



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:22 PM UTC

PDB ID : 4UEQ / pdb_00004ueq
Title : Structure of the V74C large subunit mutant of D. fructosovorans NiFe- hydrogenase
Authors : Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.
Deposited on : 2014-12-18
Resolution : 1.70 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 ⓘ 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

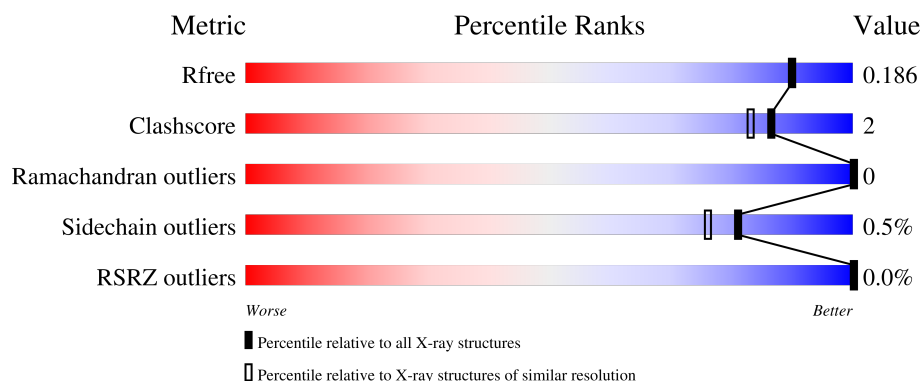
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

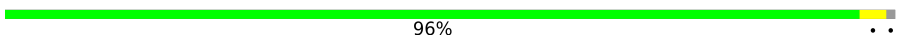
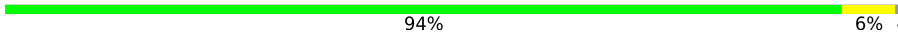
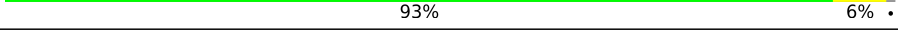
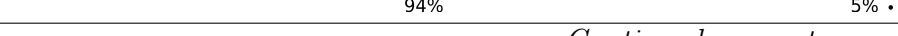
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	264	 96%
1	B	264	 94% 6%
1	C	264	 91% 7%
1	D	264	 93% 6%
1	E	264	 94% 5%

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Mol	Chain	Length	Quality of chain
1	F	264	 92% 6% .
2	Q	564	 91% 5% .
2	R	564	 91% 6% .
2	S	564	 92% . .
2	T	564	 92% 5% .
2	U	564	 93% . .
2	V	564	 92% . .

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 40973 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	2	0
			1982	1262	331	374	15			
1	B	262	Total	C	N	O	S	0	8	0
			2007	1279	334	379	15			
1	C	261	Total	C	N	O	S	0	2	0
			1977	1259	330	373	15			
1	D	262	Total	C	N	O	S	0	1	0
			1978	1259	330	374	15			
1	E	262	Total	C	N	O	S	0	6	0
			2001	1273	333	380	15			
1	F	261	Total	C	N	O	S	0	3	0
			1988	1266	333	374	15			

- Molecule 2 is a protein called NICKEL-DEPENDENT HYDROGENASE LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	21	0
			4238	2700	730	775	33			
2	R	545	Total	C	N	O	S	0	15	0
			4220	2687	729	771	33			
2	S	544	Total	C	N	O	S	0	11	0
			4205	2677	727	769	32			
2	T	544	Total	C	N	O	S	0	22	0
			4248	2706	732	776	34			
2	U	545	Total	C	N	O	S	0	15	0
			4221	2687	729	772	33			
2	V	544	Total	C	N	O	S	0	13	0
			4211	2679	726	774	32			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	expression tag	UNP E1K247
Q	-12	SER	-	expression tag	UNP E1K247
Q	-11	TRP	-	expression tag	UNP E1K247
Q	-10	SER	-	expression tag	UNP E1K247
Q	-9	HIS	-	expression tag	UNP E1K247
Q	-8	PRO	-	expression tag	UNP E1K247
Q	-7	GLN	-	expression tag	UNP E1K247
Q	-6	PHE	-	expression tag	UNP E1K247
Q	-5	GLU	-	expression tag	UNP E1K247
Q	-4	LYS	-	expression tag	UNP E1K247
Q	-3	GLY	-	expression tag	UNP E1K247
Q	-2	ALA	-	expression tag	UNP E1K247
Q	-1	SER	-	expression tag	UNP E1K247
Q	0	GLY	-	expression tag	UNP E1K247
Q	1	ALA	-	expression tag	UNP E1K247
Q	74	CYS	VAL	engineered mutation	UNP E1K247
R	-13	ALA	-	expression tag	UNP E1K247
R	-12	SER	-	expression tag	UNP E1K247
R	-11	TRP	-	expression tag	UNP E1K247
R	-10	SER	-	expression tag	UNP E1K247
R	-9	HIS	-	expression tag	UNP E1K247
R	-8	PRO	-	expression tag	UNP E1K247
R	-7	GLN	-	expression tag	UNP E1K247
R	-6	PHE	-	expression tag	UNP E1K247
R	-5	GLU	-	expression tag	UNP E1K247
R	-4	LYS	-	expression tag	UNP E1K247
R	-3	GLY	-	expression tag	UNP E1K247
R	-2	ALA	-	expression tag	UNP E1K247
R	-1	SER	-	expression tag	UNP E1K247
R	0	GLY	-	expression tag	UNP E1K247
R	1	ALA	-	expression tag	UNP E1K247
R	74	CYS	VAL	engineered mutation	UNP E1K247
S	-13	ALA	-	expression tag	UNP E1K247
S	-12	SER	-	expression tag	UNP E1K247
S	-11	TRP	-	expression tag	UNP E1K247
S	-10	SER	-	expression tag	UNP E1K247
S	-9	HIS	-	expression tag	UNP E1K247
S	-8	PRO	-	expression tag	UNP E1K247
S	-7	GLN	-	expression tag	UNP E1K247
S	-6	PHE	-	expression tag	UNP E1K247
S	-5	GLU	-	expression tag	UNP E1K247
S	-4	LYS	-	expression tag	UNP E1K247
S	-3	GLY	-	expression tag	UNP E1K247

