



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:49 PM EDT

PDB ID : 1WUK / pdb_00001wuk
Title : High resolution Structure Of The Oxidized State Of [Nife]Hydrogenase From Desulfovibrio Vulgaris Miyazaki F
Authors : Ogata, H.; Hirota, S.; Nakahara, A.; Komori, H.; Shibata, N.; Kato, T.; Kano, K.; Higuchi, Y.
Deposited on : 2004-12-07
Resolution : 1.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

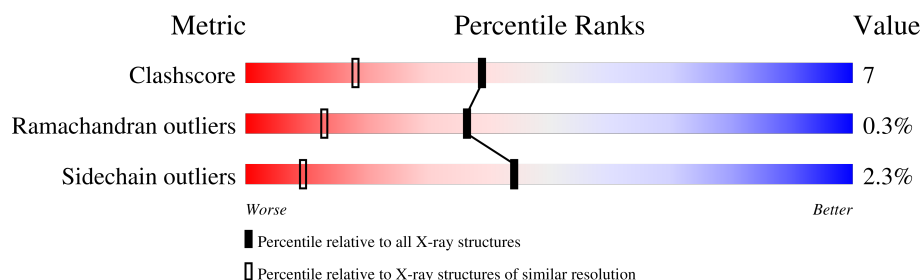
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	267	
2	L	534	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7122 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	3	0
			2022	1284	342	378	18			

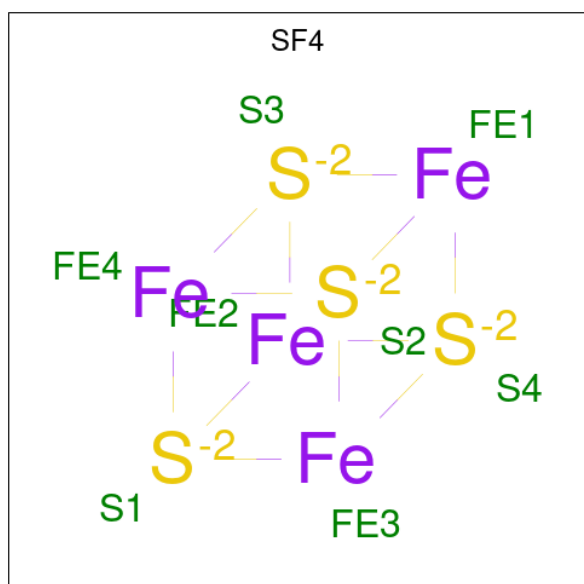
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	534	Total	C	N	O	S	0	2	0
			4187	2681	726	765	15			

There are 2 discrepancies between the modelled and reference sequences:

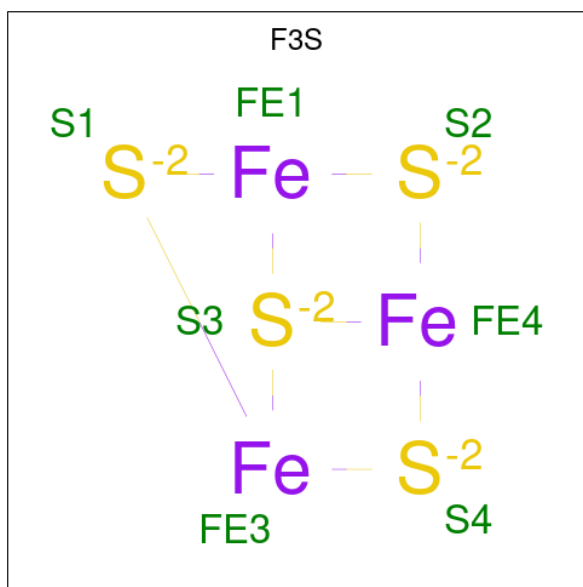
Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

