



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 02:09 PM EDT

PDB ID : 1UBH / pdb_00001ubh
Title : Three-dimensional Structure of The Carbon Monoxide Complex of [NiFe]hydrogenase From Desulfovibrio vulgaris Miyazaki F
Authors : Ogata, H.; Mizoguchi, Y.; Mizuno, N.; Miki, K.; Adachi, S.; Yasuoka, N.; Yagi, T.; Yamauchi, O.; Hirota, S.; Higuchi, Y.
Deposited on : 2003-04-04
Resolution : 1.35 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

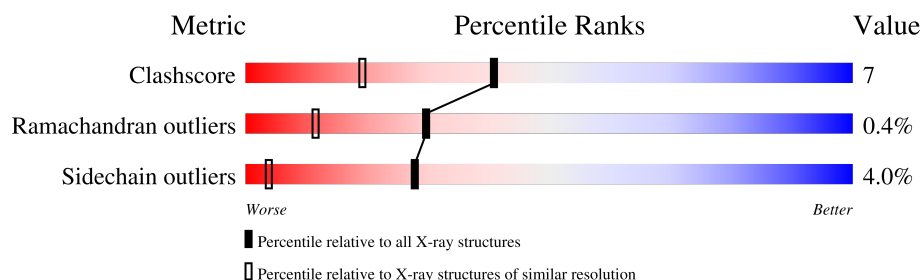
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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))
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	267	 78% 18% • •
2	L	534	 83% 15% •

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7133 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 Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	267	Total	C	N	O	S	0	0	0
			2019	1282	342	378	17			

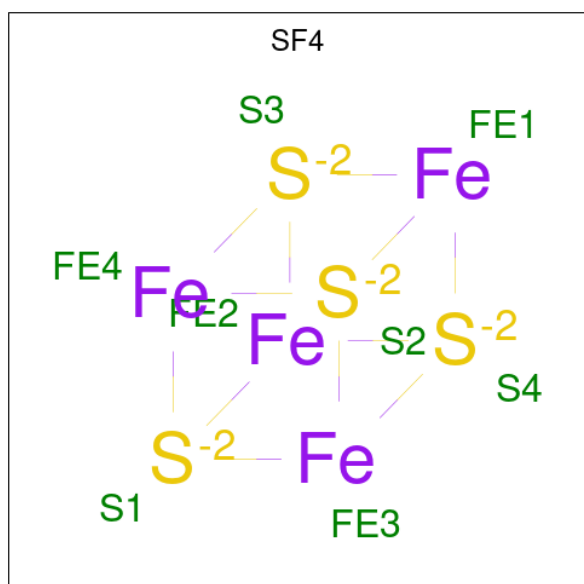
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	534	Total	C	N	O	S	0	0	0
			4177	2674	725	763	15			

There are 2 discrepancies between the modelled and reference sequences:

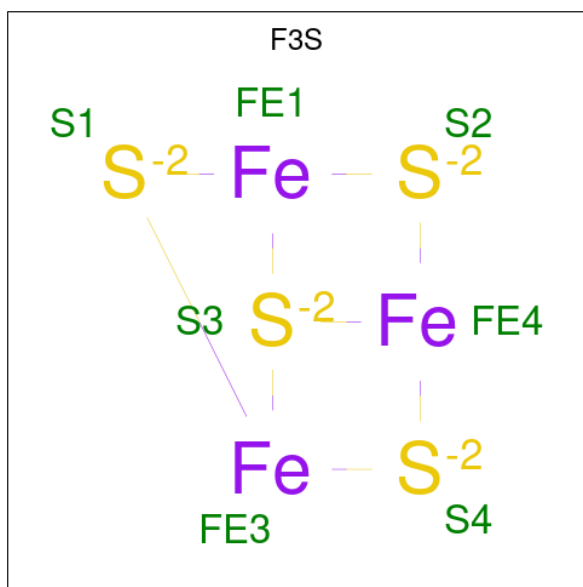
Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

