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	4	0	0	0	0
12	A	283	0	0	0	0
12	B	418	0	0	5	0
All	All	6794	6071	6005	21	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 2.

The worst 5 of 21 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:B:167:GLU:OE2	12:B:601[A]:HOH:O	1.88	0.92
7:B:502[B]:NI:NI	9:B:504[B]:H2S:S	1.59	0.85
1:A:21[B]:CYS:SG	1:A:118:VAL:HG12	2.21	0.81
2:B:489[A]:SEC:SE	6:B:501:FCO:C1	2.83	0.76
2:B:28:GLU:HB3	2:B:489[A]:SEC:CB	2.29	0.62

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	298/283 (105%)	291 (98%)	6 (2%)	1 (0%)	36 11
2	B	491/485 (101%)	482 (98%)	9 (2%)	0	100 100
All	All	789/768 (103%)	773 (98%)	15 (2%)	1 (0%)	48 14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	242/226 (107%)	242 (100%)	0	100	100
2	B	405/393 (103%)	402 (99%)	3 (1%)	76	50
All	All	647/619 (104%)	644 (100%)	3 (0%)	81	57

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	80	THR
2	B	224	VAL
2	B	403	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	261	GLN
2	B	132	GLN
1	A	282	GLN
1	A	111	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)

1 non-standard protein/DNA/RNA residue is 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	CSD	B	75[B]	7,2	4,7,8	2.09	1 (25%)	1,8,10	1.21	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	CSD	B	75[B]	7,2	-	0/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	75[B]	CSD	OD1-SG	-3.39	1.44	1.47

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 11 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	A	303[A]	1	0,12,12	-	-	-		
5	GOL	A	305[B]	-	5,5,5	0.98	0	5,5,5	1.02	0
5	GOL	A	305[A]	-	5,5,5	0.95	0	5,5,5	0.98	0
11	OXY	B	509	-	1,1,1	0.17	0	-		
6	FCO	B	501	2,9	0,6,6	-	-	-		
5	GOL	B	506	-	5,5,5	1.23	1 (20%)	5,5,5	1.06	0
4	6ML	A	304[B]	1	0,12,12	-	-	-		
11	OXY	B	508	-	1,1,1	0.18	0	-		
3	SF4	A	302	1	0,12,12	-	-	-		
3	SF4	A	301	1	0,12,12	-	-	-		
5	GOL	B	507	-	5,5,5	1.04	0	5,5,5	1.08	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
3	SF4	A	303[A]	1	-	-	0/6/5/5
5	GOL	A	305[B]	-	-	0/4/4/4	-
3	SF4	A	302	1	-	-	0/6/5/5
5	GOL	B	506	-	-	2/4/4/4	-
4	6ML	A	304[B]	1	-	-	0/2/3/3
5	GOL	A	305[A]	-	-	0/4/4/4	-
3	SF4	A	301	1	-	-	0/6/5/5
5	GOL	B	507	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	506	GOL	O2-C2	-2.34	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	506	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	506	GOL	O2-C2-C3-O3
5	B	507	GOL	O1-C1-C2-C3
5	B	507	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	305[B]	GOL	1	0
6	B	501	FCO	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

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^{th} 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^2)	Q<0.9
1	A	283/283 (100%)	-0.42	7 (2%)	58	69	5, 12, 24, 37	17 (6%)
2	B	481/485 (99%)	-0.54	2 (0%)	88	93	6, 13, 21, 34	14 (2%)
All	All	764/768 (99%)	-0.50	9 (1%)	76	85	5, 13, 22, 37	31 (4%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ASN	3.0
1	A	30	HIS	2.8
2	B	344	VAL	2.7
1	A	2	THR	2.6
1	A	96	HIS	2.3

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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
2	CSD	B	75[B]	8/9	0.99	0.04	8,9,11,11	12

6.3 Carbohydrates

There are no oligosaccharides 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^{th} 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^2)	Q<0.9
5	GOL	B	507	6/6	0.82	0.14	32,38,43,45	0
5	GOL	A	305[B]	6/6	0.87	0.12	26,31,33,33	14
5	GOL	A	305[A]	6/6	0.87	0.12	29,34,36,36	14
11	OXY	B	508	2/2	0.88	0.12	33,33,33,33	0
5	GOL	B	506	6/6	0.91	0.11	17,26,30,32	0
11	OXY	B	509	2/2	0.93	0.13	29,29,29,29	2
7	NI	B	502[B]	1/1	0.99	0.03	9,9,9,9	1
4	6ML	A	304[B]	10/10	0.99	0.05	8,9,10,10	10
7	NI	B	502[A]	1/1	0.99	0.03	10,10,10,10	1
3	SF4	A	303[A]	8/8	1.00	0.01	7,8,8,8	8
3	SF4	A	301	8/8	1.00	0.01	9,9,10,10	0
8	FE2	B	503	1/1	1.00	0.02	9,9,9,9	0
9	H2S	B	504[A]	1/1	1.00	0.01	9,9,9,9	1
9	H2S	B	504[B]	1/1	1.00	0.01	10,10,10,10	1
10	CL	B	505	1/1	1.00	0.01	8,8,8,8	0
3	SF4	A	302	8/8	1.00	0.01	8,8,9,9	0
6	FCO	B	501	7/7	1.00	0.04	9,10,10,13	0

6.5 Other polymers (i)

There are no such residues in this entry.