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



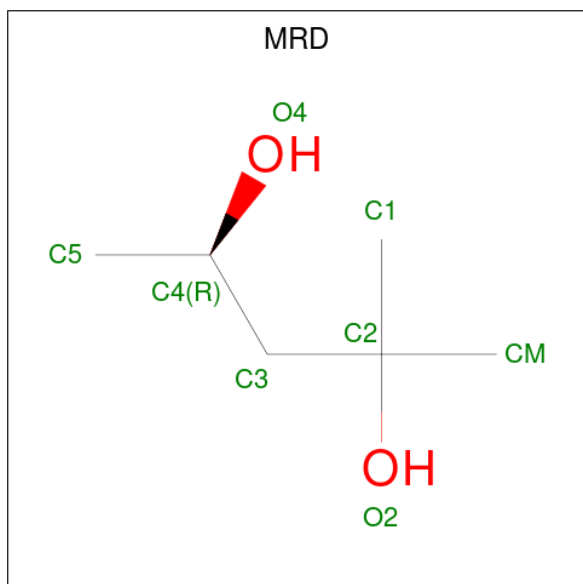
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	S	1	Total	Fe	S	0	0
			8	4	4		

- 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 (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).

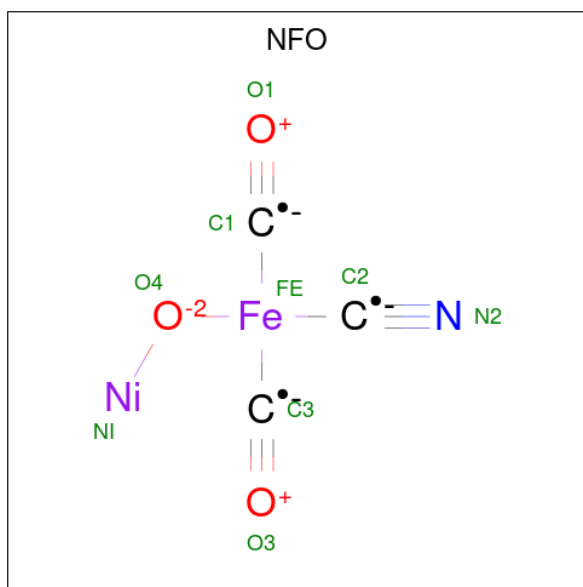


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	C	O	0	0
			8	6	2		

- 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 NI-FE OXIDIZED ACTIVE CENTER (CCD ID: NFO) (formula: C₃FeNNiO₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	L	1	Total	C	Fe	N	Ni	O	0	0
			9	3	1	1	1	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	S	302	Total	O	0	0
			302	302		
8	L	570	Total	O	0	0
			570	570		

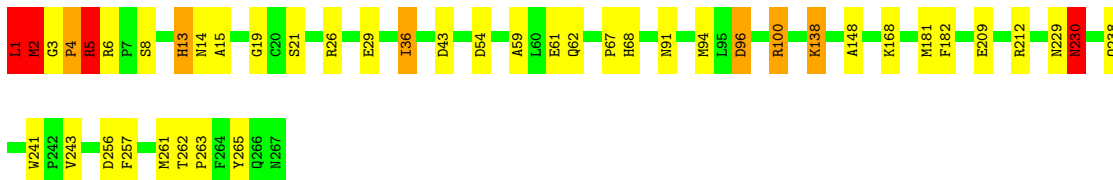
3 Residue-property plots

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.

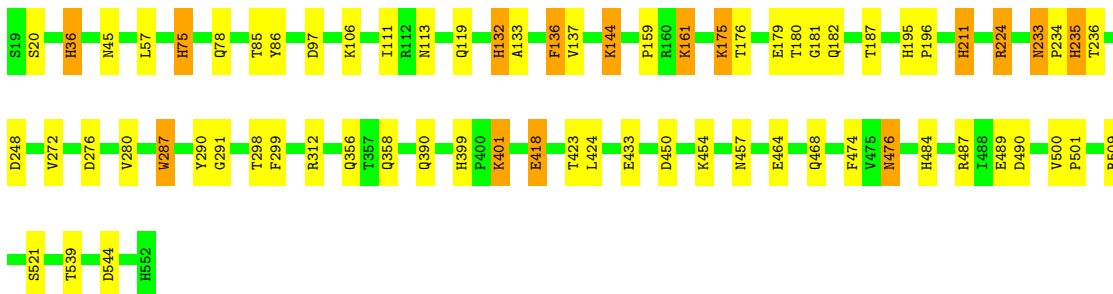
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

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	98.29Å 125.84Å 66.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.094 , 0.123	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7122	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: CSO, MRD, NFO, MG, SF4, F3S