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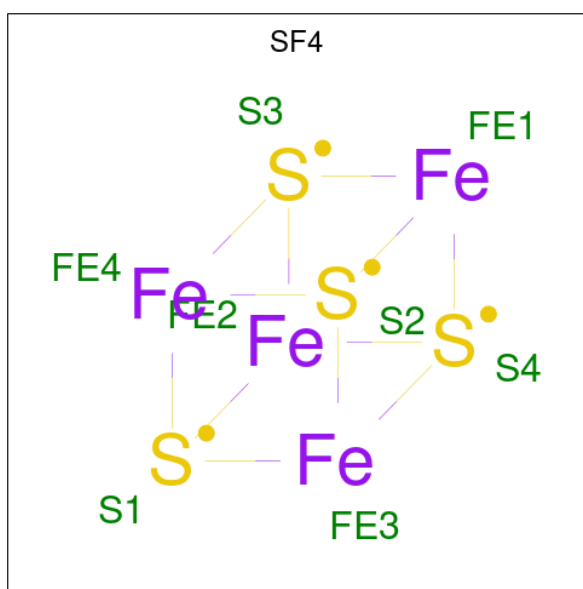
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S	-2	ALA	-	expression tag	UNP E1K247
S	-1	SER	-	expression tag	UNP E1K247
S	0	GLY	-	expression tag	UNP E1K247
S	1	ALA	-	expression tag	UNP E1K247
S	74	CYS	VAL	engineered mutation	UNP E1K247
T	-13	ALA	-	expression tag	UNP E1K247
T	-12	SER	-	expression tag	UNP E1K247
T	-11	TRP	-	expression tag	UNP E1K247
T	-10	SER	-	expression tag	UNP E1K247
T	-9	HIS	-	expression tag	UNP E1K247
T	-8	PRO	-	expression tag	UNP E1K247
T	-7	GLN	-	expression tag	UNP E1K247
T	-6	PHE	-	expression tag	UNP E1K247
T	-5	GLU	-	expression tag	UNP E1K247
T	-4	LYS	-	expression tag	UNP E1K247
T	-3	GLY	-	expression tag	UNP E1K247
T	-2	ALA	-	expression tag	UNP E1K247
T	-1	SER	-	expression tag	UNP E1K247
T	0	GLY	-	expression tag	UNP E1K247
T	1	ALA	-	expression tag	UNP E1K247
T	74	CYS	VAL	engineered mutation	UNP E1K247
U	-13	ALA	-	expression tag	UNP E1K247
U	-12	SER	-	expression tag	UNP E1K247
U	-11	TRP	-	expression tag	UNP E1K247
U	-10	SER	-	expression tag	UNP E1K247
U	-9	HIS	-	expression tag	UNP E1K247
U	-8	PRO	-	expression tag	UNP E1K247
U	-7	GLN	-	expression tag	UNP E1K247
U	-6	PHE	-	expression tag	UNP E1K247
U	-5	GLU	-	expression tag	UNP E1K247
U	-4	LYS	-	expression tag	UNP E1K247
U	-3	GLY	-	expression tag	UNP E1K247
U	-2	ALA	-	expression tag	UNP E1K247
U	-1	SER	-	expression tag	UNP E1K247
U	0	GLY	-	expression tag	UNP E1K247
U	1	ALA	-	expression tag	UNP E1K247
U	74	CYS	VAL	engineered mutation	UNP E1K247
V	-13	ALA	-	expression tag	UNP E1K247
V	-12	SER	-	expression tag	UNP E1K247
V	-11	TRP	-	expression tag	UNP E1K247
V	-10	SER	-	expression tag	UNP E1K247
V	-9	HIS	-	expression tag	UNP E1K247

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-8	PRO	-	expression tag	UNP E1K247
V	-7	GLN	-	expression tag	UNP E1K247
V	-6	PHE	-	expression tag	UNP E1K247
V	-5	GLU	-	expression tag	UNP E1K247
V	-4	LYS	-	expression tag	UNP E1K247
V	-3	GLY	-	expression tag	UNP E1K247
V	-2	ALA	-	expression tag	UNP E1K247
V	-1	SER	-	expression tag	UNP E1K247
V	0	GLY	-	expression tag	UNP E1K247
V	1	ALA	-	expression tag	UNP E1K247
V	74	CYS	VAL	engineered mutation	UNP E1K247
Q	543	CSS	CYS	microheterogeneity	UNP E1K247
R	543	CSS	CYS	microheterogeneity	UNP E1K247
S	543	CSS	CYS	microheterogeneity	UNP E1K247
T	543	CSS	CYS	microheterogeneity	UNP E1K247
U	543	CSS	CYS	microheterogeneity	UNP E1K247
V	543	CSS	CYS	microheterogeneity	UNP E1K247

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



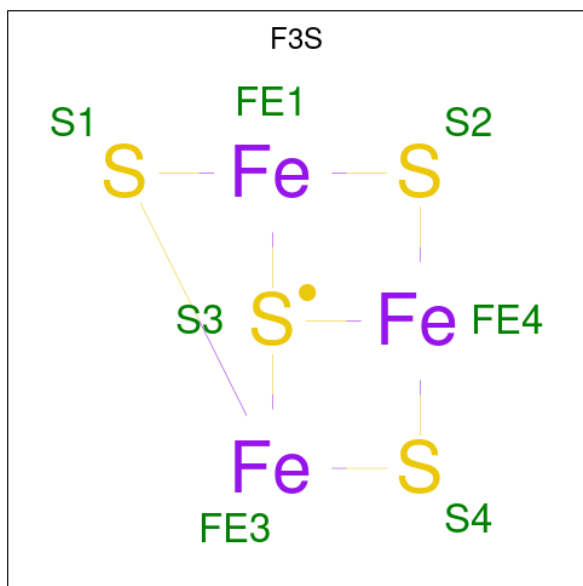
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	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	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	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	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



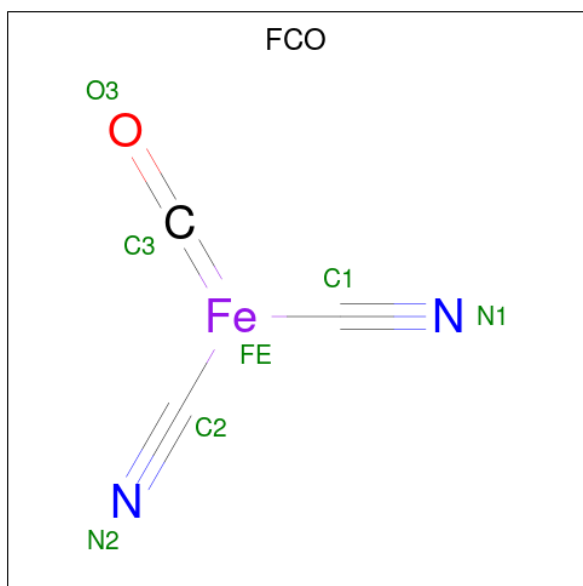
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	Fe	S	0	0
			7	3	4		
4	D	1	Total	Fe	S	0	0
			7	3	4		
4	E	1	Total	Fe	S	0	0
			7	3	4		
4	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O).

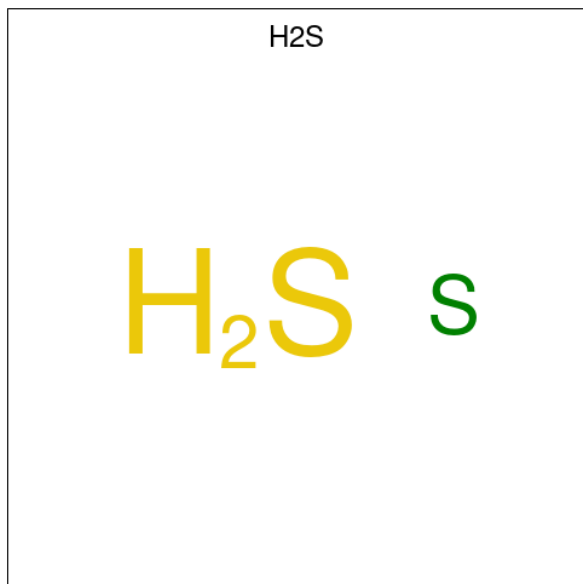


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	Q	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	R	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	S	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	T	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	U	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	V	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Q	1	Total Ni 2 2	0	1
6	R	1	Total Ni 2 2	0	1
6	S	1	Total Ni 2 2	0	1
6	T	1	Total Ni 2 2	0	1
6	U	1	Total Ni 2 2	0	1
6	V	1	Total Ni 2 2	0	1

