



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:54 AM UTC

PDB ID : 1UBM / pdb_00001ubm
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 : 1.40 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)	:	2.49

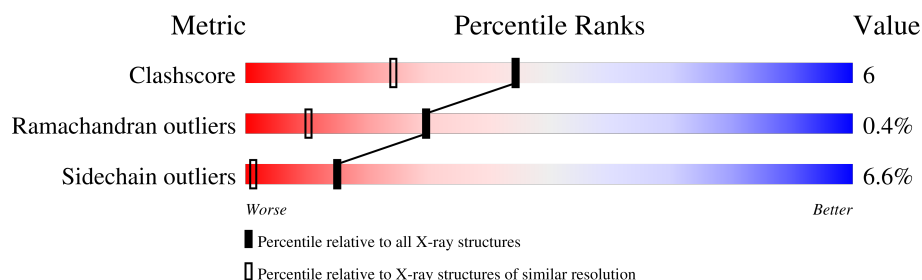
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)

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	 81% 15% . .
2	L	534	 82% 15% .

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
5	MPD	S	2004	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7084 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			

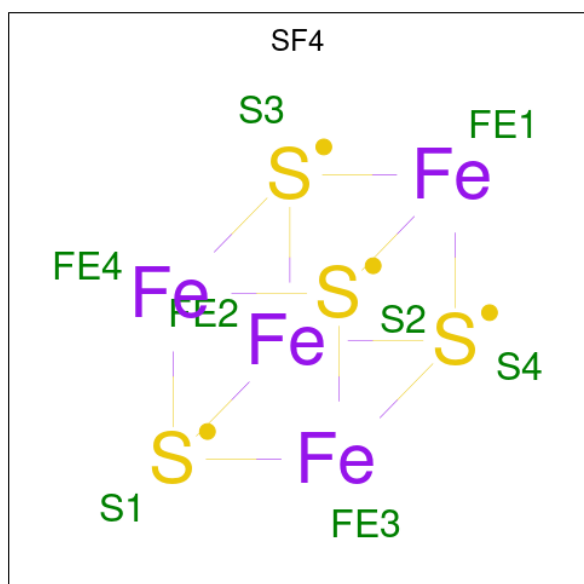
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase Large subunit.

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:

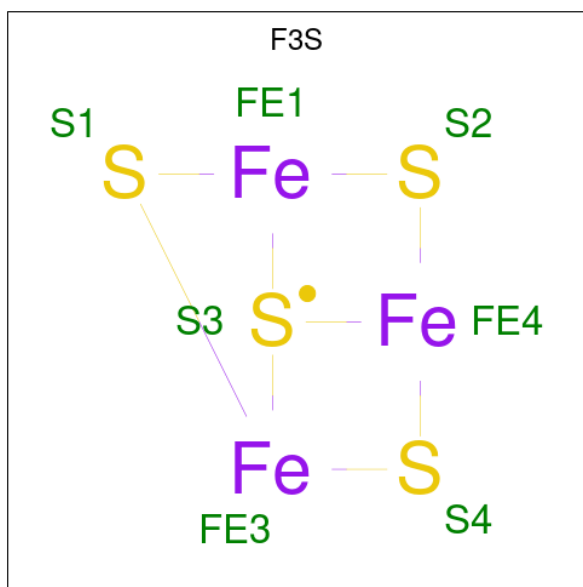
Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

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



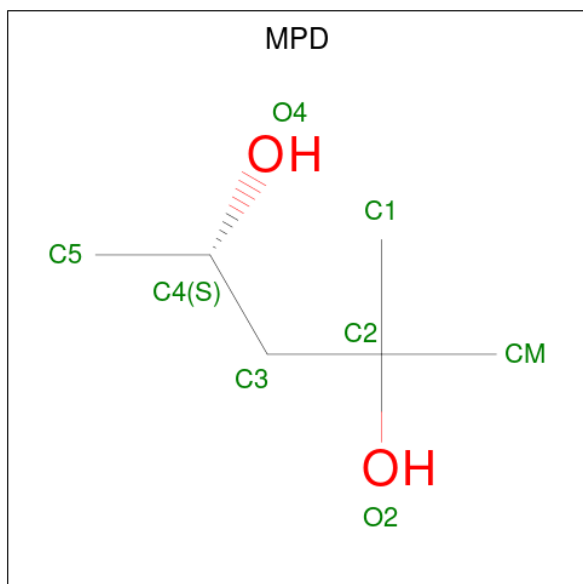
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	S	1	Total	Fe	S	0	0
			8	4	4		