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	1.00	0/2099	1.50	31/2862 (1.1%)
2	L	0.98	3/4302 (0.1%)	1.38	65/5848 (1.1%)
All	All	0.98	3/6401 (0.0%)	1.42	96/8710 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	195	HIS	CG-ND1	-9.36	1.27	1.38
2	L	509	ARG	CZ-NH2	-6.29	1.25	1.33
2	L	399	HIS	CD2-NE2	-5.73	1.31	1.37

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	2	MET	CA-C-N	19.04	151.76	121.87
1	S	2	MET	C-N-CA	19.04	151.76	121.87
1	S	100	ARG	CD-NE-CZ	16.29	147.20	124.40
1	S	1	LEU	O-C-N	14.79	146.67	123.00
2	L	424	LEU	CA-C-N	11.24	132.42	119.94
2	L	424	LEU	C-N-CA	11.24	132.42	119.94
1	S	209	GLU	CB-CG-CD	11.21	131.66	112.60
1	S	1	LEU	CA-C-O	-11.12	101.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	224	ARG	NE-CZ-NH2	10.93	129.04	119.20
2	L	136[A]	PHE	CA-CB-CG	10.51	124.31	113.80
2	L	136[B]	PHE	CA-CB-CG	10.51	124.31	113.80
2	L	487	ARG	CD-NE-CZ	9.20	137.28	124.40
1	S	256	ASP	CA-CB-CG	9.14	121.74	112.60
2	L	45	ASN	CA-CB-CG	8.44	121.03	112.60
1	S	3	GLY	O-C-N	-8.31	113.46	121.77
2	L	97	ASP	CA-CB-CG	8.19	120.79	112.60
2	L	132	HIS	CB-CG-CD2	-8.06	120.72	131.20
2	L	144	LYS	CA-CB-CG	8.04	130.18	114.10
2	L	75	HIS	CB-CG-CD2	-8.04	120.75	131.20
2	L	224	ARG	NH1-CZ-NH2	-7.95	108.97	119.30
2	L	181	GLY	CA-C-N	7.94	133.60	122.41
2	L	181	GLY	C-N-CA	7.94	133.60	122.41
1	S	2	MET	CB-CG-SD	7.75	135.96	112.70
1	S	13	HIS	CB-CG-CD2	-7.71	121.18	131.20
2	L	36	HIS	CB-CG-CD2	-7.56	121.37	131.20
1	S	2	MET	CB-CA-C	7.51	122.08	109.99
2	L	20	SER	N-CA-CB	7.35	121.49	109.88
2	L	159	PRO	O-C-N	-7.28	112.39	122.30
1	S	1	LEU	CB-CA-C	-7.21	96.40	110.10
2	L	195	HIS	ND1-CG-CD2	-7.20	98.90	106.10
2	L	418	GLU	CB-CG-CD	7.12	124.71	112.60
2	L	195	HIS	CG-ND1-CE1	7.11	121.38	109.30
1	S	5	ARG	CD-NE-CZ	-7.05	114.53	124.40
2	L	36	HIS	CB-CG-ND1	7.03	133.24	122.70
1	S	230	ASN	CA-CB-CG	6.88	119.48	112.60
2	L	489	GLU	CB-CG-CD	6.86	124.26	112.60
2	L	195	HIS	ND1-CE1-NE2	-6.70	101.70	108.40
1	S	1	LEU	CD1-CG-CD2	6.66	125.45	110.80
2	L	401	LYS	CA-C-N	6.62	128.90	120.56
2	L	401	LYS	C-N-CA	6.62	128.90	120.56
2	L	544	ASP	CA-CB-CG	6.52	119.12	112.60
2	L	161	LYS	CA-C-N	6.51	132.16	122.99
2	L	161	LYS	C-N-CA	6.51	132.16	122.99
1	S	2	MET	O-C-N	-6.46	116.71	123.56
2	L	159	PRO	CA-C-N	6.39	130.44	121.24
2	L	159	PRO	C-N-CA	6.39	130.44	121.24
2	L	211	HIS	CB-CG-ND1	6.38	132.27	122.70
2	L	235	HIS	CB-CG-CD2	-6.35	122.94	131.20
2	L	20	SER	CB-CA-C	-6.33	100.75	110.88
2	L	287	TRP	CE3-CZ3-CH2	6.19	129.15	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	61	GLU	CB-CG-CD	6.07	122.91	112.60
1	S	96	ASP	CA-CB-CG	6.06	118.66	112.60
2	L	75	HIS	CB-CG-ND1	6.00	131.71	122.70
2	L	45	ASN	CB-CG-ND2	5.99	125.39	116.40
1	S	5	ARG	CA-C-O	-5.95	112.01	120.51
2	L	113	ASN	CA-CB-CG	5.89	118.50	112.60
2	L	424	LEU	O-C-N	-5.89	116.00	122.07
2	L	132	HIS	CB-CG-ND1	5.87	131.51	122.70
2	L	401	LYS	O-C-N	-5.83	115.51	122.15
2	L	454	LYS	CG-CD-CE	5.79	124.62	111.30
1	S	212	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	L	106	LYS	CD-CE-NZ	5.73	130.23	111.90
1	S	148	ALA	CA-C-N	5.72	132.61	121.41
1	S	148	ALA	C-N-CA	5.72	132.61	121.41
1	S	67	PRO	CA-C-N	5.68	131.09	121.14
1	S	67	PRO	C-N-CA	5.68	131.09	121.14
2	L	159	PRO	CA-C-O	5.68	126.95	119.00
2	L	464	GLU	CB-CG-CD	5.66	122.23	112.60
2	L	137	VAL	CA-C-N	5.66	130.73	122.41
2	L	137	VAL	C-N-CA	5.66	130.73	122.41
2	L	433	GLU	CG-CD-OE1	5.64	131.38	118.40
1	S	13	HIS	CB-CG-ND1	5.55	131.03	122.70
2	L	399	HIS	CG-CD2-NE2	5.52	112.72	107.20
2	L	45	ASN	CB-CG-OD1	-5.48	109.84	120.80
2	L	211	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	S	1	LEU	CB-CG-CD1	-5.46	94.32	110.70
2	L	196	PRO	CA-C-N	5.42	132.19	122.38
2	L	196	PRO	C-N-CA	5.42	132.19	122.38
1	S	1	LEU	N-CA-CB	5.40	119.69	110.50
2	L	234	PRO	CA-C-N	5.32	131.70	121.54
2	L	234	PRO	C-N-CA	5.32	131.70	121.54
1	S	54	ASP	CA-CB-CG	5.31	117.91	112.60
2	L	450	ASP	CA-CB-CG	5.30	117.90	112.60
2	L	484	HIS	ND1-CE1-NE2	5.29	113.69	108.40
2	L	287	TRP	CA-CB-CG	-5.29	103.55	113.60
1	S	138	LYS	CA-C-O	5.28	126.33	120.63
2	L	248	ASP	CA-CB-CG	5.27	117.87	112.60
1	S	2	MET	CA-C-O	5.26	126.64	120.75
2	L	468	GLN	OE1-CD-NE2	-5.24	117.36	122.60
2	L	399	HIS	CB-CG-ND1	5.24	130.56	122.70
2	L	85	THR	CA-C-N	5.17	131.41	121.54
2	L	85	THR	C-N-CA	5.17	131.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	181	GLY	O-C-N	-5.13	115.82	122.34
1	S	138	LYS	CA-CB-CG	5.05	124.20	114.10
2	L	490	ASP	CA-CB-CG	5.04	117.64	112.60
2	L	358	GLN	CG-CD-NE2	5.03	123.95	116.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	4	PRO	Peptide