- Molecule 7 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Q	1	Total S 1 1	0	1
7	R	1	Total S 1 1	0	1
7	S	1	Total S 1 1	0	1
7	T	1	Total S 1 1	0	1
7	U	1	Total S 1 1	0	1
7	V	1	Total S 1 1	0	1

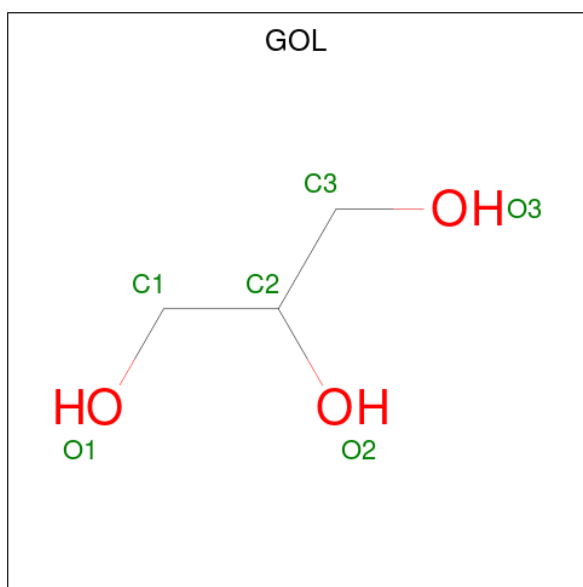
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	Q	2	Total 2	Mg 2	0	1
8	R	2	Total 2	Mg 2	0	1
8	S	1	Total 1	Mg 1	0	1
8	T	2	Total 2	Mg 2	0	1
8	U	2	Total 2	Mg 2	0	1
8	V	1	Total 1	Mg 1	0	1

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

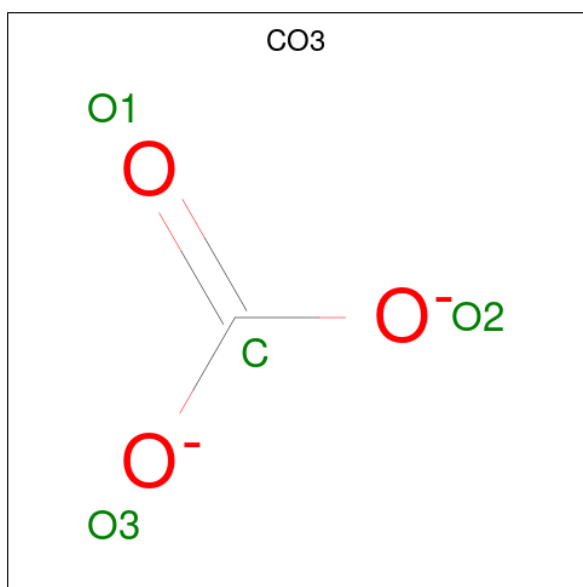
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	Q	1	Total 1	Ca 1	0	1
9	R	1	Total 1	Ca 1	0	1
9	S	1	Total 1	Ca 1	0	1
9	T	1	Total 1	Ca 1	0	1
9	U	1	Total 1	Ca 1	0	1
9	V	1	Total 1	Ca 1	0	1

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	Q	1	Total	C	O	0	0
			6	3	3		
10	Q	1	Total	C	O	0	0
			6	3	3		
10	R	1	Total	C	O	0	0
			6	3	3		
10	R	1	Total	C	O	0	0
			6	3	3		
10	S	1	Total	C	O	0	0
			6	3	3		
10	T	1	Total	C	O	0	0
			6	3	3		
10	T	1	Total	C	O	0	0
			6	3	3		
10	U	1	Total	C	O	0	0
			6	3	3		
10	U	1	Total	C	O	0	0
			6	3	3		
10	V	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	V	1	Total	C	O	0	0
			4	1	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	298	Total	O	0	7
			301	301		
12	B	198	Total	O	0	0
			198	198		
12	C	226	Total	O	0	2
			226	226		
12	D	297	Total	O	0	7
			299	299		
12	E	204	Total	O	0	2
			204	204		
12	F	209	Total	O	0	0
			209	209		
12	Q	396	Total	O	0	5
			398	398		
12	R	345	Total	O	0	4
			345	345		
12	S	247	Total	O	0	6
			247	247		
12	T	401	Total	O	0	10
			401	401		
12	U	348	Total	O	0	5
			349	349		

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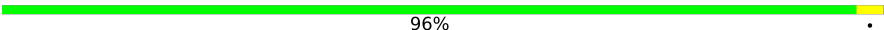
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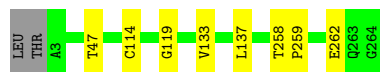
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	V	241	Total	O	0	3
			242	242		

3 Residue-property plots [i](#)

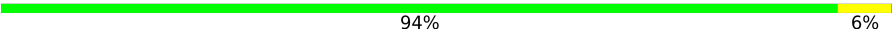
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain A:  96%



- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain B:  94% 6%

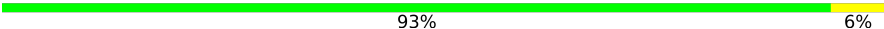


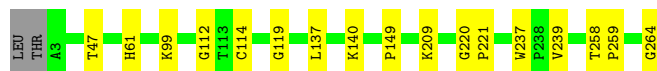
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain C:  91% 7%



- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain D:  93% 6%



- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain E:  94% 5%



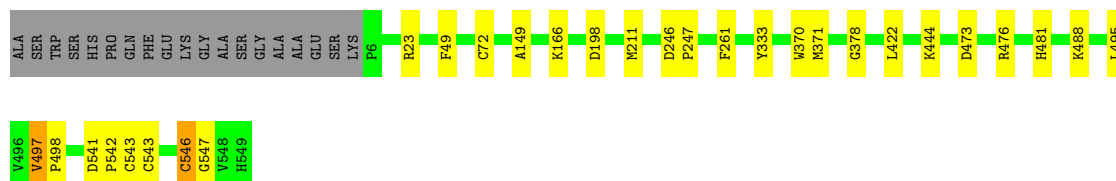
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain F:  92% 6%



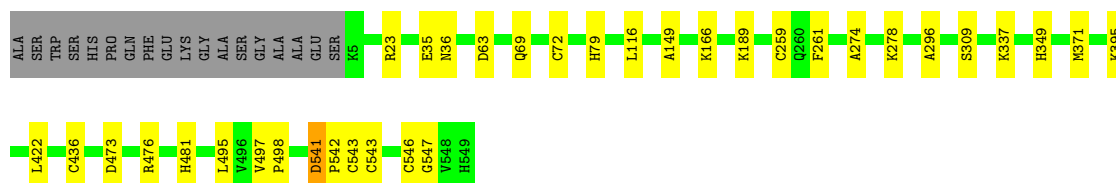
- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain Q:  91% 5%



