



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 01:28 PM UTC

PDB ID : 6Z9G / pdb_00006z9g
Title : Structure of [NiFeSe] hydrogenase G491A variant from *Desulfovibrio vulgaris* Hildenborough pressurized with Oxygen gas - structure G491A-O2
Authors : Zacarias, S.; Temporao, A.; Carpentier, P.; van der Linden, P.; Pereira, I.A.C.; Matias, P.M.
Deposited on : 2020-06-03
Resolution : 1.76 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 ⓘ 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) : 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

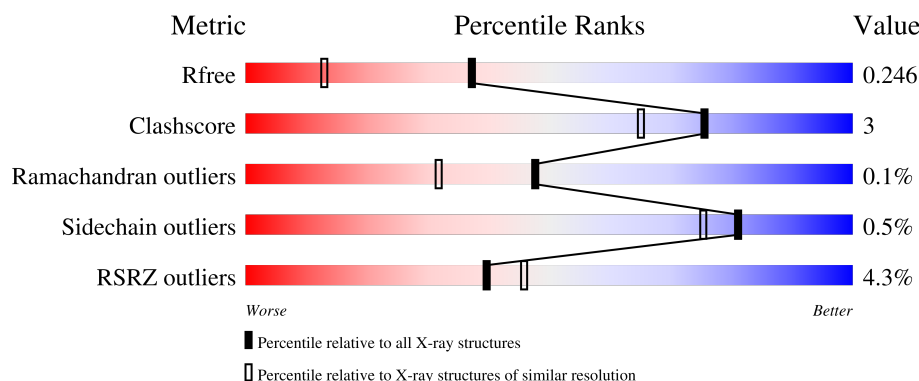
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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.



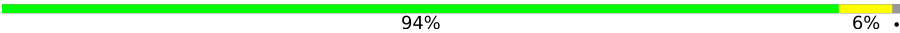
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	
1	C	283	
1	E	283	
1	G	283	
2	B	486	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	486	 94% 6% •
2	F	486	 93% 6% •
2	H	486	 88% 11% •

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
2	SEC	F	489[A]	-	-	X	-
5	FCO	D	500	-	-	X	-
5	FCO	H	500	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 47993 atoms, of which 23342 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
1	A	277	Total	C	H	N	O	S	0	5	0
			4158	1345	2051	350	392	20			
1	C	277	Total	C	H	N	O	S	0	5	0
			4160	1345	2053	350	392	20			
1	E	277	Total	C	H	N	O	S	0	5	0
			4160	1345	2053	350	392	20			
1	G	277	Total	C	H	N	O	S	0	5	0
			4160	1345	2053	350	392	20			

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	481	Total	C	H	N	O	S	Se	0	8	0
			7561	2411	3785	655	687	20	3			
2	D	481	Total	C	H	N	O	S	Se	0	7	0
			7550	2407	3780	655	685	20	3			
2	F	481	Total	C	H	N	O	S	Se	0	8	0
			7563	2411	3787	655	687	20	3			
2	H	481	Total	C	H	N	O	S	Se	0	7	0
			7550	2407	3780	655	685	20	3			

There are 4 discrepancies between the modelled and reference sequences:

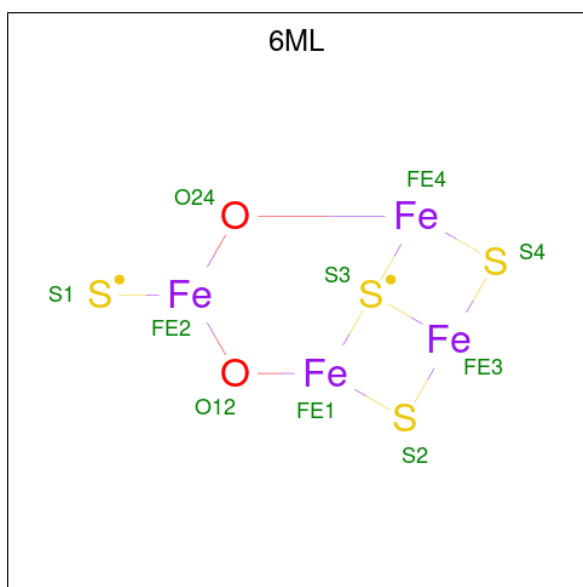
Chain	Residue	Modelled	Actual	Comment	Reference
B	491	ALA	GLY	engineered mutation	UNP Q72AS3
D	491	ALA	GLY	engineered mutation	UNP Q72AS3
F	491	ALA	GLY	engineered mutation	UNP Q72AS3
H	491	ALA	GLY	engineered mutation	UNP Q72AS3

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



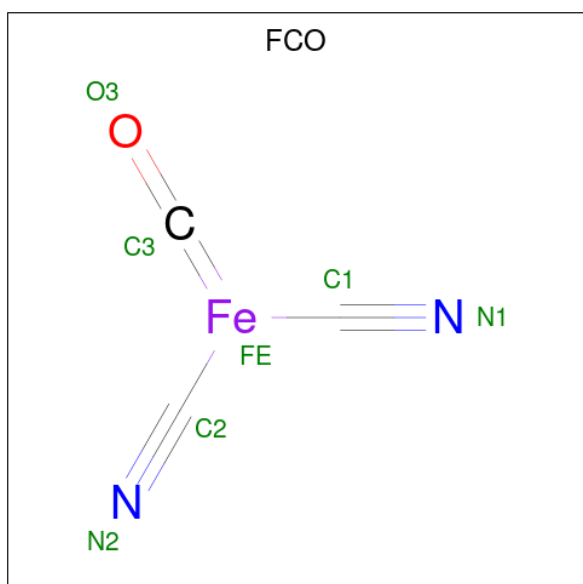
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	1
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	1
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3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

- Molecule 4 is oxygen-damaged SF4 (CCD ID: 6ML) (formula: Fe₄O₂S₄).



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		
4	E	1	Total	Fe	O	S	0	1
			10	4	2	4		
4	G	1	Total	Fe	O	S	0	1
			10	4	2	4		

- Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



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

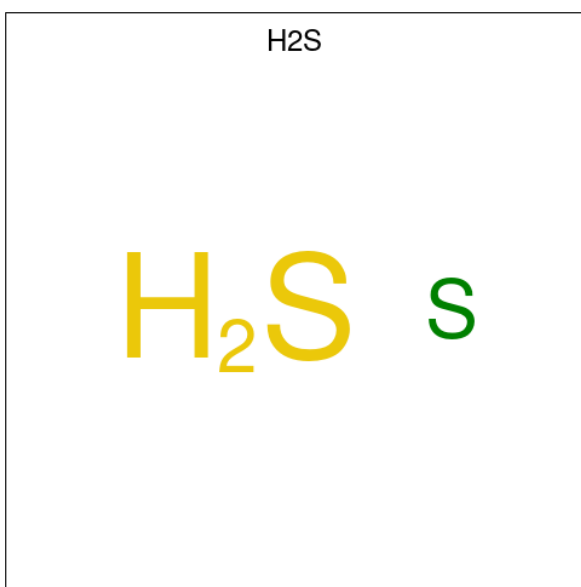
- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ni	0	1
			1	1		
6	D	1	Total	Ni	0	1
			1	1		
6	F	1	Total	Ni	0	1
			1	1		
6	H	1	Total	Ni	0	1
			1	1		

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Fe	0	0
			1	1		
7	D	1	Total	Fe	0	0
			1	1		
7	F	1	Total	Fe	0	0
			1	1		
7	H	1	Total	Fe	0	0
			1	1		

- Molecule 8 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total S 1 1	0	1
8	D	1	Total S 1 1	0	1
8	F	1	Total S 1 1	0	1
8	H	1	Total S 1 1	0	1

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0
9	D	1	Total Cl 1 1	0	0
9	F	1	Total Cl 1 1	0	0
9	H	1	Total Cl 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	80	Total O 81 81	0	2

Continued on next page...