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	2022	0	1948	40	0
2	L	4187	0	4133	54	0
3	S	16	0	0	0	0
4	S	7	0	0	0	0
5	S	8	0	13	1	0
6	L	1	0	0	0	0
7	L	9	0	0	0	0
8	L	570	0	0	26	0
8	S	302	0	0	16	0
All	All	7122	0	6094	84	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 (84) 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:2:MET:HA	2:L:182:GLN:HG2	1.40	1.03
1:S:2:MET:HB2	2:L:182:GLN:HE21	1.29	0.96
2:L:390:GLN:HA	8:L:5636:HOH:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:423:THR:HG21	8:L:5622:HOH:O	1.73	0.86
2:L:176:THR:O	2:L:180:THR:HG23	1.84	0.76
1:S:94:MET:HE1	8:S:5589:HOH:O	1.85	0.75
1:S:2:MET:HG2	1:S:8:SER:HB2	1.69	0.75
1:S:1:LEU:HD11	1:S:62:GLN:HG2	1.69	0.75
8:S:5589:HOH:O	2:L:57:LEU:HD13	1.89	0.72
1:S:5:ARG:HB2	8:L:5362:HOH:O	1.90	0.72
8:S:5625:HOH:O	2:L:180:THR:HG21	1.90	0.72
1:S:1:LEU:HD21	1:S:59:ALA:O	1.93	0.69
2:L:86:TYR:HB3	8:L:5641:HOH:O	1.91	0.69
1:S:1:LEU:HG	2:L:187:THR:HG21	1.73	0.69
2:L:175:LYS:O	2:L:179:GLU:HG3	1.94	0.68
2:L:233:ASN:C	2:L:233:ASN:HD22	2.05	0.65
2:L:299:PHE:HB3	8:L:5626:HOH:O	1.97	0.64
1:S:26:ARG:HH21	2:L:233:ASN:HD21	1.43	0.64
1:S:68:HIS:HB2	8:S:5285:HOH:O	1.99	0.62
2:L:78:GLN:HE21	2:L:86:TYR:H	1.48	0.61
2:L:539:THR:N	8:L:5622:HOH:O	2.34	0.61
2:L:287:TRP:CZ3	8:L:5622:HOH:O	2.52	0.60
2:L:272:VAL:HG22	8:L:5576:HOH:O	2.02	0.59
2:L:211:HIS:HD2	2:L:276:ASP:OD2	1.85	0.59
2:L:211:HIS:HE1	8:L:5412:HOH:O	1.86	0.59
2:L:133:ALA:HA	2:L:136[B]:PHE:CZ	2.37	0.59
8:S:5589:HOH:O	2:L:57:LEU:HD22	2.02	0.59
1:S:29:GLU:HG3	8:S:5658:HOH:O	2.02	0.58
2:L:36:HIS:HD2	8:L:5118:HOH:O	1.86	0.58
2:L:290:TYR:HE2	8:L:5650:HOH:O	1.86	0.58
2:L:133:ALA:HA	2:L:136[B]:PHE:CE1	2.39	0.57
2:L:474:PHE:HB3	8:L:5626:HOH:O	2.03	0.57
5:S:2001:MRD:H5C2	8:S:5359:HOH:O	2.04	0.57
2:L:119:GLN:HG2	8:L:5641:HOH:O	2.04	0.57
1:S:2:MET:HB3	1:S:43:ASP:OD1	2.05	0.56
1:S:257:PHE:HB2	1:S:261[B]:MET:HG2	1.86	0.56
1:S:1:LEU:HD22	1:S:43:ASP:HB3	1.87	0.56
2:L:298:THR:HG21	8:L:5636:HOH:O	2.05	0.56
1:S:2:MET:CB	2:L:182:GLN:HE21	2.12	0.55
1:S:238:GLN:HE21	2:L:224:ARG:HH21	1.55	0.54
1:S:2:MET:CG	1:S:8:SER:HB2	2.37	0.54