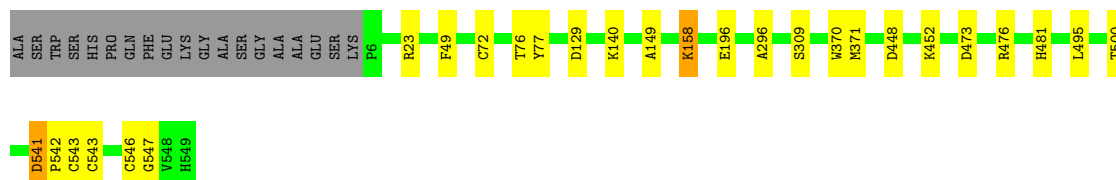
- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain R:  91% 6%

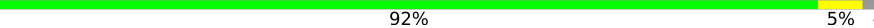


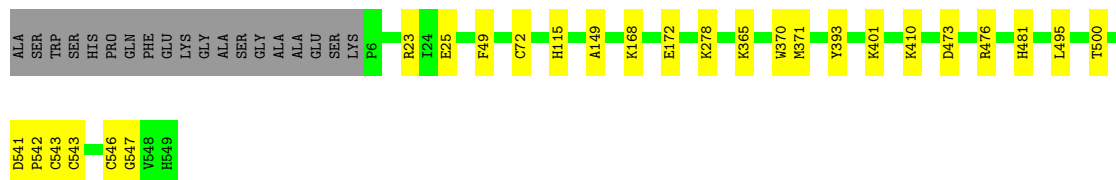
- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain S:  92%

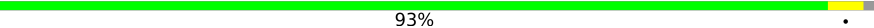


- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain T:  92% 5%



- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

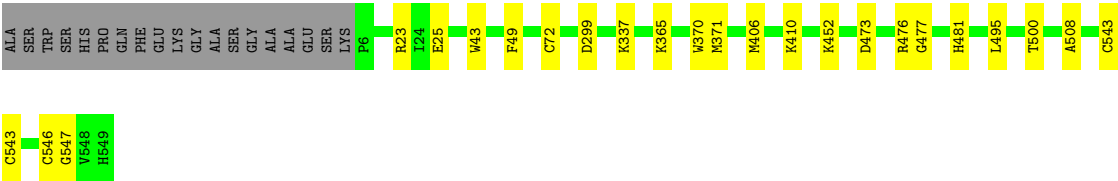
Chain U:  93%



● Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain V:

92%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.72Å 99.80Å 190.80Å 90.21° 98.61° 90.11°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	85.0 (20.00-1.70) 85.0 (20.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.137 , 0.185 0.137 , 0.186	Depositor DCC
R_{free} test set	20976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-h-l 0.439 for -h,k,-l 0.054 for -h,-k,h+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	40973	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CSS, F3S, MG, FCO, H2S, GOL, NI, CA, CO3, 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	0.82	0/2045	0.89	1/2782 (0.0%)
1	B	0.74	0/2098	0.83	0/2853
1	C	0.79	0/2041	0.89	2/2777 (0.1%)
1	D	0.81	0/2036	0.88	0/2771
1	E	0.75	0/2087	0.86	0/2839
1	F	0.80	0/2052	0.85	5/2792 (0.2%)
2	Q	0.78	1/4433 (0.0%)	0.90	2/6010 (0.0%)
2	R	0.76	1/4387 (0.0%)	0.88	2/5950 (0.0%)
2	S	0.71	1/4351 (0.0%)	0.85	1/5901 (0.0%)
2	T	0.78	0/4437	0.88	2/6016 (0.0%)
2	U	0.76	2/4387 (0.0%)	0.88	1/5951 (0.0%)
2	V	0.68	0/4367	0.83	1/5923 (0.0%)
All	All	0.76	5/38721 (0.0%)	0.87	17/52565 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	541	ASP	C-O	8.18	1.27	1.23
2	S	541	ASP	C-O	6.21	1.26	1.23
2	U	541	ASP	C-O	5.49	1.26	1.23
2	U	541	ASP	N-CA	5.41	1.50	1.46
2	Q	198	ASP	CG-OD2	5.08	1.34	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	497	VAL	N-CA-CB	-6.59	107.28	111.83
2	R	149	ALA	N-CA-C	6.51	114.08	108.22
2	T	149	ALA	N-CA-C	6.14	113.74	108.22
1	F	235	VAL	N-CA-C	6.01	119.42	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	VAL	N-CA-C	5.88	116.07	110.42
2	U	149	ALA	N-CA-C	5.77	113.41	108.22
2	Q	149	ALA	N-CA-C	5.71	113.36	108.22
2	R	189	LYS	N-CA-C	5.63	118.18	111.71
1	F	227	CYS	CA-C-N	-5.58	113.92	119.56
1	F	227	CYS	C-N-CA	-5.58	113.92	119.56
1	F	28	ILE	CA-C-N	-5.29	117.13	122.74
1	F	28	ILE	C-N-CA	-5.29	117.13	122.74
2	V	477	GLY	N-CA-C	5.22	118.22	110.60
2	T	115	HIS	N-CA-C	5.09	116.83	111.28
1	C	227	CYS	CA-C-N	-5.08	113.81	119.19
1	C	227	CYS	C-N-CA	-5.08	113.81	119.19
2	S	149	ALA	N-CA-C	5.01	112.73	108.22

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	1982	0	1922	4	0
1	B	2007	0	1950	12	0
1	C	1977	0	1921	13	0
1	D	1978	0	1913	11	0
1	E	2001	0	1937	11	0
1	F	1988	0	1927	10	0
2	Q	4238	0	4224	19	0
2	R	4220	0	4196	30	0
2	S	4205	0	4175	16	0
2	T	4248	0	4227	15	0
2	U	4221	0	4191	12	0
2	V	4211	0	4173	15	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	16	0	0	0	0
3	F	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
4	E	7	0	0	0	0
4	F	7	0	0	0	0
5	Q	7	0	0	0	0
5	R	7	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
5	U	7	0	0	0	0
5	V	7	0	0	0	0
6	Q	2	0	0	1	0
6	R	2	0	0	1	0
6	S	2	0	0	1	0
6	T	2	0	0	1	0
6	U	2	0	0	1	0
6	V	2	0	0	1	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
8	Q	2	0	0	0	0
8	R	2	0	0	0	0
8	S	1	0	0	0	0
8	T	2	0	0	0	0
8	U	2	0	0	0	0
8	V	1	0	0	0	0
9	Q	1	0	0	0	0
9	R	1	0	0	0	0
9	S	1	0	0	0	0
9	T	1	0	0	0	0
9	U	1	0	0	0	0
9	V	1	0	0	0	0
10	Q	12	0	16	0	0
10	R	12	0	16	0	0
10	S	6	0	8	0	0
10	T	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	U	12	0	16	0	0
10	V	6	0	8	0	0
11	V	4	0	0	0	0
12	A	301	0	0	0	0
12	B	198	0	0	0	0
12	C	226	0	0	2	0
12	D	299	0	0	5	0
12	E	204	0	0	1	0
12	F	209	0	0	1	0
12	Q	398	0	0	2	0
12	R	345	0	0	3	0
12	S	247	0	0	1	0
12	T	401	0	0	3	0
12	U	349	0	0	2	0
12	V	242	0	0	1	0
All	All	40973	0	36836	159	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.