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



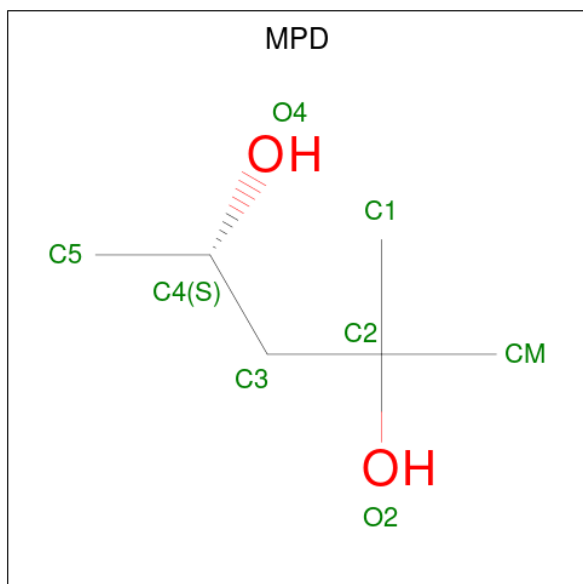
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	S	1	Total	Fe	S	0	0
			8	4	4		

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



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).

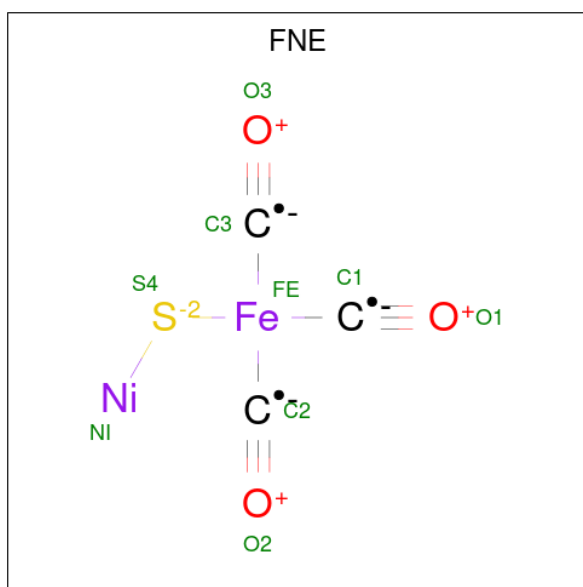


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

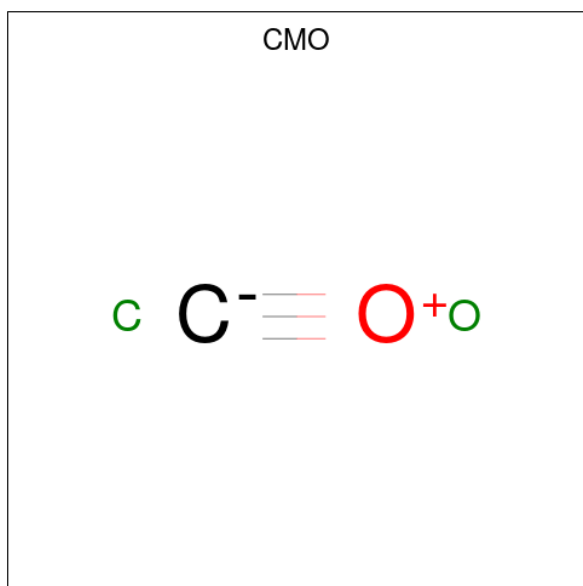
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total Mg 1 1	0	0

- Molecule 7 is (MU-SULPHIDO)-BIS(MU-CYS,S)-[TRICARBONYLIRON-DI-(CYS,S)NIC KEL(II)](FE-NI) (CCD ID: FNE) (formula: C₃FeNiO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Fe	Ni	O	0	0
			8	3	1	1	3		

- Molecule 8 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			2	1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	268	Total 268	O 268	0	0
9	L	547	Total 547	O 547	0	0

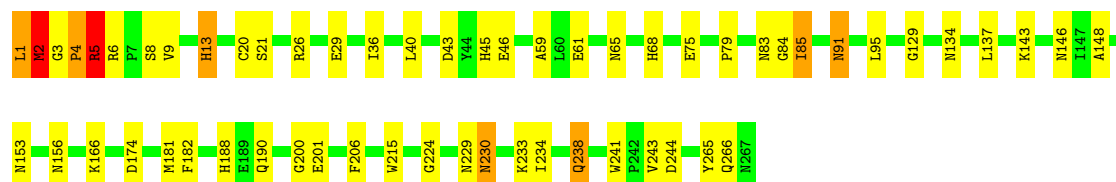
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