1:S:2:MET:HE3	8:S:5177:HOH:O	2.07	0.53
2:L:233:ASN:HA	8:L:5606:HOH:O	2.08	0.53
1:S:1:LEU:CG	2:L:187:THR:HG21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:75:HIS:HD2	8:L:5021:HOH:O	1.91	0.52
1:S:265:TYR:OH	2:L:75:HIS:HE1	1.93	0.52
1:S:15:ALA:HA	8:S:5589:HOH:O	2.10	0.51
1:S:1:LEU:HD12	1:S:2:MET:H	1.76	0.50
2:L:136[B]:PHE:CD1	2:L:280:VAL:HG11	2.46	0.50
2:L:111:ILE:HD13	8:L:5642:HOH:O	2.12	0.50
1:S:2:MET:HB2	2:L:182:GLN:NE2	2.12	0.49
1:S:19:GLY:HA3	8:L:5666:HOH:O	2.13	0.48
1:S:29:GLU:N	8:S:5658:HOH:O	2.46	0.48
1:S:1:LEU:HD12	1:S:1:LEU:H3	1.79	0.47
1:S:1:LEU:HB3	2:L:187:THR:OG1	2.14	0.47
2:L:312:ARG:NH1	8:L:5626:HOH:O	2.48	0.47
1:S:14:ASN:O	8:S:5589:HOH:O	2.20	0.47
1:S:1:LEU:HA	2:L:187:THR:OG1	2.15	0.47
2:L:418:GLU:H	2:L:418:GLU:CD	2.23	0.47
1:S:96:ASP:OD2	1:S:100:ARG:NH1	2.49	0.46
1:S:1:LEU:HD13	8:S:5328:HOH:O	2.14	0.46
2:L:401:LYS:HG2	8:L:5670:HOH:O	2.16	0.45
1:S:5:ARG:HB3	1:S:6:ARG:H	1.65	0.45
2:L:236:THR:N	8:L:5606:HOH:O	2.50	0.45
1:S:36:ILE:N	1:S:36:ILE:HD13	2.32	0.44
2:L:235:HIS:N	8:L:5606:HOH:O	2.50	0.44
2:L:356:GLN:N	8:L:5567:HOH:O	2.49	0.44
1:S:36:ILE:HG23	8:S:5075:HOH:O	2.18	0.44
2:L:287:TRP:HZ3	8:L:5622:HOH:O	1.96	0.44
2:L:287:TRP:NE1	8:L:5650:HOH:O	2.49	0.44
8:S:5589:HOH:O	2:L:57:LEU:CD1	2.58	0.43
1:S:262:THR:HA	1:S:263:PRO:C	2.44	0.43
1:S:241:TRP:CH2	1:S:243:VAL:HB	2.54	0.43
1:S:2:MET:HG3	8:S:5328:HOH:O	2.18	0.43
1:S:13:HIS:HE1	1:S:21:SER:OG	2.02	0.42
1:S:229:ASN:HD22	1:S:230:ASN:H	1.67	0.42
2:L:500:VAL:CG1	2:L:501:PRO:HD2	2.50	0.42
1:S:181:MET:HE3	1:S:182:PHE:CE2	2.55	0.41
2:L:86:TYR:HD1	8:L:5641:HOH:O	2.03	0.41
2:L:299:PHE:H	2:L:476:ASN:ND2	2.18	0.41
2:L:291:GLY:HA2	2:L:521:SER:O	2.21	0.41
2:L:211:HIS:CD2	2:L:276:ASP:OD2	2.70	0.40
2:L:233:ASN:C	2:L:233:ASN:ND2	2.72	0.40
8:S:5589:HOH:O	2:L:57:LEU:CD2	2.67	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	268/267 (100%)	261 (97%)	5 (2%)	2 (1%)	18	4
2	L	533/534 (100%)	518 (97%)	15 (3%)	0	100	100
All	All	801/801 (100%)	779 (97%)	20 (2%)	2 (0%)	36	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	5	ARG
1	S	4	PRO