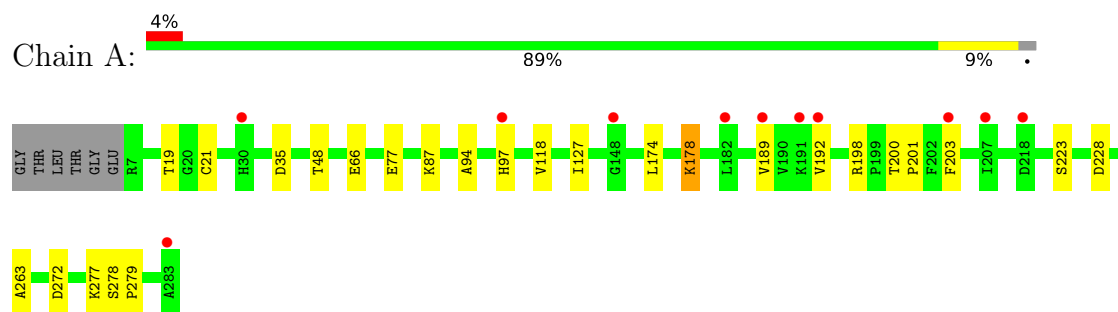
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	153	Total 154	O 154	0	1
10	C	96	Total 96	O 96	0	1
10	D	175	Total 177	O 177	0	2
10	E	101	Total 101	O 101	0	1
10	F	160	Total 161	O 161	0	1
10	G	81	Total 81	O 81	0	1
10	H	100	Total 100	O 100	0	0

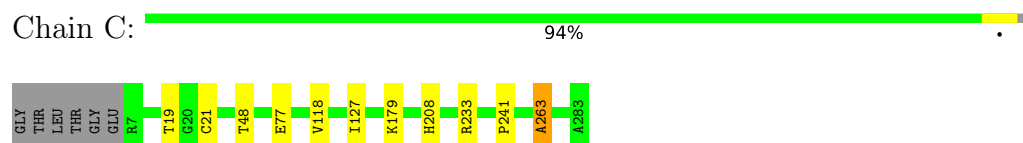
3 Residue-property plots [i](#)

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.

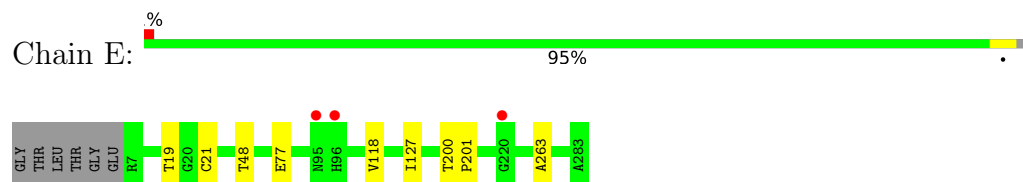
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit



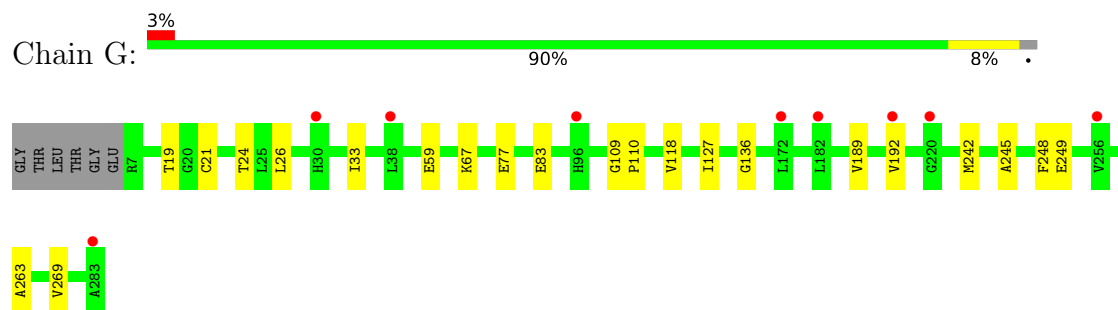
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit



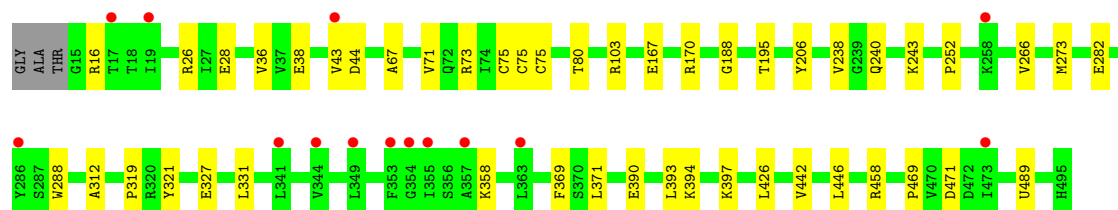
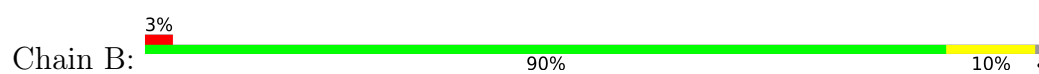
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit



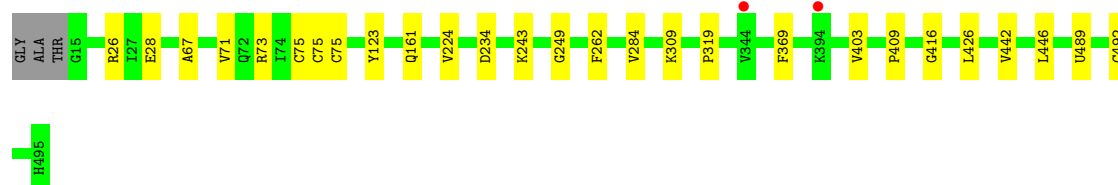
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit



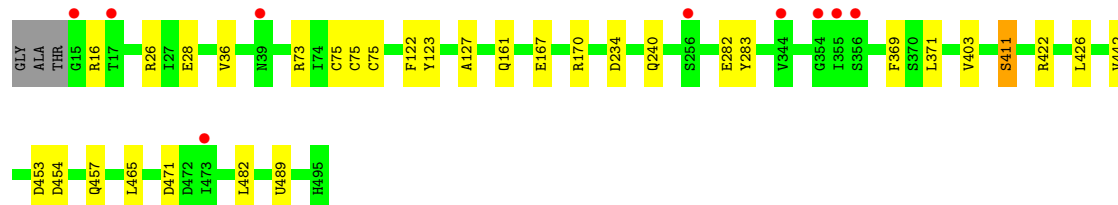
- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing



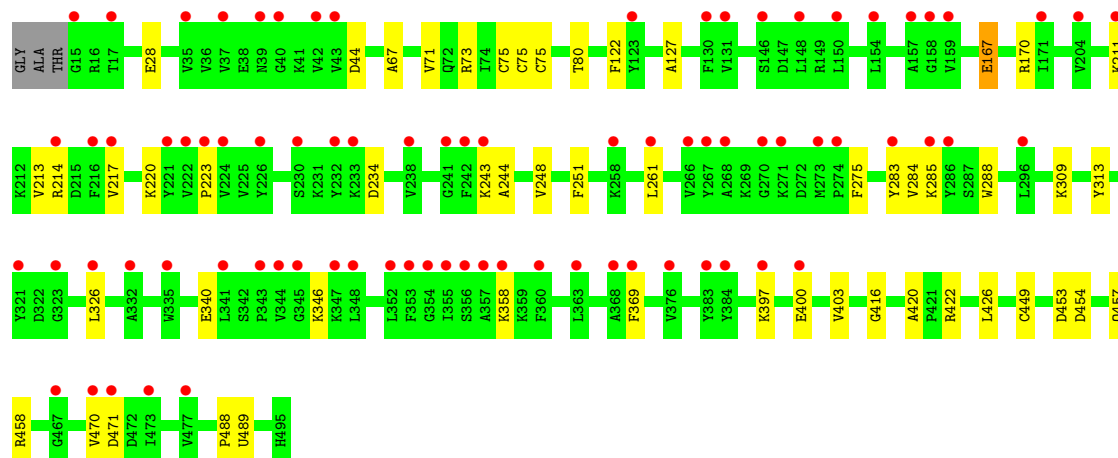
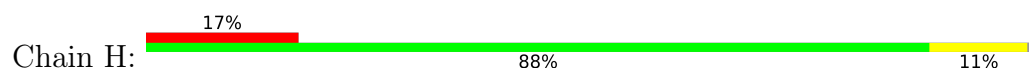
- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing



- 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, α , β , γ	120.31Å 93.81Å 126.95Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	61.20 – 1.76 61.20 – 1.76	Depositor EDS
% Data completeness (in resolution range)	70.3 (61.20-1.76) 70.3 (61.20-1.76)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.192 , 0.240 0.201 , 0.246	Depositor DCC
R_{free} test set	9499 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	47993	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.30 % 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 2.7936e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 6ML, FCO, CSD, OCS, FE2, NI, H2S, CL, SEC, 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	0.23	0/2174	0.46	0/2954
1	C	0.26	0/2174	0.47	0/2954
1	E	0.24	0/2174	0.47	0/2954
1	G	0.24	0/2174	0.47	0/2954
2	B	0.27	0/3863	0.48	0/5221
2	D	0.26	0/3854	0.49	0/5209
2	F	0.25	0/3863	0.47	0/5221
2	H	0.24	0/3853	0.46	0/5206
All	All	0.25	0/24129	0.47	0/32673

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	A	2107	2051	2046	16	2
1	C	2107	2053	2046	8	0
1	E	2107	2053	2046	6	0
1	G	2107	2053	2046	14	0
2	B	3776	3785	3773	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3770	3780	3767	16	0
2	F	3776	3787	3773	25	0
2	H	3770	3780	3767	31	2
3	A	24	0	0	0	0
3	C	24	0	0	0	0
3	E	24	0	0	0	0
3	G	24	0	0	0	0
4	A	10	0	0	0	0
4	C	10	0	0	0	0
4	E	10	0	0	0	0
4	G	10	0	0	1	0
5	B	7	0	0	1	0
5	D	7	0	0	2	0
5	F	7	0	0	1	0
5	H	7	0	0	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
10	A	81	0	0	4	0
10	B	154	0	0	2	0
10	C	96	0	0	1	0
10	D	177	0	0	0	0
10	E	101	0	0	2	0
10	F	161	0	0	1	0
10	G	81	0	0	2	0
10	H	100	0	0	1	0
All	All	24651	23342	23264	136	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 3.