- 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: $\text{C}_6\text{H}_{14}\text{O}_2$).

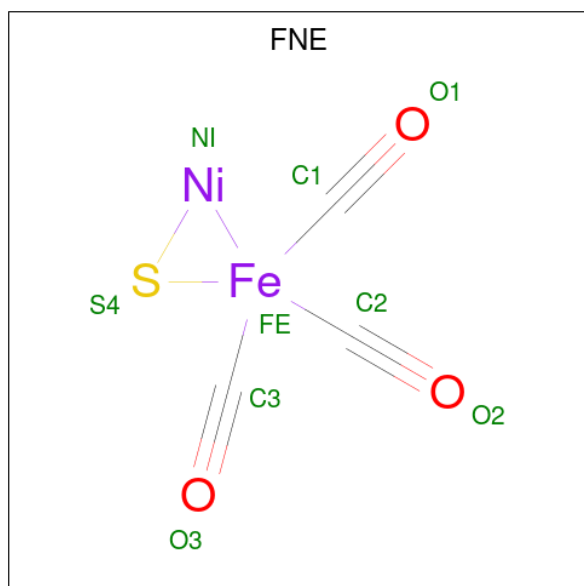


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	C	O	0	0
			8	6	2		
5	S	1	Total	C	O	0	0
			8	6	2		
5	S	1	Total	C	O	0	0
			8	6	2		
5	L	1	Total	C	O	0	0
			8	6	2		
5	L	1	Total	C	O	0	0
			8	6	2		

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

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

- Molecule 7 is (MU-SULPHIDO)-BIS(MU-CYS,S)-[TRICARBONYLIRON-DI-(CYS,S)NICKEL(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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	S	276	Total 276	O 276	0	0
8	L	540	Total 540	O 540	0	0

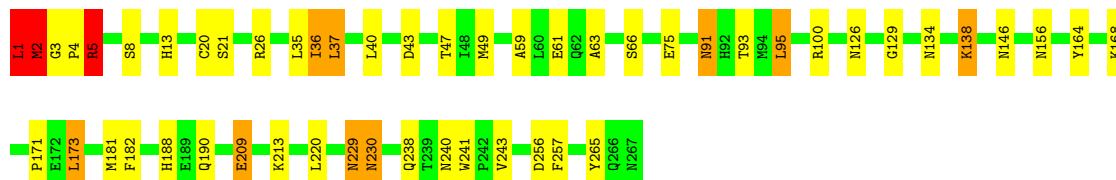
3 Residue-property plots

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.

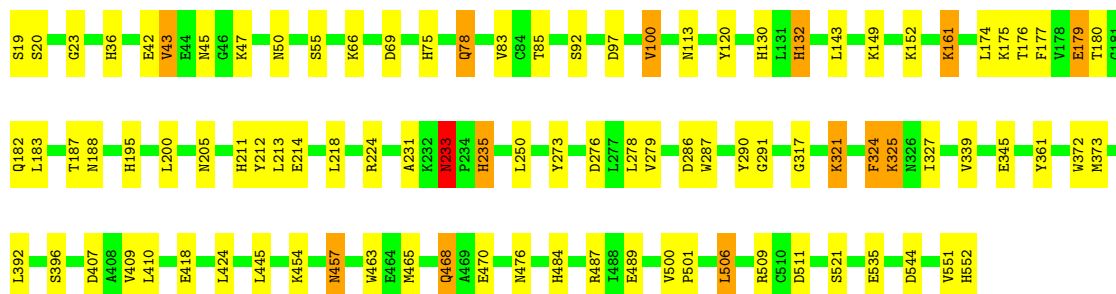
• Molecule 1: Periplasmic [NiFe] hydrogenase Small subunit