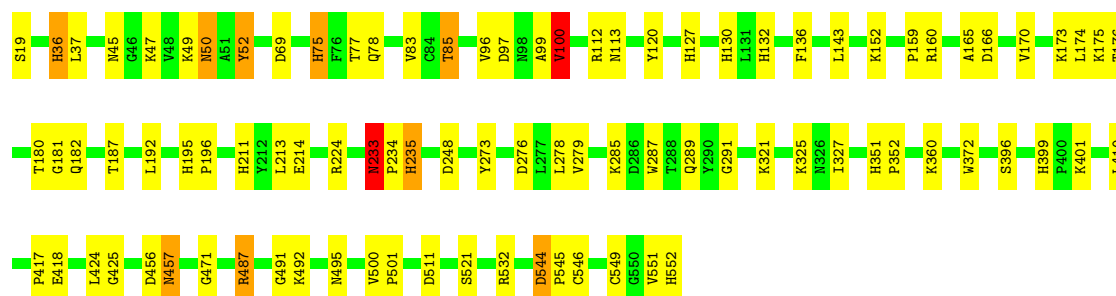
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain S: 



- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain L: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.06Å 126.21Å 66.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.35	Depositor
% Data completeness (in resolution range)	77.1 (20.00-1.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.125 , 0.178	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7133	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FNE, MPD, F3S, CMO, SF4, MG

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	S	0.80	1/2075 (0.0%)	1.71	48/2830 (1.7%)
2	L	0.80	2/4288 (0.0%)	1.65	84/5831 (1.4%)
All	All	0.80	3/6363 (0.0%)	1.67	132/8661 (1.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	552	HIS	C-O	5.83	1.35	1.23
2	L	85	THR	C-N	-5.61	1.25	1.33
1	S	85	ILE	CA-CB	5.57	1.63	1.54