The worst 5 of 136 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:G:77[B]:GLU:OE1	10:G:401[B]:HOH:O	1.71	1.04
1:A:77[B]:GLU:OE1	10:A:401[B]:HOH:O	1.78	0.99
1:E:77[B]:GLU:OE1	10:E:401[B]:HOH:O	1.88	0.91
1:C:77[B]:GLU:OE1	10:C:401[B]:HOH:O	1.97	0.81
2:F:282:GLU:OE1	10:F:601:HOH:O	2.04	0.75

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)
1:A:200:THR:OG1	2:H:285:LYS:NZ[1_455]	1.96	0.24
1:A:200:THR:OG1	2:H:285:LYS:HZ2[1_455]	1.60	0.00

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	280/283 (99%)	268 (96%)	11 (4%)	1 (0%)	30	15
1	C	280/283 (99%)	269 (96%)	10 (4%)	1 (0%)	30	15
1	E	280/283 (99%)	270 (96%)	9 (3%)	1 (0%)	30	15
1	G	280/283 (99%)	270 (96%)	9 (3%)	1 (0%)	30	15
2	B	483/486 (99%)	473 (98%)	10 (2%)	0	100	100
2	D	482/486 (99%)	472 (98%)	10 (2%)	0	100	100
2	F	483/486 (99%)	474 (98%)	9 (2%)	0	100	100
2	H	482/486 (99%)	471 (98%)	11 (2%)	0	100	100
All	All	3050/3076 (99%)	2967 (97%)	79 (3%)	4 (0%)	48	32

All (4) Ramachandran outliers are listed below:

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

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	A	227/226 (100%)	226 (100%)	1 (0%)	84	80
1	C	227/226 (100%)	227 (100%)	0	100	100
1	E	227/226 (100%)	227 (100%)	0	100	100
1	G	227/226 (100%)	225 (99%)	2 (1%)	70	60
2	B	397/392 (101%)	394 (99%)	3 (1%)	73	64
2	D	396/392 (101%)	394 (100%)	2 (0%)	81	75
2	F	397/392 (101%)	395 (100%)	2 (0%)	81	75
2	H	396/392 (101%)	393 (99%)	3 (1%)	73	64
All	All	2494/2472 (101%)	2481 (100%)	13 (0%)	81	75

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	411	SER
1	G	242[A]	MET
2	H	403	VAL
2	H	80	THR
2	H	167	GLU

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	F	260	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	457	GLN
2	B	161	GLN
2	B	474	GLN
1	C	30	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