All (159) 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:R:259[B]:CYS:CB	2:R:436[B]:CYS:HG	1.75	0.99
2:S:543[A]:CSS:SD	6:S:1551[A]:NI:NI	1.40	0.93
2:V:543[A]:CSS:SD	6:V:1551[A]:NI:NI	1.38	0.91
2:R:543[A]:CSS:SD	6:R:1551[A]:NI:NI	1.46	0.89
2:U:543[A]:CSS:SD	6:U:1551[A]:NI:NI	1.46	0.89
2:T:543[A]:CSS:SD	6:T:1551[A]:NI:NI	1.37	0.86
2:Q:543[A]:CSS:SD	6:Q:1551[A]:NI:NI	1.48	0.78
2:Q:444[A]:LYS:HG2	12:Q:2351:HOH:O	1.87	0.74
2:R:259[B]:CYS:CB	2:R:436[B]:CYS:SG	2.82	0.68
2:S:140:LYS:HG2	2:S:196:GLU:HG2	1.79	0.64
2:Q:211[B]:MET:HE2	2:Q:261:PHE:HB2	1.79	0.63
2:V:43:TRP:CE2	2:V:365:LYS:HE2	2.37	0.59
2:T:72[D]:CYS:SG	2:T:546:CYS:SG	3.00	0.59
1:B:37:LEU:HD13	2:R:166[B]:LYS:HD3	1.84	0.58
2:R:72[D]:CYS:SG	2:R:546:CYS:SG	3.03	0.57
2:V:543[A]:CSS:HB2	2:V:546:CYS:HB2	1.89	0.53
2:T:168:LYS:O	2:T:172:GLU:HG3	2.08	0.53
1:E:258:THR:HA	1:E:259:PRO:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:THR:O	2:V:23:ARG:HA	2.08	0.53
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.89	0.53
2:S:371:MET:HE2	2:S:547:GLY:HA3	1.90	0.53
1:E:171:GLU:H	1:E:171:GLU:CD	2.17	0.52
2:R:337:LYS:NZ	12:R:2255:HOH:O	2.39	0.51
1:B:258:THR:HA	1:B:259:PRO:C	2.36	0.51
2:R:476:ARG:NE	2:R:543[A]:CSS:SG	2.84	0.51
2:R:116[B]:LEU:HD11	2:R:261:PHE:CE2	2.46	0.51
2:R:481:HIS:CD2	2:R:495[B]:LEU:HG	2.46	0.50
2:S:543[A]:CSS:HB2	2:S:546:CYS:HB2	1.93	0.50
2:T:543[A]:CSS:HB2	2:T:546:CYS:HB2	1.94	0.50
1:F:71:TYR:CE1	1:F:106:LYS:HD2	2.46	0.50
2:T:371:MET:HE2	2:T:547:GLY:HA3	1.94	0.50
2:V:72[D]:CYS:SG	2:V:546:CYS:SG	3.09	0.50
1:C:71:TYR:CE1	1:C:106:LYS:HD2	2.47	0.50
2:U:481:HIS:CD2	2:U:495[B]:LEU:HG	2.47	0.49
2:Q:371:MET:HE2	2:Q:547:GLY:HA3	1.93	0.49
2:R:259[B]:CYS:HG	2:R:436[B]:CYS:CB	2.25	0.49
2:U:72[D]:CYS:SG	2:U:546:CYS:SG	3.10	0.49
2:Q:543[A]:CSS:HB2	2:Q:546:CYS:HB2	1.95	0.49
2:Q:72[D]:CYS:SG	2:Q:546:CYS:SG	3.10	0.49
2:S:448:ASP:O	2:S:452:LYS:HG2	2.12	0.49
2:S:72[D]:CYS:SG	2:S:546:CYS:SG	3.11	0.48
2:R:371:MET:HE2	2:R:547:GLY:HA3	1.95	0.48
2:V:476:ARG:NE	2:V:543[A]:CSS:SG	2.87	0.48
1:E:57:GLU:HG2	1:E:61[B]:HIS:CE1	2.49	0.48
2:R:543[A]:CSS:HB2	2:R:546:CYS:HB2	1.95	0.48
2:Q:476:ARG:NE	2:Q:543[A]:CSS:SG	2.87	0.48
2:Q:481:HIS:CD2	2:Q:495[B]:LEU:HG	2.49	0.48
2:V:481:HIS:CD2	2:V:495[B]:LEU:HG	2.49	0.48
1:F:99:LYS:HG3	1:F:137:LEU:HD22	1.96	0.47
12:U:2131:HOH:O	2:V:452:LYS:HE2	2.14	0.47
1:C:47:THR:O	2:S:23:ARG:HA	2.13	0.47
2:T:481:HIS:CD2	2:T:495[B]:LEU:HG	2.48	0.47
2:R:259[B]:CYS:HB2	2:R:436[B]:CYS:SG	2.55	0.47
2:S:476:ARG:NE	2:S:543[A]:CSS:SG	2.88	0.47
2:U:541:ASP:N	2:U:542:PRO:HD3	2.30	0.47
1:D:140:LYS:HE3	12:D:2180:HOH:O	2.14	0.47
2:U:476:ARG:NE	2:U:543[A]:CSS:SG	2.88	0.47
1:C:140:LYS:HD2	2:R:349:HIS:HB2	1.97	0.47
2:R:116[B]:LEU:HD11	2:R:261:PHE:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:TRP:CZ2	1:E:239:VAL:HB	2.50	0.46
2:Q:246:ASP:HB2	2:Q:247:PRO:HD3	1.97	0.46
2:R:274:ALA:HA	2:R:422[A]:LEU:HD11	1.97	0.46
2:V:365:LYS:HD2	2:V:365:LYS:HA	1.74	0.46
1:B:37:LEU:CD1	2:R:166[B]:LYS:HD3	2.44	0.46
1:D:264:GLY:HA3	12:D:2293:HOH:O	2.14	0.46
1:C:100[A]:LYS:HG3	12:C:2085:HOH:O	2.14	0.46
2:Q:488:LYS:HE2	12:Q:2364:HOH:O	2.14	0.46
1:E:237:TRP:CH2	1:E:239:VAL:HB	2.51	0.46
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.45	0.46
2:S:49:PHE:HB2	2:S:370:TRP:CD2	2.50	0.46
2:R:541:ASP:N	2:R:542:PRO:HD3	2.31	0.46
2:R:278:LYS:HG2	12:R:2194:HOH:O	2.15	0.46
1:E:229[A]:LYS:NZ	12:E:2152:HOH:O	2.49	0.46
1:B:259:PRO:HA	2:R:63:ASP:OD2	2.16	0.45
1:A:114:CYS:HA	1:A:119:GLY:HA3	1.98	0.45
2:T:476:ARG:NE	2:T:543[A]:CSS:SG	2.88	0.45
2:R:395:LYS:HE3	12:R:2226:HOH:O	2.16	0.45
2:V:371:MET:HE2	2:V:547:GLY:HA3	1.97	0.45
1:B:47:THR:O	2:R:23:ARG:HA	2.16	0.45
2:T:278:LYS:HG3	12:T:2225:HOH:O	2.17	0.45
1:D:47:THR:O	2:T:23:ARG:HA	2.17	0.45
1:D:61:HIS:HE1	12:D:2087:HOH:O	2.00	0.45
2:V:49:PHE:HB2	2:V:370:TRP:CD2	2.51	0.45
2:S:158:LYS:HD2	2:S:158:LYS:C	2.42	0.45
2:T:393:TYR:CE1	2:T:401[A]:LYS:HD3	2.52	0.45
1:E:142:ILE:HD11	1:E:166:ILE:HD12	1.99	0.44
1:E:223:THR:OG1	1:E:247:GLY:HA2	2.18	0.44
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.53	0.44
2:U:49:PHE:HB2	2:U:370:TRP:CD2	2.52	0.44
2:U:464:GLU:OE2	2:U:488:LYS:HE3	2.18	0.44