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	487	ARG	CD-NE-CZ	17.37	148.71	124.40
2	L	424	LEU	CA-C-N	16.01	137.71	119.94
2	L	424	LEU	C-N-CA	16.01	137.71	119.94
1	S	95	LEU	CA-C-N	13.88	138.49	120.44
1	S	95	LEU	C-N-CA	13.88	138.49	120.44
1	S	26	ARG	NE-CZ-NH2	13.40	131.26	119.20
1	S	129	GLY	O-C-N	-12.23	110.43	122.41
1	S	95	LEU	O-C-N	-11.63	110.09	122.07
2	L	224	ARG	NE-CZ-NH2	11.46	129.51	119.20
2	L	78	GLN	OE1-CD-NE2	-10.88	111.72	122.60
1	S	148	ALA	CA-C-N	9.86	136.28	122.57
1	S	148	ALA	C-N-CA	9.86	136.28	122.57
1	S	229	ASN	O-C-N	-9.76	113.53	123.29
2	L	85	THR	O-C-N	-9.39	111.76	122.75
2	L	233	ASN	CB-CG-OD1	9.26	139.31	120.80
1	S	238	GLN	OE1-CD-NE2	-9.21	113.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	234	PRO	CA-C-N	9.18	139.07	121.54
2	L	234	PRO	C-N-CA	9.18	139.07	121.54
2	L	196	PRO	CA-C-N	9.10	138.99	122.06
2	L	196	PRO	C-N-CA	9.10	138.99	122.06
1	S	129	GLY	CA-C-N	9.09	134.05	121.05
1	S	129	GLY	C-N-CA	9.09	134.05	121.05
2	L	181	GLY	CA-C-N	8.93	135.00	122.41
2	L	181	GLY	C-N-CA	8.93	135.00	122.41
2	L	424	LEU	O-C-N	-8.80	112.79	122.12
2	L	233	ASN	OD1-CG-ND2	-8.77	113.83	122.60
2	L	273	TYR	CA-C-N	-8.72	114.75	120.24
2	L	273	TYR	C-N-CA	-8.72	114.75	120.24
2	L	50	ASN	OD1-CG-ND2	-8.65	113.95	122.60
1	S	229	ASN	CA-C-N	8.63	136.39	122.67
1	S	229	ASN	C-N-CA	8.63	136.39	122.67
1	S	84	GLY	CA-C-N	8.62	134.76	120.62
1	S	84	GLY	C-N-CA	8.62	134.76	120.62
2	L	85	THR	CA-C-N	8.53	137.82	121.54
2	L	85	THR	C-N-CA	8.53	137.82	121.54
2	L	372	TRP	O-C-N	-8.52	109.98	122.43
2	L	224	ARG	NH1-CZ-NH2	-8.51	108.23	119.30
2	L	196	PRO	O-C-N	-8.42	111.36	122.22
2	L	195	HIS	CB-CG-CD2	8.25	141.93	131.20
1	S	229	ASN	CA-CB-CG	8.06	120.66	112.60
1	S	26	ARG	NH1-CZ-NH2	-7.97	108.93	119.30
1	S	190	GLN	OE1-CD-NE2	7.97	130.57	122.60
1	S	83	ASN	CA-CB-CG	-7.96	104.64	112.60
2	L	50	ASN	CA-CB-CG	7.95	120.55	112.60
1	S	230	ASN	CA-CB-CG	7.72	120.32	112.60
2	L	181	GLY	O-C-N	-7.67	112.39	122.28
2	L	69	ASP	CA-CB-CG	7.61	120.21	112.60
2	L	99	ALA	CA-C-N	7.57	132.45	121.02
2	L	99	ALA	C-N-CA	7.57	132.45	121.02
2	L	195	HIS	ND1-CE1-NE2	-7.40	101.00	108.40
2	L	136	PHE	CA-CB-CG	7.37	121.17	113.80
2	L	165	ALA	CA-C-N	7.22	129.82	120.44
2	L	165	ALA	C-N-CA	7.22	129.82	120.44
2	L	401	LYS	CA-C-N	7.07	129.47	120.56
2	L	401	LYS	C-N-CA	7.07	129.47	120.56
1	S	153	ASN	OD1-CG-ND2	7.02	129.62	122.60
2	L	195	HIS	ND1-CG-CD2	-6.99	99.11	106.10
2	L	78	GLN	CG-CD-OE1	6.97	134.74	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	45	ASN	CA-CB-CG	6.86	119.46	112.60
2	L	456	ASP	CA-C-O	6.85	127.91	120.58
2	L	130	HIS	CA-CB-CG	-6.85	106.95	113.80
2	L	195	HIS	CG-ND1-CE1	6.83	120.92	109.30
2	L	85	THR	CA-C-O	6.81	129.36	121.87
2	L	113	ASN	CA-CB-CG	6.68	119.28	112.60
2	L	97	ASP	CA-CB-CG	6.65	119.25	112.60
