Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 04:52 am BST

PDB ID	:	6RTP / pdb_00006rtp
Title	:	THE 3D STRUCTURE OF [NIFESE] HYDROGENASE G50T VaRIANT FROM DESULFOVIBRIO VULGARIS HILDENBOROUGH AT 1.10 ANGSTROM RESOLUTION
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Deposited on	:	2019-05-24
Resolution	:	1.10 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*
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 (i)) were used in the production of this report:

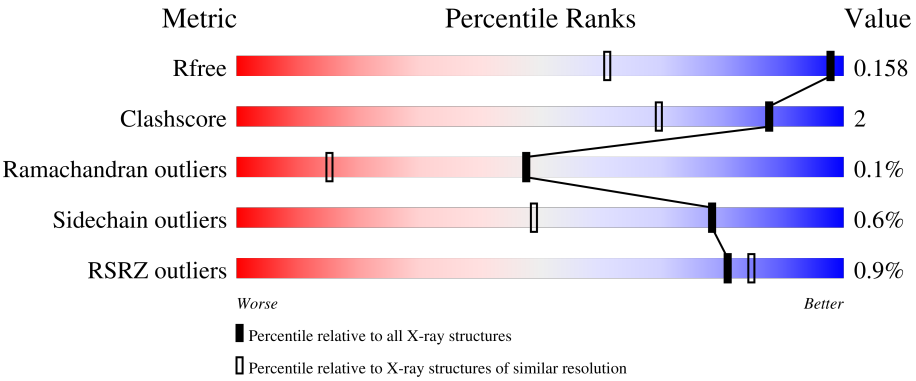
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.10 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	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	% 96% .
2	B	492	% 94% . .

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13099 atoms, of which 6111 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	4395	1420	2181	365	409	20	0	16	0

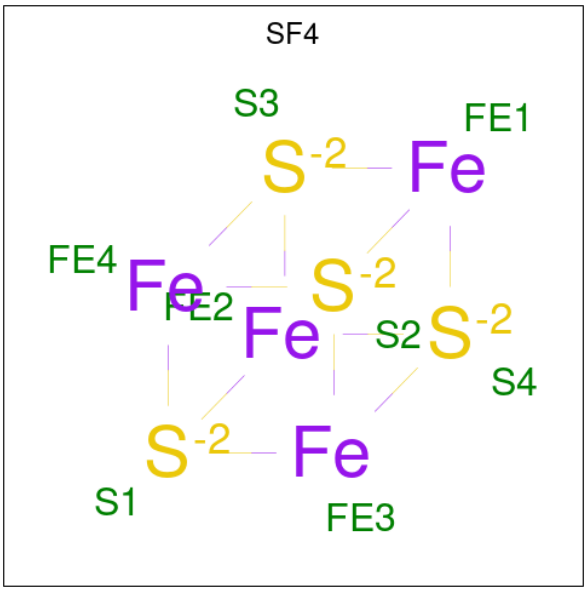
- Molecule 2 is a protein called Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
2	B	484	7798	2490	3913	667	703	22	3	0	24	0

There are 9 discrepancies between the modelled and reference sequences:

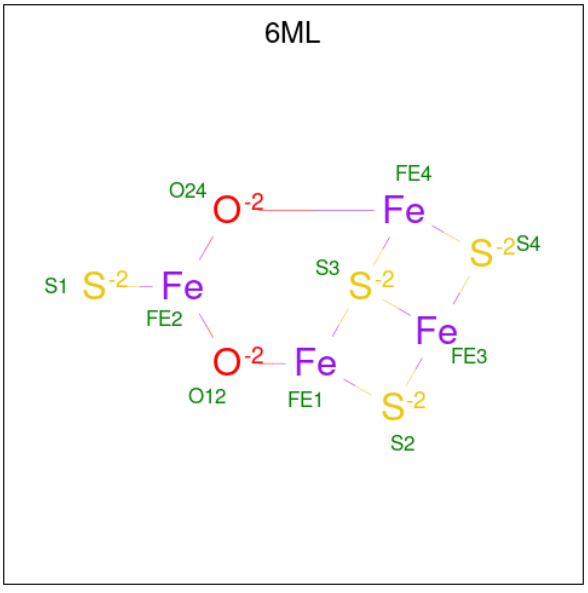
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	TRP	-	expression tag	UNP Q72AS3
B	5	SER	-	expression tag	UNP Q72AS3
B	6	HIS	-	expression tag	UNP Q72AS3
B	7	PRO	-	expression tag	UNP Q72AS3
B	8	GLN	-	expression tag	UNP Q72AS3
B	9	PHE	-	expression tag	UNP Q72AS3
B	10	GLU	-	expression tag	UNP Q72AS3
B	11	LYS	-	expression tag	UNP Q72AS3
B	50	THR	GLY	engineered mutation	UNP Q72AS3