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	97.66 Å 125.30 Å 66.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40	Depositor
% Data completeness (in resolution range)	87.3 (20.00-1.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.112 , 0.189	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7084	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: SF4, F3S, MPD, MG, FNE

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	0.64	0/2075	1.67	42/2830 (1.5%)
2	L	0.66	1/4288 (0.0%)	1.63	71/5831 (1.2%)
All	All	0.65	1/6363 (0.0%)	1.64	113/8661 (1.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	552	HIS	C-O	10.17	1.43	1.23

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	424	LEU	CA-C-N	15.43	137.07	119.94
2	L	424	LEU	C-N-CA	15.43	137.07	119.94
1	S	26	ARG	NE-CZ-NH2	14.09	131.88	119.20
1	S	95	LEU	CA-C-N	13.05	137.40	120.44
1	S	95	LEU	C-N-CA	13.05	137.40	120.44
2	L	233	ASN	OD1-CG-ND2	-11.37	111.23	122.60
2	L	235	HIS	CG-CD2-NE2	11.34	118.54	107.20
2	L	233	ASN	CB-CG-OD1	10.85	142.49	120.80
2	L	484	HIS	CB-CG-CD2	10.61	144.99	131.20
1	S	230	ASN	CA-CB-CG	10.39	122.99	112.60
2	L	20	SER	CA-C-O	10.14	131.05	120.40
2	L	97	ASP	CA-CB-CG	9.52	122.12	112.60
1	S	229	ASN	CA-CB-CG	9.15	121.75	112.60
2	L	130	HIS	CA-CB-CG	-9.13	104.67	113.80
1	S	229	ASN	O-C-N	-8.78	114.51	123.29
1	S	95	LEU	O-C-N	-8.76	112.98	122.09
2	L	78	GLN	OE1-CD-NE2	-8.32	114.28	122.60
1	S	238	GLN	OE1-CD-NE2	-8.19	114.41	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	235	HIS	CB-CG-ND1	8.15	134.92	122.70
1	S	126	ASN	CA-CB-CG	8.12	120.72	112.60
2	L	85	THR	CA-C-N	7.97	136.76	121.54
2	L	85	THR	C-N-CA	7.97	136.76	121.54
2	L	50	ASN	CA-CB-CG	7.95	120.55	112.60
2	L	235	HIS	ND1-CG-CD2	-7.88	98.22	106.10
2	L	224	ARG	NE-CZ-NH2	7.82	126.24	119.20
1	S	156	ASN	OD1-CG-ND2	7.76	130.36	122.60
2	L	235	HIS	CE1-NE2-CD2	-7.43	101.57	109.00
2	L	69	ASP	CA-CB-CG	7.40	120.00	112.60
2	L	372	TRP	CA-C-N	7.40	132.00	121.42
2	L	372	TRP	C-N-CA	7.40	132.00	121.42
2	L	113	ASN	CA-CB-CG	7.37	119.97	112.60
2	L	544	ASP	CA-CB-CG	7.27	119.87	112.60
1	S	229	ASN	CA-C-N	7.11	133.98	122.67
1	S	229	ASN	C-N-CA	7.11	133.98	122.67
1	S	3	GLY	O-C-N	-7.08	114.69	121.77
1	S	129	GLY	CA-C-N	7.05	131.13	121.05
1	S	129	GLY	C-N-CA	7.05	131.13	121.05
2	L	465	MET	CA-C-O	7.03	124.87	119.46
2	L	372	TRP	O-C-N	-7.01	112.19	122.43
1	S	238	GLN	CG-CD-OE1	6.98	134.76	120.80
2	L	50	ASN	OD1-CG-ND2	-6.87	115.73	122.60
2	L	484	HIS	CB-CG-ND1	-6.81	112.49	122.70
2	L	233	ASN	CB-CG-ND2	-6.80	106.20	116.40
2	L	224	ARG	NH1-CZ-NH2	-6.74	110.54	119.30
2	L	195	HIS	CB-CG-CD2	6.70	139.91	131.20
2	L	287	TRP	CA-CB-CG	-6.68	100.91	113.60
1	S	126	ASN	OD1-CG-ND2	-6.63	115.97	122.60
2	L	233	ASN	CA-CB-CG	6.62	119.22	112.60