1	S	46	GLU	CA-C-N	6.48	129.49	120.29
1	S	46	GLU	C-N-CA	6.48	129.49	120.29
2	L	159	PRO	CA-C-N	6.47	131.54	121.26
2	L	159	PRO	C-N-CA	6.47	131.54	121.26
2	L	532	ARG	CD-NE-CZ	6.43	133.41	124.40
2	L	233	ASN	CB-CG-ND2	-6.37	106.84	116.40
2	L	372	TRP	CA-C-N	6.33	129.85	120.87
2	L	372	TRP	C-N-CA	6.33	129.85	120.87
2	L	372	TRP	CA-C-O	6.30	127.18	119.11
2	L	544	ASP	CA-CB-CG	6.27	118.87	112.60
2	L	351	HIS	CA-CB-CG	-6.22	107.58	113.80
1	S	238	GLN	CG-CD-OE1	6.22	133.24	120.80
2	L	166	ASP	CA-CB-CG	6.20	118.80	112.60
2	L	50	ASN	CA-C-O	-6.14	114.66	121.23
1	S	229	ASN	OD1-CG-ND2	-6.14	116.46	122.60
2	L	181	GLY	CA-C-O	6.11	125.52	119.04
1	S	6	ARG	NE-CZ-NH2	6.07	124.67	119.20
2	L	551	VAL	CB-CA-C	-6.05	104.59	111.55
2	L	532	ARG	CG-CD-NE	6.03	125.25	112.00
2	L	287	TRP	CA-CB-CG	-5.98	102.25	113.60
2	L	401	LYS	O-C-N	-5.96	115.36	122.15
1	S	26	ARG	CG-CD-NE	-5.96	98.89	112.00
2	L	248	ASP	CA-CB-CG	5.96	118.56	112.60
1	S	156	ASN	OD1-CG-ND2	5.93	128.53	122.60
2	L	487	ARG	CG-CD-NE	5.90	124.99	112.00
2	L	170	VAL	CA-C-O	5.89	127.08	120.95
1	S	85	ILE	CA-CB-CG1	-5.87	100.42	110.40
2	L	511	ASP	CA-CB-CG	5.87	118.47	112.60
2	L	85	THR	CA-CB-OG1	-5.82	100.87	109.60
2	L	425	GLY	N-CA-C	-5.82	105.75	112.50
2	L	36	HIS	CB-CG-ND1	5.81	131.41	122.70
2	L	83	VAL	N-CA-C	-5.79	105.48	110.74
2	L	75	HIS	CA-CB-CG	-5.78	108.03	113.80
1	S	148	ALA	CA-C-O	5.75	128.61	121.89
2	L	75	HIS	CB-CG-ND1	5.73	131.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	120	TYR	CA-CB-CG	5.63	124.03	113.90
1	S	95	LEU	CA-C-O	5.61	126.71	120.82
2	L	77	THR	CA-CB-OG1	-5.61	101.18	109.60
1	S	91	ASN	CA-CB-CG	5.58	118.18	112.60
2	L	36	HIS	CB-CG-CD2	-5.56	123.97	131.20
2	L	399	HIS	ND1-CG-CD2	-5.55	100.55	106.10
2	L	75	HIS	CB-CG-CD2	-5.52	124.02	131.20
2	L	399	HIS	CG-CD2-NE2	5.46	112.66	107.20
2	L	457	ASN	CA-CB-CG	5.43	118.03	112.60
1	S	45	HIS	CB-CG-CD2	5.35	138.16	131.20
2	L	352	PRO	O-C-N	-5.35	115.07	122.24
2	L	112	ARG	NE-CZ-NH2	5.35	124.01	119.20
2	L	127	HIS	CA-CB-CG	-5.34	108.46	113.80
1	S	65	ASN	CA-C-O	5.33	125.88	119.43
1	S	200	GLY	O-C-N	5.33	128.16	122.41
1	S	137	LEU	O-C-N	5.28	129.08	122.22
1	S	2	MET	CA-CB-CG	5.25	124.60	114.10
1	S	174	ASP	CA-CB-CG	5.25	117.84	112.60
1	S	2	MET	CA-C-N	5.22	130.07	121.87
1	S	2	MET	C-N-CA	5.22	130.07	121.87
2	L	495	ASN	CA-CB-CG	5.21	117.81	112.60
1	S	29	GLU	CB-CG-CD	-5.20	103.75	112.60
1	S	79	PRO	O-C-N	5.18	128.52	123.03
1	S	13	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	S	148	ALA	O-C-N	-5.14	116.67	122.68
2	L	100	VAL	CG1-CB-CG2	5.11	122.05	110.80
2	L	52	TYR	O-C-N	5.11	129.28	123.31
1	S	266	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	L	471	GLY	O-C-N	5.08	128.30	123.57
1	S	91	ASN	CB-CG-ND2	5.07	124.01	116.40
1	S	65	ASN	O-C-N	-5.06	115.86	122.39
1	S	206	PHE	CA-CB-CG	-5.01	108.79	113.80