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



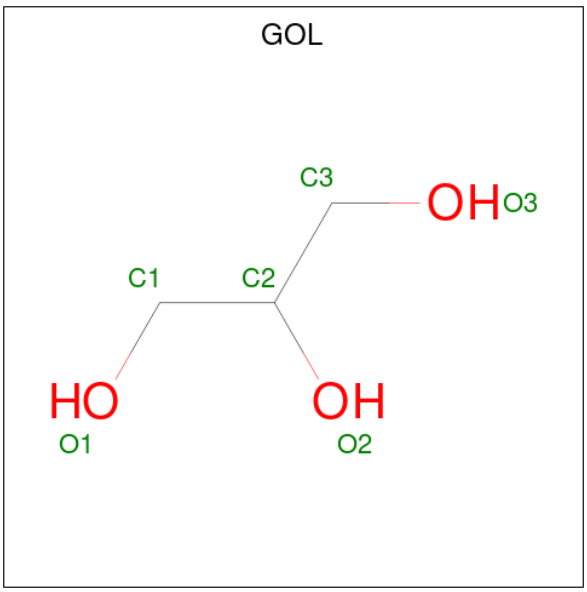
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	1

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



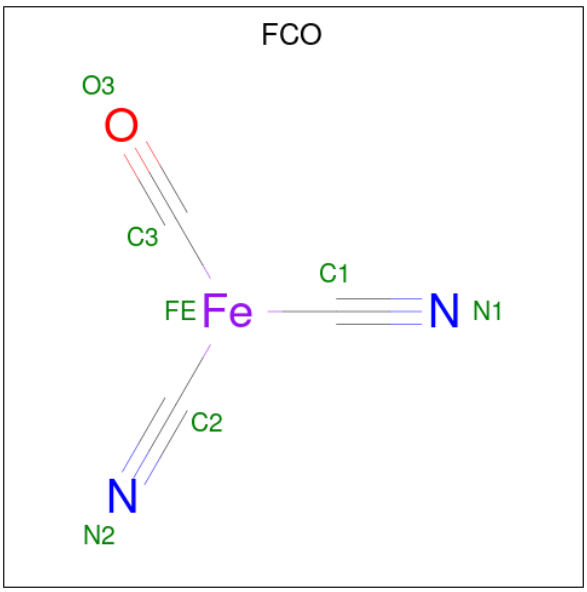
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe O S 10 4 2 4	0	1

- 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 11 3 5 3	0	1
5	B	1	Total C H O 13 3 7 3	0	0
5	B	1	Total C H O 11 3 5 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		

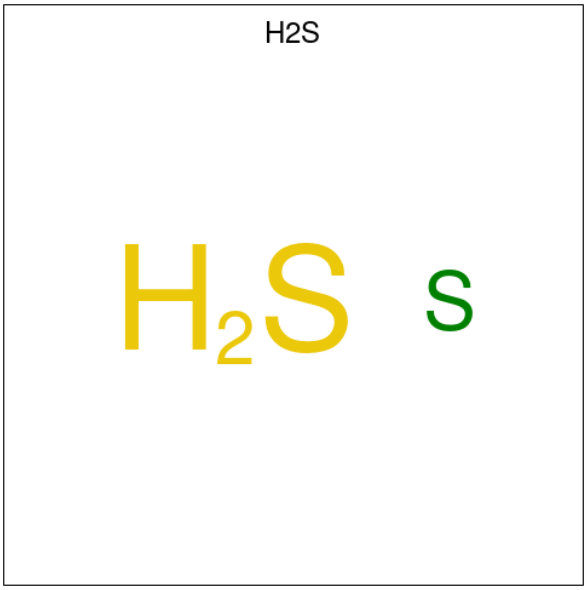
- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- 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
			1	1		