1	S	1	LEU	O-C-N	6.60	133.56	123.00
1	S	26	ARG	CD-NE-CZ	6.51	133.51	124.40
2	L	345	GLU	CA-C-O	6.49	128.32	120.92
1	S	26	ARG	NH1-CZ-NH2	-6.39	110.99	119.30
2	L	42	GLU	CA-C-N	-6.33	114.32	123.06
2	L	42	GLU	C-N-CA	-6.33	114.32	123.06
1	S	126	ASN	CB-CG-OD1	6.26	133.33	120.80
2	L	457	ASN	CA-CB-CG	6.19	118.79	112.60
2	L	83	VAL	N-CA-C	-6.18	105.11	110.74
2	L	372	TRP	CA-C-O	6.13	126.96	119.11
1	S	47	THR	CA-C-N	-6.11	115.35	122.14
1	S	47	THR	C-N-CA	-6.11	115.35	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	324	PHE	CA-CB-CG	-6.04	107.76	113.80
2	L	85	THR	O-C-N	-5.99	115.74	122.75
1	S	100	ARG	CD-NE-CZ	5.92	132.69	124.40
2	L	78	GLN	CG-CD-OE1	5.89	132.59	120.80
2	L	361	TYR	O-C-N	5.89	129.99	123.16
1	S	129	GLY	O-C-N	-5.85	115.09	122.70
2	L	100	VAL	CA-CB-CG2	-5.83	100.48	110.40
2	L	273	TYR	CB-CG-CD1	5.81	129.52	120.80
2	L	214	GLU	CA-C-O	5.80	126.70	120.55
2	L	273	TYR	CA-C-N	-5.79	116.59	120.24
2	L	273	TYR	C-N-CA	-5.79	116.59	120.24
2	L	551	VAL	CB-CA-C	-5.77	104.92	111.55
1	S	91	ASN	OD1-CG-ND2	-5.76	116.84	122.60
2	L	45	ASN	CA-CB-CG	5.72	118.32	112.60
1	S	257	PHE	CA-CB-CG	5.66	119.46	113.80
1	S	36	ILE	CA-CB-CG1	5.65	120.01	110.40
2	L	509	ARG	NE-CZ-NH1	5.64	127.14	121.50
2	L	424	LEU	O-C-N	-5.62	116.28	122.07
1	S	2	MET	CA-C-N	5.55	130.59	121.87
1	S	2	MET	C-N-CA	5.55	130.59	121.87
2	L	506	LEU	CA-CB-CG	5.53	135.67	116.30
1	S	49	MET	CA-C-O	5.51	127.56	121.56
2	L	476	ASN	CB-CG-ND2	-5.50	108.15	116.40
2	L	468	GLN	CA-CB-CG	5.49	125.07	114.10
1	S	93	THR	OG1-CB-CG2	-5.48	98.33	109.30
2	L	132	HIS	CA-CB-CG	5.48	119.28	113.80
2	L	511	ASP	CA-CB-CG	5.47	118.07	112.60
2	L	85	THR	CA-C-O	5.46	127.88	121.87
2	L	233	ASN	CB-CA-C	5.41	117.36	110.16
2	L	92	SER	CA-CB-OG	5.37	121.84	111.10
1	S	1	LEU	CA-C-O	-5.35	111.71	120.80
2	L	476	ASN	CA-CB-CG	-5.35	107.25	112.60
1	S	188	HIS	CB-CG-CD2	-5.34	124.26	131.20
2	L	212	TYR	CA-CB-CG	5.33	123.49	113.90
2	L	339	VAL	CA-C-O	-5.30	115.32	119.46
1	S	35	LEU	CA-C-O	-5.27	115.28	120.82
2	L	205	ASN	CA-CB-CG	5.26	117.86	112.60
2	L	489	GLU	CB-CG-CD	5.25	121.52	112.60
2	L	409	VAL	O-C-N	5.24	127.04	121.91
2	L	120	TYR	CA-CB-CG	5.24	123.32	113.90
1	S	138	LYS	CA-C-O	5.22	126.49	120.90
2	L	188	ASN	CA-CB-CG	5.15	117.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	190	GLN	OE1-CD-NE2	5.14	127.74	122.60
2	L	321	LYS	CA-CB-CG	5.13	124.36	114.10
2	L	50	ASN	CA-C-O	-5.12	115.80	121.33
1	S	5	ARG	CA-C-O	-5.12	113.19	120.51
1	S	91	ASN	CA-CB-CG	5.10	117.70	112.60
2	L	407	ASP	CA-C-O	5.09	125.94	120.55
2	L	290	TYR	CA-C-N	5.06	129.92	120.87
2	L	290	TYR	C-N-CA	5.06	129.92	120.87
1	S	240	ASN	OD1-CG-ND2	5.05	127.65	122.60
1	S	209	GLU	CB-CG-CD	5.03	121.15	112.60
1	S	229	ASN	OD1-CG-ND2	-5.02	117.58	122.60