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	S	2019	0	1949	45	0
2	L	4177	0	4129	41	0
3	S	16	0	0	0	0
4	S	7	0	0	0	0
5	L	40	0	70	10	0
5	S	48	0	84	13	0
6	L	1	0	0	0	0
7	L	8	0	0	0	0
8	L	2	0	0	0	0
9	L	547	0	0	14	0
9	S	268	0	0	7	0
All	All	7133	0	6232	82	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 7.

All (82) 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:S:146:ASN:HD21	5:S:2004:MPD:H13	1.24	1.00
1:S:134:ASN:HB2	5:S:2004:MPD:H12	1.59	0.84
2:L:417:PRO:HB3	5:L:2005:MPD:H4	1.63	0.79
1:S:5:ARG:HB2	2:L:182:GLN:OE1	1.82	0.79
1:S:2:MET:HB3	1:S:43:ASP:OD1	1.84	0.76
5:L:2009:MPD:H51	9:L:3494:HOH:O	1.87	0.75
1:S:238:GLN:HA	5:S:2008:MPD:H31	1.71	0.73
2:L:176:THR:O	2:L:180:THR:HG23	1.89	0.72
1:S:1:LEU:HD21	1:S:59:ALA:O	1.89	0.72
1:S:146:ASN:ND2	5:S:2004:MPD:H13	2.03	0.71
2:L:321:LYS:HE2	9:L:3514:HOH:O	1.89	0.70
2:L:289:GLN:HG3	9:L:3455:HOH:O	1.91	0.70
1:S:2:MET:HB2	2:L:182:GLN:HE21	1.57	0.68
2:L:192:LEU:HB3	5:L:2002:MPD:H13	1.74	0.68
1:S:2:MET:HE3	1:S:8:SER:HB2	1.75	0.67
2:L:360:LYS:HE3	9:L:3558:HOH:O	1.94	0.66
1:S:2:MET:HA	2:L:182:GLN:HG2	1.83	0.60
2:L:160:ARG:HB3	9:L:3743:HOH:O	2.01	0.60
2:L:52:TYR:CD2	5:L:2010:MPD:H53	2.36	0.60
1:S:2:MET:HG2	9:S:3509:HOH:O	2.00	0.59
2:L:233:ASN:C	2:L:233:ASN:HD22	2.10	0.59
1:S:13:HIS:HD2	9:S:3139:HOH:O	1.84	0.59
2:L:211:HIS:HE1	9:L:3263:HOH:O	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2:MET:HE2	2:L:182:GLN:NE2	2.20	0.57
1:S:166:LYS:HD3	9:S:3600:HOH:O	2.04	0.56
2:L:417:PRO:HB3	5:L:2005:MPD:C4	2.33	0.55
1:S:5:ARG:HH11	1:S:5:ARG:HB3	1.71	0.54
1:S:1:LEU:HB3	2:L:187:THR:OG1	2.07	0.54
2:L:360:LYS:HG2	9:L:3558:HOH:O	2.08	0.53
2:L:36:HIS:HD2	9:L:3241:HOH:O	1.91	0.53
1:S:233:LYS:HD3	9:S:3296:HOH:O	2.09	0.53
2:L:75:HIS:HD2	9:L:3039:HOH:O	1.91	0.53
5:L:2002:MPD:H53	9:L:3427:HOH:O	2.09	0.53
1:S:238:GLN:HG3	5:S:2008:MPD:C3	2.39	0.53
2:L:192:LEU:CB	5:L:2002:MPD:H13	2.39	0.52
1:S:238:GLN:OE1	5:S:2008:MPD:H11	2.10	0.52
1:S:181:MET:HE3	1:S:182:PHE:CE2	2.45	0.51
2:L:52:TYR:HD2	5:L:2010:MPD:H53	1.75	0.50
2:L:214:GLU:OE1	5:L:2003:MPD:H11	2.11	0.50