1:F:112:GLY:HA2	1:F:149:PRO:HD3	2.00	0.43
2:U:543[A]:CSS:HB2	2:U:546:CYS:HB2	2.00	0.43
1:B:223:THR:OG1	1:B:247:GLY:HA2	2.17	0.43
1:C:114:CYS:HA	1:C:119:GLY:HA3	2.00	0.43
2:S:481:HIS:CD2	2:S:495[B]:LEU:HG	2.53	0.43
2:Q:333:TYR:OH	2:Q:378:GLY:HA2	2.17	0.43
1:B:7:PRO:HD2	1:B:39:THR:O	2.18	0.43
2:R:259[B]:CYS:SG	2:R:436[B]:CYS:HB3	2.59	0.43
1:A:259:PRO:HG2	1:A:262:GLU:HB2	2.01	0.43
1:E:171:GLU:CD	1:E:171:GLU:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:O	2:Q:23:ARG:HA	2.18	0.43
2:V:337:LYS:HD2	2:V:508:ALA:O	2.18	0.43
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.49	0.42
2:T:49:PHE:HB2	2:T:370:TRP:CD2	2.54	0.42
2:T:365:LYS:HE3	12:T:2324:HOH:O	2.19	0.42
2:U:296:ALA:HA	2:U:309:SER:HA	2.01	0.42
1:C:40:ILE:HG22	1:C:162:LEU:CD1	2.50	0.42
2:S:296:ALA:HA	2:S:309:SER:HA	2.02	0.42
2:V:299:ASP:HB3	12:V:2161:HOH:O	2.19	0.42
1:A:258:THR:HA	1:A:259:PRO:C	2.45	0.42
2:V:25:GLU:HG3	2:V:72[A]:CYS:SG	2.60	0.42
1:C:112:GLY:HA2	1:C:149:PRO:HD3	2.02	0.42
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.54	0.42
1:D:114:CYS:HA	1:D:119:GLY:HA3	2.01	0.42
1:E:44:TYR:CD1	1:E:60:LEU:HB2	2.55	0.42
2:R:35:GLU:HG2	2:R:36[A]:ASN:ND2	2.35	0.42
1:D:220:GLY:N	1:D:221:PRO:CD	2.83	0.41
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.56	0.41
2:R:259[B]:CYS:SG	2:R:436[B]:CYS:CB	3.07	0.41
2:R:296:ALA:HA	2:R:309:SER:HA	2.02	0.41
2:S:541:ASP:N	2:S:542:PRO:HD3	2.35	0.41
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.55	0.41
1:C:67:LYS:HD2	1:C:67:LYS:N	2.35	0.41
1:F:258:THR:HA	1:F:259:PRO:C	2.45	0.41
2:S:129:ASP:OD1	2:S:129:ASP:C	2.64	0.41
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.55	0.41
2:S:476:ARG:HD2	12:S:2042[A]:HOH:O	2.20	0.41
2:T:25:GLU:HG3	2:T:72[A]:CYS:SG	2.61	0.41
1:D:99:LYS:HD2	12:D:2141:HOH:O	2.20	0.41
1:D:209:LYS:NZ	12:D:2245:HOH:O	2.45	0.41
1:D:237:TRP:CZ2	1:D:239:VAL:HB	2.56	0.41
1:F:14:ASN:ND2	12:F:2011:HOH:O	2.44	0.41
1:F:237:TRP:CH2	1:F:239:VAL:HB	2.55	0.41
2:Q:541:ASP:N	2:Q:542:PRO:HD3	2.35	0.41
2:U:125:LEU:HG	12:U:2114:HOH:O	2.21	0.41
2:U:371:MET:HE2	2:U:547:GLY:HA3	2.03	0.41
2:V:406:MET:O	2:V:410:LYS:HG2	2.20	0.41
1:F:237:TRP:CZ2	1:F:239:VAL:HB	2.56	0.40
2:R:69:GLN:HA	2:R:79:HIS:HB2	2.03	0.40
2:T:541:ASP:N	2:T:542:PRO:HD3	2.36	0.40
2:U:315:VAL:HG13	2:U:381[B]:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:GLY:HA2	1:D:149:PRO:HD3	2.03	0.40
1:D:258:THR:HA	1:D:259:PRO:C	2.46	0.40
1:E:229[A]:LYS:HE2	1:E:229[A]:LYS:HB3	1.87	0.40
2:T:476:ARG:HD2	12:T:2078[A]:HOH:O	2.21	0.40
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	2.03	0.40
1:B:44:TYR:CD1	1:B:60:LEU:HB2	2.57	0.40
2:S:76:THR:O	2:S:77:TYR:HB3	2.21	0.40
1:C:135:GLU:HG3	12:C:2117:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
1	B	268/264 (102%)	260 (97%)	8 (3%)	0	100	100
1	C	261/264 (99%)	254 (97%)	7 (3%)	0	100	100
1	D	261/264 (99%)	254 (97%)	7 (3%)	0	100	100
1	E	267/264 (101%)	260 (97%)	7 (3%)	0	100	100
1	F	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
2	Q	563/564 (100%)	553 (98%)	10 (2%)	0	100	100
2	R	558/564 (99%)	546 (98%)	12 (2%)	0	100	100
2	S	553/564 (98%)	542 (98%)	11 (2%)	0	100	100
2	T	564/564 (100%)	553 (98%)	11 (2%)	0	100	100
2	U	558/564 (99%)	548 (98%)	10 (2%)	0	100	100
2	V	555/564 (98%)	545 (98%)	10 (2%)	0	100	100
All	All	4932/4968 (99%)	4825 (98%)	107 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/210 (100%)	209 (100%)	1 (0%)	81	76
1	B	216/210 (103%)	215 (100%)	1 (0%)	81	76
1	C	210/210 (100%)	209 (100%)	1 (0%)	81	76
1	D	209/210 (100%)	208 (100%)	1 (0%)	81	76
1	E	215/210 (102%)	215 (100%)	0	100	100
1	F	211/210 (100%)	210 (100%)	1 (0%)	81	76
2	Q	457/448 (102%)	454 (99%)	3 (1%)	76	69
2	R	451/448 (101%)	450 (100%)	1 (0%)	87	84
2	S	447/448 (100%)	444 (99%)	3 (1%)	76	69
2	T	457/448 (102%)	454 (99%)	3 (1%)	76	69
2	U	451/448 (101%)	448 (99%)	3 (1%)	76	69
2	V	449/448 (100%)	447 (100%)	2 (0%)	84	80
All	All	3983/3948 (101%)	3963 (100%)	20 (0%)	81	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	B	171	GLU
1	C	67	LYS
1	D	137	LEU
1	F	88	MET
2	Q	166	LYS
2	Q	473	ASP
2	Q	546	CYS
2	R	473	ASP
2	S	158	LYS
2	S	473	ASP