16 non-standard protein/DNA/RNA residues are 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	OCS	H	75[B]	2	2,7,9	1.07	0	2,8,13	3.14	2 (100%)
2	CSD	D	75[B]	2	4,7,8	2.43	2 (50%)	1,8,10	1.82	0
2	CSD	B	75[B]	2	4,7,8	2.44	2 (50%)	1,8,10	2.11	1 (100%)
2	CSD	F	75[B]	2	4,7,8	2.63	2 (50%)	1,8,10	1.86	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	OCS	H	75[B]	2	-	0/3/6/9	-
2	CSD	D	75[B]	2	-	1/2/6/8	-
2	CSD	B	75[B]	2	-	1/2/6/8	-
2	CSD	F	75[B]	2	-	2/2/6/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	75[B]	CSD	OD1-SG	-4.49	1.43	1.47
2	D	75[B]	CSD	OD1-SG	-4.03	1.44	1.47
2	B	75[B]	CSD	OD1-SG	-4.03	1.44	1.47
2	F	75[B]	CSD	CB-SG	-2.35	1.66	1.79
2	D	75[B]	CSD	CB-SG	-2.34	1.66	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	75[B]	OCS	OD1-SG-CB	3.45	110.31	105.35
2	H	75[B]	OCS	OD3-SG-CB	2.81	109.39	105.35
2	B	75[B]	CSD	OD1-SG-CB	2.11	109.49	105.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	75[B]	CSD	N-CA-CB-SG
2	D	75[B]	CSD	N-CA-CB-SG
2	F	75[B]	CSD	CA-CB-SG-OD1
2	F	75[B]	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 36 ligands modelled in this entry, 12 are monoatomic and 4 are modelled with single atom - leaving 20 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	G	301	1	0,12,12	-	-	-		
3	SF4	C	301	1	0,12,12	-	-	-		
5	FCO	H	500	2	0,6,6	-	-	-		
3	SF4	A	302	1	0,12,12	-	-	-		
3	SF4	E	303[A]	1	0,12,12	-	-	-		
3	SF4	C	303[A]	1	0,12,12	-	-	-		
3	SF4	A	303[A]	1	0,12,12	-	-	-		
4	6ML	E	304[B]	1	0,12,12	-	-	-		
3	SF4	A	301	1	0,12,12	-	-	-		
3	SF4	C	302	1	0,12,12	-	-	-		
4	6ML	G	304[B]	1	0,12,12	-	-	-		
5	FCO	D	500	2	0,6,6	-	-	-		
5	FCO	F	500	2	0,6,6	-	-	-		
3	SF4	G	302	1	0,12,12	-	-	-		
5	FCO	B	500	2	0,6,6	-	-	-		
4	6ML	A	304[B]	1	0,12,12	-	-	-		
4	6ML	C	304[B]	1	0,12,12	-	-	-		
3	SF4	G	303[A]	1	0,12,12	-	-	-		
3	SF4	E	301	1	0,12,12	-	-	-		
3	SF4	E	302	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	301	1	-	-	0/6/5/5
4	6ML	A	304[B]	1	-	-	0/2/3/3
3	SF4	G	301	1	-	-	0/6/5/5
3	SF4	C	302	1	-	-	0/6/5/5
3	SF4	A	303[A]	1	-	-	0/6/5/5
4	6ML	E	304[B]	1	-	-	0/2/3/3
4	6ML	G	304[B]	1	-	-	0/2/3/3
4	6ML	C	304[B]	1	-	-	0/2/3/3
3	SF4	G	303[A]	1	-	-	0/6/5/5
3	SF4	C	301	1	-	-	0/6/5/5
3	SF4	G	302	1	-	-	0/6/5/5
3	SF4	A	302	1	-	-	0/6/5/5
3	SF4	E	303[A]	1	-	-	0/6/5/5
3	SF4	C	303[A]	1	-	-	0/6/5/5
3	SF4	E	301	1	-	-	0/6/5/5
3	SF4	E	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.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	500	FCO	2	0
4	G	304[B]	6ML	1	0
5	D	500	FCO	2	0
5	F	500	FCO	1	0
5	B	500	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	277/283 (97%)	0.44	11 (3%) 42 48	8, 30, 51, 73	6 (2%)
1	C	277/283 (97%)	-0.18	0 100 100	6, 22, 41, 68	7 (2%)
1	E	277/283 (97%)	-0.06	3 (1%) 78 83	7, 23, 45, 68	7 (2%)
1	G	277/283 (97%)	0.25	9 (3%) 50 57	9, 26, 51, 70	9 (3%)
2	B	479/486 (98%)	0.25	14 (2%) 53 60	10, 28, 49, 86	5 (1%)
2	D	479/486 (98%)	-0.18	2 (0%) 88 91	9, 24, 43, 73	8 (1%)
2	F	479/486 (98%)	0.03	9 (1%) 66 73	8, 26, 49, 81	7 (1%)
2	H	479/486 (98%)	0.89	81 (16%) 4 4	11, 38, 66, 104	6 (1%)
All	All	3024/3076 (98%)	0.20	129 (4%) 40 46	6, 27, 53, 104	55 (1%)

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	368	ALA	5.5
2	H	15	GLY	5.4
2	H	323	GLY	4.9
1	A	192	VAL	4.4
2	H	355	ILE	4.4