2:L:96:VAL:O	2:L:100:VAL:HB	2.12	0.50
1:S:238:GLN:HG3	5:S:2008:MPD:H32	1.94	0.49
2:L:47:LYS:HE3	9:L:3784:HOH:O	2.13	0.49
1:S:13:HIS:HE1	1:S:21:SER:OG	1.95	0.49
1:S:265:TYR:OH	2:L:75:HIS:HE1	1.95	0.49
5:L:2002:MPD:H31	9:L:3427:HOH:O	2.12	0.49
1:S:1:LEU:HD22	1:S:43:ASP:HB3	1.94	0.48
5:S:2011:MPD:H52	9:S:3407:HOH:O	2.13	0.48
5:S:2011:MPD:O4	5:S:2011:MPD:H12	2.13	0.48
1:S:1:LEU:HG	2:L:187:THR:HG21	1.96	0.47
1:S:2:MET:HB2	1:S:2:MET:HE2	1.82	0.47
2:L:211:HIS:HD2	2:L:276:ASP:OD2	1.98	0.47
2:L:491:GLY:O	2:L:492:LYS:HD3	2.14	0.46
1:S:3:GLY:O	1:S:4:PRO:O	2.34	0.46
2:L:37:LEU:N	9:L:3748:HOH:O	2.49	0.46
1:S:241:TRP:CH2	1:S:243:VAL:HB	2.51	0.45
2:L:85:THR:OG1	2:L:235:HIS:HD2	2.00	0.45
1:S:234:ILE:O	5:S:2008:MPD:H4	2.17	0.45
1:S:2:MET:HA	2:L:182:GLN:CG	2.46	0.44
1:S:9:VAL:HG21	1:S:40:LEU:HD23	2.00	0.44
1:S:2:MET:CE	1:S:8:SER:HB2	2.47	0.44
2:L:175:LYS:NZ	9:L:3632:HOH:O	2.50	0.44
1:S:188:HIS:HB2	1:S:224:GLY:C	2.44	0.43
1:S:1:LEU:HD12	1:S:1:LEU:N	2.33	0.43
1:S:201:GLU:HB3	1:S:215:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:143:LYS:NZ	9:S:3721:HOH:O	2.49	0.43
2:L:327:ILE:HD11	2:L:396:SER:CB	2.49	0.43
1:S:20:CYS:HB2	1:S:75:GLU:CD	2.43	0.43
1:S:233:LYS:HE2	9:S:3417:HOH:O	2.19	0.43
2:L:500:VAL:CG1	2:L:501:PRO:HD2	2.48	0.43
2:L:321:LYS:N	2:L:321:LYS:HD3	2.34	0.42
1:S:134:ASN:CB	5:S:2004:MPD:H12	2.38	0.42
1:S:4:PRO:HB2	1:S:5:ARG:H	1.58	0.42
1:S:2:MET:CG	1:S:8:SER:HB2	2.49	0.42
2:L:546:CYS:SG	2:L:549:CYS:HB2	2.60	0.42
1:S:1:LEU:HD12	1:S:1:LEU:H3	1.84	0.41
1:S:2:MET:SD	1:S:68:HIS:HB2	2.61	0.41
2:L:491:GLY:C	2:L:492:LYS:HD3	2.45	0.41
1:S:2:MET:CA	2:L:182:GLN:HG2	2.50	0.41
2:L:544:ASP:N	2:L:545:PRO:HD3	2.36	0.41
2:L:291:GLY:HA2	2:L:521:SER:O	2.20	0.41
1:S:244:ASP:O	5:S:2007:MPD:H52	2.21	0.40
5:S:2011:MPD:H32	2:L:173:LYS:HD3	2.03	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	S	265/267 (99%)	257 (97%)	6 (2%)	2 (1%)	16	3
2	L	532/534 (100%)	520 (98%)	11 (2%)	1 (0%)	43	19
All	All	797/801 (100%)	777 (98%)	17 (2%)	3 (0%)	30	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	4	PRO
1	S	5	ARG
2	L	235	HIS