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	S	2019	0	1949	42	0
2	L	4177	0	4129	41	0
3	S	16	0	0	0	0
4	S	7	0	0	0	0
5	L	16	0	28	7	0
5	S	24	0	42	10	0
6	L	1	0	0	0	0
7	L	8	0	0	0	0
8	L	540	0	0	12	0
8	S	276	0	0	5	0
All	All	7084	0	6148	75	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 6.

All (75) 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	1.23	0.97
1:S:2:MET:HB2	2:L:182:GLN:HE21	1.38	0.88
1:S:1:LEU:HG	2:L:187:THR:HG21	1.58	0.85
1:S:2:MET:HA	2:L:182:GLN:HG2	1.63	0.81
1:S:2:MET:HG2	1:S:8:SER:HB2	1.64	0.77
1:S:134:ASN:HB2	5:S:2004:MPD:H12	1.67	0.77
1:S:2:MET:HG3	8:S:3298:HOH:O	1.85	0.74
2:L:175:LYS:O	2:L:179:GLU:HG3	1.87	0.74
2:L:176:THR:O	2:L:180:THR:HG23	1.87	0.73
1:S:5:ARG:HH11	1:S:5:ARG:HA	1.55	0.72
2:L:325:LYS:HD2	8:L:3643:HOH:O	1.91	0.70
1:S:1:LEU:HD21	1:S:59:ALA:O	1.91	0.70
1:S:146:ASN:ND2	5:S:2004:MPD:H13	2.02	0.69
2:L:392:LEU:HD22	5:L:2006:MPD:H11	1.77	0.66
5:L:2010:MPD:HM3	8:L:3335:HOH:O	1.99	0.62
1:S:2:MET:HB3	1:S:43:ASP:OD1	1.99	0.62
1:S:1:LEU:HD12	1:S:1:LEU:H3	1.67	0.59
1:S:2:MET:HE2	2:L:182:GLN:NE2	2.18	0.59
1:S:37:LEU:HD12	2:L:177:PHE:CD2	2.36	0.59
1:S:13:HIS:HD2	8:S:3034:HOH:O	1.85	0.58
1:S:256:ASP:HB3	8:S:3418:HOH:O	2.03	0.58
2:L:325:LYS:N	2:L:325:LYS:HE3	2.17	0.58
1:S:181:MET:HE3	1:S:182:PHE:CZ	2.39	0.57
2:L:454:LYS:HE2	8:L:3326:HOH:O	2.05	0.57
2:L:211:HIS:HE1	8:L:3220:HOH:O	1.87	0.56
1:S:2:MET:HB2	2:L:182:GLN:NE2	2.16	0.55
2:L:75:HIS:HD2	8:L:3074:HOH:O	1.90	0.54
1:S:1:LEU:HA	2:L:187:THR:OG1	2.08	0.54
2:L:535:GLU:HB2	8:L:3725:HOH:O	2.08	0.53
2:L:233:ASN:C	2:L:233:ASN:HD22	2.17	0.52
1:S:265:TYR:OH	2:L:75:HIS:HE1	1.92	0.52
1:S:241:TRP:CH2	1:S:243:VAL:HB	2.44	0.52
2:L:392:LEU:HD22	5:L:2006:MPD:H31	1.92	0.52
1:S:181:MET:HE3	1:S:182:PHE:CE2	2.44	0.51