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Mol	Chain	Res	Type
2	S	500	THR
2	T	410	LYS
2	T	473	ASP
2	T	500	THR
2	U	395	LYS
2	U	452	LYS
2	U	473	ASP
2	V	473	ASP
2	V	500	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	92	HIS
1	A	240	GLN
1	B	14	ASN
1	B	234	GLN
1	C	14	ASN
1	C	129	GLN
1	C	234	GLN
1	C	240	GLN
1	D	14	ASN
1	D	92	HIS
1	D	240	GLN
1	E	14	ASN
1	E	92	HIS
1	E	234	GLN
1	F	14	ASN
1	F	234	GLN
1	F	240	GLN
2	Q	47	GLN
2	Q	241	GLN
2	R	47	GLN
2	R	263	ASN
2	S	47	GLN
2	S	164	GLN
2	S	241	GLN
2	S	263	ASN
2	T	47	GLN
2	T	241	GLN
2	T	509	GLN

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Mol	Chain	Res	Type
2	U	47	GLN
2	U	139	ASN
2	V	47	GLN
2	V	164	GLN
2	V	241	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	CSS	V	543[A]	2,5	4,6,7	1.16	0	2,6,8	1.14	0
2	CSS	S	543[A]	2,5	4,6,7	1.00	0	2,6,8	1.03	0
2	CSS	Q	543[A]	2,5	4,6,7	1.02	0	2,6,8	1.07	0
2	CSS	T	543[A]	2,5	4,6,7	0.91	0	2,6,8	1.07	0
2	CSS	R	543[A]	2,5	4,6,7	1.12	0	2,6,8	1.23	0
2	CSS	U	543[A]	2,5	4,6,7	1.04	0	2,6,8	1.03	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	CSS	V	543[A]	2,5	-	0/1/5/7	-
2	CSS	S	543[A]	2,5	-	0/1/5/7	-
2	CSS	Q	543[A]	2,5	-	0/1/5/7	-
2	CSS	T	543[A]	2,5	-	0/1/5/7	-
2	CSS	R	543[A]	2,5	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSS	U	543[A]	2,5	-	0/1/5/7	-

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.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	543[A]	CSS	3	0
2	S	543[A]	CSS	3	0
2	Q	543[A]	CSS	3	0
2	T	543[A]	CSS	3	0
2	R	543[A]	CSS	3	0
2	U	543[A]	CSS	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 28 are monoatomic and 6 are modelled with single atom - leaving 35 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	E	1267	1	0,12,12	-	-	-		
4	F3S	B	1266	1	0,9,9	-	-	-		
10	GOL	T	1562	-	5,5,5	0.32	0	5,5,5	0.32	0
3	SF4	D	1265	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	C	1267	1	0,12,12	-	-	-		
10	GOL	T	1561	-	5,5,5	0.35	0	5,5,5	0.52	0
4	F3S	A	1266	1	0,9,9	-	-	-		
3	SF4	F	1267	1	0,12,12	-	-	-		
5	FCO	S	1550	2,7,12	0,6,6	-	-	-		
3	SF4	A	1265	1	0,12,12	-	-	-		
10	GOL	V	1561	-	5,5,5	0.28	0	5,5,5	0.46	0
3	SF4	E	1265	1	0,12,12	-	-	-		
3	SF4	B	1267	1	0,12,12	-	-	-		
3	SF4	C	1265	1	0,12,12	-	-	-		
10	GOL	Q	1562	-	5,5,5	0.41	0	5,5,5	0.30	0
10	GOL	Q	1561	-	5,5,5	0.38	0	5,5,5	0.53	0
10	GOL	U	1561	-	5,5,5	0.35	0	5,5,5	0.32	0
4	F3S	C	1266	1	0,9,9	-	-	-		
3	SF4	F	1265	1	0,12,12	-	-	-		
5	FCO	R	1550	2,7,12	0,6,6	-	-	-		
5	FCO	T	1550	2,7,12	0,6,6	-	-	-		
11	CO3	V	1562	-	3,3,3	1.15	0	2,3,3	0.53	0
10	GOL	R	1563	-	5,5,5	0.45	0	5,5,5	0.66	0
5	FCO	V	1550	2,7,12	0,6,6	-	-	-		
10	GOL	S	1561	-	5,5,5	0.30	0	5,5,5	0.57	0
5	FCO	Q	1550	2,7,12	0,6,6	-	-	-		
3	SF4	B	1265	1	0,12,12	-	-	-		
4	F3S	E	1266	1	0,9,9	-	-	-		
3	SF4	A	1267	1	0,12,12	-	-	-		
4	F3S	F	1266	1	0,9,9	-	-	-		
10	GOL	R	1561	-	5,5,5	0.28	0	5,5,5	0.54	0
10	GOL	U	1563	-	5,5,5	0.37	0	5,5,5	0.54	0
3	SF4	D	1267	1	0,12,12	-	-	-		
5	FCO	U	1550	2,7,12	0,6,6	-	-	-		
4	F3S	D	1266	1	0,9,9	-	-	-		

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	E	1267	1	-	-	0/6/5/5
4	F3S	B	1266	1	-	-	0/3/3/3
10	GOL	T	1562	-	-	0/4/4/4	-
3	SF4	D	1265	1	-	-	0/6/5/5
3	SF4	C	1267	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	T	1561	-	-	2/4/4/4	-
4	F3S	A	1266	1	-	-	0/3/3/3
3	SF4	F	1267	1	-	-	0/6/5/5
3	SF4	A	1265	1	-	-	0/6/5/5
10	GOL	V	1561	-	-	0/4/4/4	-
3	SF4	E	1265	1	-	-	0/6/5/5
3	SF4	B	1267	1	-	-	0/6/5/5
10	GOL	Q	1562	-	-	0/4/4/4	-
3	SF4	C	1265	1	-	-	0/6/5/5
10	GOL	U	1561	-	-	0/4/4/4	-
10	GOL	Q	1561	-	-	0/4/4/4	-
4	F3S	C	1266	1	-	-	0/3/3/3
3	SF4	F	1265	1	-	-	0/6/5/5
10	GOL	R	1563	-	-	0/4/4/4	-
10	GOL	S	1561	-	-	0/4/4/4	-
3	SF4	B	1265	1	-	-	0/6/5/5
4	F3S	E	1266	1	-	-	0/3/3/3
3	SF4	A	1267	1	-	-	0/6/5/5
4	F3S	F	1266	1	-	-	0/3/3/3
10	GOL	R	1561	-	-	0/4/4/4	-
10	GOL	U	1563	-	-	0/4/4/4	-
3	SF4	D	1267	1	-	-	0/6/5/5
4	F3S	D	1266	1	-	-	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	T	1561	GOL	C1-C2-C3-O3
10	T	1561	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	262/264 (99%)	-0.77	0 100 100	9, 15, 27, 53	8 (3%)
1	B	262/264 (99%)	-0.48	1 (0%) 88 90	13, 22, 35, 54	12 (4%)
1	C	261/264 (98%)	-0.70	0 100 100	10, 17, 29, 45	10 (3%)
1	D	262/264 (99%)	-0.74	0 100 100	9, 15, 26, 55	6 (2%)
1	E	262/264 (99%)	-0.53	0 100 100	13, 21, 35, 49	14 (5%)
1	F	261/264 (98%)	-0.67	0 100 100	10, 17, 29, 44	8 (3%)
2	Q	543/564 (96%)	-0.71	0 100 100	9, 16, 30, 42	29 (5%)
2	R	544/564 (96%)	-0.69	0 100 100	8, 17, 32, 46	20 (3%)
2	S	543/564 (96%)	-0.49	0 100 100	10, 23, 36, 45	18 (3%)
2	T	543/564 (96%)	-0.72	0 100 100	8, 16, 29, 38	30 (5%)
2	U	544/564 (96%)	-0.69	0 100 100	8, 17, 31, 44	23 (4%)
2	V	543/564 (96%)	-0.46	0 100 100	10, 23, 37, 50	18 (3%)
All	All	4830/4968 (97%)	-0.63	1 (0%) 100 100	8, 18, 33, 55	196 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	2.8