- 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		

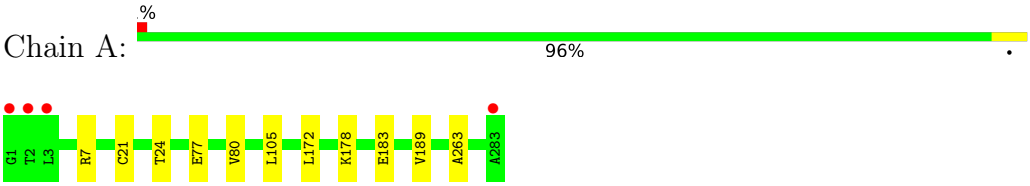
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	309	Total O 325 325	0	21
11	B	490	Total O 501 501	0	15

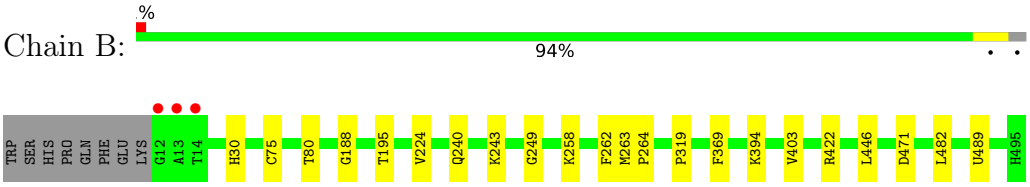
3 Residue-property plots (i)

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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.14Å 62.71Å 110.24Å 90.00° 105.11° 90.00°	Depositor
Resolution (Å)	45.38 – 1.10 45.38 – 1.10	Depositor EDS
% Data completeness (in resolution range)	79.8 (45.38-1.10) 93.3 (45.38-1.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 1.10Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.139 , 0.158 0.139 , 0.158	Depositor DCC
R_{free} test set	13323 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	11.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13099	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: 6ML, SEC, NI, H2S, FE2, FCO, GOL, CL, CSD, SF4

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	0.33	0/2307	0.56	0/3135
2	B	0.31	0/4009	0.58	0/5414
All	All	0.32	0/6316	0.57	0/8549

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	2214	2181	2191	7	0
2	B	3885	3913	3937	18	0
3	A	24	0	0	0	0
4	A	10	0	0	0	0
5	A	6	5	8	0	0
5	B	12	12	15	0	0
6	B	7	0	0	1	0
7	B	1	0	0	0	0
8	B	1	0	0	0	0
9	B	1	0	0	0	0
10	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	325	0	0	3	1
11	B	501	0	0	6	1
All	All	6988	6111	6151	25	2

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.

All (25) 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:183:GLU:OE1	11:A:401:HOH:O	1.76	1.02
1:A:7[A]:ARG:NH2	11:A:402:HOH:O	2.21	0.74
2:B:489[A]:SEC:SE	6:B:501:FCO:C1	2.85	0.74
2:B:30[B]:HIS:NE2	11:B:602:HOH:O	2.24	0.69
2:B:471[B]:ASP:OD2	11:B:601[B]:HOH:O	2.11	0.68
1:A:80:VAL:HG21	1:A:105[B]:LEU:CD1	2.27	0.64
2:B:258:LYS:NZ	11:B:606:HOH:O	2.33	0.61
1:A:80:VAL:HG21	1:A:105[B]:LEU:HD11	1.86	0.55
1:A:21[B]:CYS:HB2	1:A:77[B]:GLU:CD	2.32	0.55
2:B:30[B]:HIS:HD2	11:B:874:HOH:O	1.91	0.53
11:A:633[A]:HOH:O	2:B:30[A]:HIS:HD2	1.92	0.53
2:B:482:LEU:C	2:B:482:LEU:HD13	2.39	0.47
1:A:172[B]:LEU:HD23	1:A:189:VAL:HG22	1.97	0.46
2:B:394:LYS:HG3	11:B:628:HOH:O	2.16	0.45
2:B:422:ARG:CD	2:B:489[A]:SEC:SE	3.15	0.44
2:B:249:GLY:HA2	2:B:262:PHE:O	2.17	0.43
2:B:243:LYS:NZ	11:B:604:HOH:O	2.32	0.43
2:B:263[A]:MET:HE3	2:B:264:PRO:HD2	2.00	0.43
1:A:21[B]:CYS:O	1:A:24:THR:HG22	2.19	0.42
2:B:319:PRO:HG3	2:B:446:LEU:HG	2.02	0.42
2:B:240:GLN:HA	2:B:369:PHE:O	2.20	0.41
2:B:422:ARG:HD2	2:B:489[A]:SEC:SE	2.72	0.40
2:B:188:GLY:HA2	2:B:195:THR:OG1	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:503:HOH:O	11:A:583:HOH:O[2_658]	1.76	0.44
11:B:613:HOH:O	11:B:885:HOH:O[3_445]	1.88	0.32