1:S:164:TYR:OH	5:S:2007:MPD:H53	2.11	0.51
2:L:291:GLY:HA2	2:L:521:SER:O	2.12	0.50
2:L:470:GLU:HB2	8:L:3600:HOH:O	2.12	0.49
1:S:1:LEU:HD22	1:S:43:ASP:HB3	1.94	0.49
1:S:2:MET:HA	2:L:182:GLN:CG	2.38	0.48
1:S:209:GLU:O	1:S:213:LYS:HG3	2.13	0.48
1:S:134:ASN:HD22	5:S:2004:MPD:H12	1.78	0.48
1:S:134:ASN:CB	5:S:2004:MPD:H12	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:324:PHE:CD2	5:L:2006:MPD:H13	2.48	0.48
1:S:5:ARG:HA	1:S:5:ARG:HD3	1.53	0.48
1:S:37:LEU:HD12	2:L:177:PHE:CE2	2.50	0.47
5:S:2004:MPD:H11	8:S:3119:HOH:O	2.14	0.47
2:L:317:GLY:HA2	8:L:3788:HOH:O	2.14	0.47
2:L:55:SER:OG	2:L:373:MET:HE3	2.15	0.47
2:L:36:HIS:HD2	8:L:3070:HOH:O	1.97	0.46
1:S:164:TYR:CZ	5:S:2007:MPD:H53	2.51	0.46
1:S:171:PRO:O	1:S:173:LEU:HD13	2.15	0.46
2:L:463:TRP:CH2	5:L:2010:MPD:H32	2.51	0.45
1:S:20:CYS:HB2	1:S:75:GLU:CD	2.42	0.45
2:L:23:GLY:O	2:L:43:VAL:HG13	2.17	0.45
1:S:2:MET:CG	1:S:8:SER:HB2	2.40	0.45
2:L:470:GLU:OE1	2:L:487:ARG:NE	2.49	0.45
1:S:1:LEU:HB3	2:L:187:THR:OG1	2.17	0.45
2:L:211:HIS:HD2	2:L:276:ASP:OD2	1.99	0.45
2:L:327:ILE:HD11	2:L:396:SER:CB	2.47	0.45
1:S:2:MET:HG2	1:S:8:SER:CB	2.41	0.44
2:L:161:LYS:HG3	8:L:3180:HOH:O	2.17	0.44
1:S:1:LEU:HD13	8:S:3298:HOH:O	2.16	0.44
2:L:78:GLN:HG2	2:L:235:HIS:CD2	2.53	0.43
2:L:500:VAL:CG1	2:L:501:PRO:HD2	2.48	0.43
2:L:535:GLU:N	8:L:3725:HOH:O	2.50	0.43
1:S:1:LEU:HD12	1:S:1:LEU:N	2.32	0.43
1:S:13:HIS:HE1	1:S:21:SER:OG	2.01	0.43
5:L:2006:MPD:O4	5:L:2006:MPD:O2	2.30	0.43
1:S:1:LEU:HD22	1:S:63:ALA:HB2	2.01	0.42
1:S:134:ASN:HB3	5:S:2004:MPD:H4	2.01	0.42
2:L:286:ASP:OD2	2:L:286:ASP:N	2.50	0.42
2:L:149:LYS:NZ	8:L:3687:HOH:O	2.49	0.42
5:S:2007:MPD:H12	5:S:2007:MPD:H4	1.97	0.41
2:L:392:LEU:CD2	5:L:2006:MPD:H31	2.49	0.41
1:S:1:LEU:CG	2:L:187:THR:HG21	2.40	0.41