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, 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
2	CSS	S	543[A]	7/8	0.91	0.09	14,15,17,17	7
2	CSS	V	543[A]	7/8	0.94	0.09	15,15,17,18	7
2	CSS	Q	543[A]	7/8	0.95	0.07	10,11,13,13	7
2	CSS	R	543[A]	7/8	0.96	0.07	10,11,13,15	7
2	CSS	T	543[A]	7/8	0.98	0.05	11,12,13,14	7
2	CSS	U	543[A]	7/8	0.99	0.06	10,12,13,15	7

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
10	GOL	U	1563	6/6	0.94	0.08	15,18,18,22	6
11	CO3	V	1562	4/4	0.95	0.04	38,40,42,43	0
10	GOL	Q	1561	6/6	0.97	0.05	17,19,20,22	0
10	GOL	V	1561	6/6	0.97	0.06	17,18,21,22	6
10	GOL	S	1561	6/6	0.97	0.04	19,22,22,24	0
8	MG	U	1560	1/1	0.98	0.05	13,13,13,13	1
10	GOL	T	1561	6/6	0.98	0.04	13,15,16,20	0
10	GOL	U	1561	6/6	0.98	0.04	16,18,21,21	0
10	GOL	Q	1562	6/6	0.98	0.04	10,12,12,12	6
10	GOL	R	1561	6/6	0.98	0.03	17,18,19,20	0
10	GOL	R	1563	6/6	0.98	0.04	16,19,21,22	0
6	NI	U	1551[B]	1/1	0.99	0.02	15,15,15,15	1
6	NI	V	1551[A]	1/1	0.99	0.03	20,20,20,20	1
6	NI	V	1551[B]	1/1	0.99	0.03	17,17,17,17	1
7	H2S	Q	1552[B]	1/1	0.99	0.03	14,14,14,14	1
7	H2S	R	1552[B]	1/1	0.99	0.02	12,12,12,12	1
7	H2S	S	1552[B]	1/1	0.99	0.06	16,16,16,16	1
7	H2S	U	1552[B]	1/1	0.99	0.04	12,12,12,12	1
7	H2S	V	1552[B]	1/1	0.99	0.07	17,17,17,17	1
8	MG	R	1560	1/1	0.99	0.02	14,14,14,14	1
8	MG	S	1553[A]	1/1	0.99	0.02	15,15,15,15	1
8	MG	T	1560	1/1	0.99	0.02	16,16,16,16	1
3	SF4	B	1265	8/8	0.99	0.03	24,27,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CA	S	1554[B]	1/1	0.99	0.02	16,16,16,16	1
9	CA	T	1554[B]	1/1	0.99	0.01	11,11,11,11	1
9	CA	U	1554[B]	1/1	0.99	0.03	12,12,12,12	1
3	SF4	E	1265	8/8	0.99	0.03	23,24,26,28	0
6	NI	Q	1551[A]	1/1	0.99	0.04	16,16,16,16	1
6	NI	Q	1551[B]	1/1	0.99	0.04	14,14,14,14	1
6	NI	R	1551[A]	1/1	0.99	0.02	18,18,18,18	1
6	NI	R	1551[B]	1/1	0.99	0.02	15,15,15,15	1
6	NI	S	1551[A]	1/1	0.99	0.03	21,21,21,21	1
10	GOL	T	1562	6/6	0.99	0.05	15,17,18,22	0
6	NI	S	1551[B]	1/1	0.99	0.03	17,17,17,17	1
6	NI	T	1551[A]	1/1	0.99	0.03	16,16,16,16	1
6	NI	T	1551[B]	1/1	0.99	0.03	13,13,13,13	1
6	NI	U	1551[A]	1/1	0.99	0.02	19,19,19,19	1
4	F3S	D	1266	7/7	1.00	0.02	10,11,13,14	0
4	F3S	E	1266	7/7	1.00	0.02	17,18,19,19	0
7	H2S	T	1552[B]	1/1	1.00	0.02	13,13,13,13	1
4	F3S	F	1266	7/7	1.00	0.01	12,12,12,13	0
5	FCO	Q	1550	7/7	1.00	0.03	10,11,13,14	0
8	MG	Q	1553[A]	1/1	1.00	0.01	11,11,11,11	1
8	MG	Q	1560	1/1	1.00	0.01	9,9,9,9	1
8	MG	R	1553[A]	1/1	1.00	0.03	12,12,12,12	1
5	FCO	R	1550	7/7	1.00	0.03	8,11,12,13	0
5	FCO	S	1550	7/7	1.00	0.04	13,15,16,17	0
8	MG	T	1553[A]	1/1	1.00	0.01	11,11,11,11	1
5	FCO	T	1550	7/7	1.00	0.03	10,11,12,14	0
8	MG	U	1553[A]	1/1	1.00	0.04	12,12,12,12	1
5	FCO	U	1550	7/7	1.00	0.02	11,12,13,13	0
8	MG	V	1553[A]	1/1	1.00	0.02	16,16,16,16	1
9	CA	Q	1554[B]	1/1	1.00	0.01	11,11,11,11	1
9	CA	R	1554[D]	1/1	1.00	0.03	13,13,13,13	1
5	FCO	V	1550	7/7	1.00	0.04	13,16,17,18	0
3	SF4	A	1265	8/8	1.00	0.01	11,12,13,14	0
3	SF4	B	1267	8/8	1.00	0.02	14,16,16,17	0
9	CA	V	1554[B]	1/1	1.00	0.02	15,15,15,15	1
3	SF4	C	1265	8/8	1.00	0.01	11,12,13,13	0
3	SF4	C	1267	8/8	1.00	0.02	11,12,13,14	0
3	SF4	D	1265	8/8	1.00	0.01	12,12,14,14	0
3	SF4	D	1267	8/8	1.00	0.02	10,10,10,10	0
3	SF4	A	1267	8/8	1.00	0.01	9,10,11,11	0
3	SF4	E	1267	8/8	1.00	0.02	14,15,15,15	0
3	SF4	F	1265	8/8	1.00	0.01	10,12,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SF4	F	1267	8/8	1.00	0.02	11,12,13,14	0
4	F3S	A	1266	7/7	1.00	0.02	10,11,12,12	0
4	F3S	B	1266	7/7	1.00	0.01	18,18,20,21	0
4	F3S	C	1266	7/7	1.00	0.01	11,12,12,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.