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	SEC	H	489[A]	6/7	0.96	0.12	30,36,37,39	6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SEC	H	489[B]	6/7	0.96	0.12	27,36,37,40	6
2	SEC	H	489[C]	6/7	0.96	0.12	30,36,37,40	6
2	SEC	F	489[A]	6/7	0.97	0.11	22,24,26,26	6
2	SEC	F	489[B]	6/7	0.97	0.11	20,24,25,26	6
2	SEC	F	489[C]	6/7	0.97	0.11	22,24,25,26	6
2	SEC	D	489[A]	6/7	0.97	0.08	20,22,23,24	6
2	SEC	D	489[B]	6/7	0.97	0.08	17,22,23,24	6
2	SEC	D	489[C]	6/7	0.97	0.08	20,22,23,24	6
2	SEC	B	489[A]	6/7	0.99	0.07	18,21,22,24	6
2	SEC	B	489[B]	6/7	0.99	0.07	14,21,22,22	6
2	SEC	B	489[C]	6/7	0.99	0.07	19,21,22,22	6
2	CSD	B	75[B]	8/9	-	-	9,14,20,20	12
2	CSD	D	75[B]	8/9	-	-	9,12,18,21	12
2	CSD	F	75[B]	8/9	-	-	10,13,20,20	12
2	OCS	H	75[B]	8/10	-	-	13,18,27,27	12

6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	SF4	A	301	8/8	0.96	0.06	17,22,25,26	0
6	NI	D	501[A]	1/1	0.96	0.04	19,19,19,19	1
3	SF4	G	301	8/8	0.97	0.05	16,19,25,27	0
3	SF4	E	301	8/8	0.97	0.05	16,18,21,24	0
6	NI	F	501[A]	1/1	0.97	0.04	21,21,21,21	1
8	H2S	B	503[A]	1/1	0.97	0.04	11,11,11,11	1
8	H2S	D	503[A]	1/1	0.97	0.04	10,10,10,10	1
8	H2S	F	503[A]	1/1	0.97	0.04	11,11,11,11	1
8	H2S	H	503[A]	1/1	0.97	0.05	21,21,21,21	1
3	SF4	G	302	8/8	0.98	0.03	13,15,16,17	0
3	SF4	G	303[A]	8/8	0.98	0.04	10,13,19,22	8
6	NI	B	501[A]	1/1	0.98	0.05	18,18,18,18	1
3	SF4	C	301	8/8	0.98	0.04	18,20,24,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SF4	C	302	8/8	0.98	0.03	14,14,15,16	0
3	SF4	C	303[A]	8/8	0.98	0.04	9,10,12,15	8
3	SF4	A	302	8/8	0.98	0.04	11,15,19,20	0
3	SF4	E	303[A]	8/8	0.98	0.04	7,10,14,14	8
3	SF4	A	303[A]	8/8	0.98	0.03	11,12,14,15	8
5	FCO	F	500	7/7	0.99	0.06	8,16,19,20	0
5	FCO	H	500	7/7	0.99	0.06	14,19,25,28	0
3	SF4	E	302	8/8	0.99	0.02	10,13,15,19	0
4	6ML	A	304[B]	10/10	0.99	0.04	9,11,15,15	10
4	6ML	C	304[B]	10/10	0.99	0.04	7,10,10,13	10
6	NI	H	501[A]	1/1	0.99	0.05	22,22,22,22	1
7	FE2	B	502	1/1	0.99	0.02	18,18,18,18	0
7	FE2	D	502	1/1	0.99	0.02	12,12,12,12	0
7	FE2	F	502	1/1	0.99	0.02	16,16,16,16	0
7	FE2	H	502	1/1	0.99	0.03	22,22,22,22	0
4	6ML	E	304[B]	10/10	0.99	0.04	7,9,10,14	10
4	6ML	G	304[B]	10/10	0.99	0.03	11,13,17,19	10
5	FCO	B	500	7/7	0.99	0.03	6,11,14,15	0
5	FCO	D	500	7/7	0.99	0.04	8,12,17,19	0
9	CL	B	504	1/1	0.99	0.03	10,10,10,10	0
9	CL	D	504	1/1	0.99	0.03	11,11,11,11	0
9	CL	H	504	1/1	0.99	0.07	18,18,18,18	0
9	CL	F	504	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.