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	S	213/213 (100%)	205 (96%)	8 (4%)	29	4
2	L	438/438 (100%)	420 (96%)	18 (4%)	27	4
All	All	651/651 (100%)	625 (96%)	26 (4%)	28	4

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	1	LEU
1	S	2	MET
1	S	5	ARG
1	S	36	ILE
1	S	61	GLU
1	S	85	ILE
1	S	91	ASN
1	S	230	ASN
2	L	19	SER
2	L	49	LYS
2	L	50	ASN
2	L	100	VAL
2	L	132	HIS
2	L	143	LEU
2	L	152	LYS
2	L	174	LEU
2	L	213	LEU
2	L	233	ASN
2	L	278	LEU
2	L	279	VAL
2	L	285	LYS

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Mol	Chain	Res	Type
2	L	325	LYS
2	L	410	LEU
2	L	418	GLU
2	L	457	ASN
2	L	487	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	13	HIS
1	S	45	HIS
1	S	68	HIS
1	S	126	ASN
1	S	139	HIS
1	S	146	ASN
1	S	229	ASN
1	S	230	ASN
1	S	266	GLN
2	L	36	HIS
2	L	50	ASN
2	L	75	HIS
2	L	78	GLN
2	L	113	ASN
2	L	132	HIS
2	L	188	ASN
2	L	205	ASN
2	L	211	HIS
2	L	233	ASN
2	L	235	HIS
2	L	289	GLN
2	L	334	GLN
2	L	457	ASN
2	L	476	ASN
2	L	513	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	FNE	L	1004	2,8	3,6,8	0.91	0	-		
5	MPD	L	2003	-	7,7,7	0.44	0	9,10,10	0.79	0
5	MPD	L	2009	-	7,7,7	0.33	0	9,10,10	0.68	0
5	MPD	S	2011	-	7,7,7	0.45	0	9,10,10	0.72	0
5	MPD	S	2001	-	7,7,7	0.48	0	9,10,10	0.89	1 (11%)
4	F3S	S	1003	1	0,9,9	-	-	-		
5	MPD	S	2006	-	7,7,7	0.53	0	9,10,10	0.64	0
3	SF4	S	1001	1	0,12,12	-	-	-		
8	CMO	L	1006	7	0,1,1	-	-	-		
3	SF4	S	1002	1	0,12,12	-	-	-		
5	MPD	L	2005	-	7,7,7	0.37	0	9,10,10	0.71	0
5	MPD	L	2010	-	7,7,7	0.39	0	9,10,10	0.58	0
5	MPD	S	2004	-	7,7,7	0.53	0	9,10,10	1.03	0
5	MPD	S	2007	-	7,7,7	0.60	0	9,10,10	0.95	0
5	MPD	L	2002	-	7,7,7	0.41	0	9,10,10	0.60	0
5	MPD	S	2008	-	7,7,7	0.38	0	9,10,10	0.95	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
5	MPD	L	2003	-	-	2/5/5/5	-
5	MPD	L	2009	-	-	0/5/5/5	-
5	MPD	S	2011	-	-	1/5/5/5	-
5	MPD	S	2001	-	-	0/5/5/5	-
4	F3S	S	1003	1	-	-	0/3/3/3
5	MPD	S	2006	-	-	3/5/5/5	-
3	SF4	S	1001	1	-	-	0/6/5/5
5	MPD	L	2010	-	-	2/5/5/5	-
5	MPD	L	2005	-	-	3/5/5/5	-
3	SF4	S	1002	1	-	-	0/6/5/5
5	MPD	S	2004	-	-	1/5/5/5	-
5	MPD	S	2007	-	-	1/5/5/5	-
5	MPD	L	2002	-	-	4/5/5/5	-
5	MPD	S	2008	-	-	3/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2001	MPD	CM-C2-C1	2.07	115.27	110.63

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	2006	MPD	C2-C3-C4-O4
5	S	2006	MPD	C2-C3-C4-C5
5	L	2002	MPD	C2-C3-C4-O4
5	L	2005	MPD	C1-C2-C3-C4
5	S	2007	MPD	O2-C2-C3-C4
5	L	2005	MPD	O2-C2-C3-C4
5	S	2004	MPD	C1-C2-C3-C4
5	S	2006	MPD	C1-C2-C3-C4
5	S	2008	MPD	C1-C2-C3-C4
5	L	2002	MPD	C1-C2-C3-C4
5	L	2002	MPD	CM-C2-C3-C4
5	L	2005	MPD	CM-C2-C3-C4
5	L	2002	MPD	C2-C3-C4-C5
5	S	2008	MPD	O2-C2-C3-C4
5	L	2010	MPD	O2-C2-C3-C4
5	S	2011	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	S	2008	MPD	CM-C2-C3-C4
5	L	2003	MPD	C1-C2-C3-C4
5	L	2003	MPD	CM-C2-C3-C4
5	L	2010	MPD	CM-C2-C3-C4

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2003	MPD	1	0
5	L	2009	MPD	1	0
5	S	2011	MPD	3	0
5	L	2005	MPD	2	0
5	L	2010	MPD	2	0
5	S	2004	MPD	4	0
5	S	2007	MPD	1	0
5	L	2002	MPD	4	0
5	S	2008	MPD	5	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.