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	297/283 (105%)	289 (97%)	7 (2%)	1 (0%)	36 13
2	B	501/492 (102%)	491 (98%)	10 (2%)	0	100 100
All	All	798/775 (103%)	780 (98%)	17 (2%)	1 (0%)	48 15

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	241/226 (107%)	240 (100%)	1 (0%)	84 60
2	B	413/400 (103%)	410 (99%)	3 (1%)	76 45
All	All	654/626 (104%)	650 (99%)	4 (1%)	78 49

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LYS
2	B	80	THR
2	B	224	VAL
2	B	403	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	180	ASN
1	A	261	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)

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[A]	2,7	3,7,8	1.29	0	1,8,10	2.15	1 (100%)

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[A]	2,7	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	75[A]	CSD	OD1-SG-CB	-2.15	101.44	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	75[A]	CSD	N-CA-CB-SG

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 12 ligands modelled in this entry, 3 are monoatomic and 1 is modelled with single atom - leaving 8 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[A]	-	5,5,5	1.04	0	5,5,5	0.80	0
6	FCO	B	501	2	1,6,6	2.06	1 (100%)	-		
5	GOL	B	506	-	5,5,5	1.61	1 (20%)	5,5,5	1.23	0
5	GOL	B	507	-	5,5,5	1.02	0	5,5,5	1.05	0
3	SF4	A	302	1	0,12,12	-	-	-		
3	SF4	A	301	1	0,12,12	-	-	-		
4	6ML	A	304[B]	1	0,12,12	-	-	-		

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	305[A]	-	-	3/4/4/4	-
4	6ML	A	304[B]	1	-	-	0/2/3/3
5	GOL	B	506	-	-	1/4/4/4	-
5	GOL	B	507	-	-	2/4/4/4	-
3	SF4	A	301	1	-	-	0/6/5/5
3	SF4	A	302	1	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	506	GOL	O3-C3	-2.70	1.31	1.42
6	B	501	FCO	O3-C3	-2.06	1.13	1.16

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	305[A]	GOL	C1-C2-C3-O3
5	B	506	GOL	O1-C1-C2-C3
5	B	507	GOL	O1-C1-C2-C3
5	B	507	GOL	O1-C1-C2-O2
5	A	305[A]	GOL	O2-C2-C3-O3
5	A	305[A]	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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, 95th 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%)	-0.39	4 (1%)	73	78	5, 13, 24, 38	21 (7%)
2	B	482/492 (97%)	-0.46	3 (0%)	85	88	6, 14, 21, 62	36 (7%)
All	All	765/775 (98%)	-0.43	7 (0%)	81	85	5, 13, 23, 62	57 (7%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	13	ALA	7.8
2	B	12	GLY	5.4
1	A	2	THR	3.4
1	A	3	LEU	2.9
2	B	14	THR	2.8
1	A	1	GLY	2.5
1	A	283	ALA	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, 95th 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[A]	8/9	0.99	0.04	9,12,14,14	3

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, 95th 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	44,46,55,55	0
5	GOL	B	506	6/6	0.87	0.13	30,37,41,44	0
5	GOL	A	305[A]	6/6	0.90	0.12	23,26,31,32	11
9	H2S	B	504[A]	1/1	0.99	0.03	13,13,13,13	1
3	SF4	A	301	8/8	1.00	0.01	10,10,11,12	0
3	SF4	A	302	8/8	1.00	0.01	9,9,9,10	0
3	SF4	A	303[A]	8/8	1.00	0.01	7,7,9,10	8
6	FCO	B	501	7/7	1.00	0.04	10,12,14,16	0
7	NI	B	502[A]	1/1	1.00	0.01	12,12,12,12	1
8	FE2	B	503	1/1	1.00	0.01	9,9,9,9	0
4	6ML	A	304[B]	10/10	1.00	0.03	8,8,9,9	10
10	CL	B	505	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.