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%)	255 (96%)	8 (3%)	2 (1%)	16	3
2	L	532/534 (100%)	521 (98%)	10 (2%)	1 (0%)	43	19
All	All	797/801 (100%)	776 (97%)	18 (2%)	3 (0%)	30	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	5	ARG
1	S	4	PRO
2	L	231	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	S	213/213 (100%)	197 (92%)	16 (8%)	12	1
2	L	438/438 (100%)	411 (94%)	27 (6%)	16	1
All	All	651/651 (100%)	608 (93%)	43 (7%)	15	1

All (43) 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

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Mol	Chain	Res	Type
1	S	36	ILE
1	S	37	LEU
1	S	40	LEU
1	S	61	GLU
1	S	66	SER
1	S	91	ASN
1	S	95	LEU
1	S	138	LYS
1	S	168	LYS
1	S	173	LEU
1	S	220	LEU
1	S	229	ASN
1	S	230	ASN
2	L	19	SER
2	L	43	VAL
2	L	47	LYS
2	L	66	LYS
2	L	100	VAL
2	L	132	HIS
2	L	143	LEU
2	L	152	LYS
2	L	161	LYS
2	L	174	LEU
2	L	179	GLU
2	L	183	LEU
2	L	200	LEU
2	L	213	LEU
2	L	218	LEU
2	L	233	ASN
2	L	250	LEU
2	L	278	LEU
2	L	279	VAL
2	L	321	LYS
2	L	325	LYS
2	L	410	LEU
2	L	418	GLU
2	L	445	LEU
2	L	457	ASN
2	L	468	GLN
2	L	506	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	13	HIS
1	S	45	HIS
1	S	68	HIS
1	S	92	HIS
1	S	126	ASN
1	S	139	HIS
1	S	146	ASN
1	S	229	ASN
1	S	266	GLN
1	S	267	ASN
2	L	36	HIS
2	L	50	ASN
2	L	75	HIS
2	L	132	HIS
2	L	211	HIS
2	L	233	ASN
2	L	235	HIS
2	L	310	ASN
2	L	451	ASN
2	L	476	ASN
2	L	513	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	S	1001	1	0,12,12	-	-	-		
3	SF4	S	1002	1	0,12,12	-	-	-		
5	MPD	S	2001	-	7,7,7	0.47	0	9,10,10	0.94	1 (11%)
7	FNE	L	1004	2	3,7,9	2.15	2 (66%)	-		
5	MPD	S	2004	-	7,7,7	0.44	0	9,10,10	0.51	0
5	MPD	L	2010	-	7,7,7	0.39	0	9,10,10	0.50	0
5	MPD	L	2006	-	7,7,7	0.47	0	9,10,10	0.53	0
4	F3S	S	1003	1	0,9,9	-	-	-		
5	MPD	S	2007	-	7,7,7	0.46	0	9,10,10	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	S	1001	1	-	-	0/6/5/5
3	SF4	S	1002	1	-	-	0/6/5/5
5	MPD	S	2001	-	-	0/5/5/5	-
5	MPD	S	2004	-	-	0/5/5/5	-
5	MPD	L	2010	-	-	2/5/5/5	-
5	MPD	L	2006	-	-	3/5/5/5	-
4	F3S	S	1003	1	-	-	0/3/3/3
5	MPD	S	2007	-	-	5/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1004	FNE	O2-C2	-3.04	1.10	1.16
7	L	1004	FNE	O1-C1	2.15	1.20	1.16

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2001	MPD	CM-C2-C1	2.15	115.45	110.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	2004	MPD	7	0
5	L	2010	MPD	2	0
5	L	2006	MPD	5	0
5	S	2007	MPD	3	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.