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	216/213 (101%)	208 (96%)	8 (4%)	30	3
2	L	439/437 (100%)	432 (98%)	7 (2%)	55	19
All	All	655/650 (101%)	640 (98%)	15 (2%)	44	9

All (15) 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

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Mol	Chain	Res	Type
1	S	91	ASN
1	S	138	LYS
1	S	168	LYS
1	S	230	ASN
2	L	132	HIS
2	L	144	LYS
2	L	161	LYS
2	L	175	LYS
2	L	233	ASN
2	L	457	ASN
2	L	476	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	13	HIS
1	S	45	HIS
1	S	68	HIS
1	S	139	HIS
1	S	229	ASN
1	S	230	ASN
1	S	238	GLN
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	457	ASN
2	L	468	GLN
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 ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSO	L	546	7,2	3,6,7	0.55	0	1,6,8	0.90	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	CSO	L	546	7,2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	546	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	1002	1	0,12,12	-	-	-		
3	SF4	S	1001	1	0,12,12	-	-	-		
5	MRD	S	2001	-	7,7,7	1.03	0	9,10,10	1.10	0
4	F3S	S	1003	1	0,9,9	-	-	-		
7	NFO	L	1004	2	3,8,8	1.08	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	1002	1	-	-	0/6/5/5
3	SF4	S	1001	1	-	-	0/6/5/5
5	MRD	S	2001	-	-	3/5/5/5	-
4	F3S	S	1003	1	-	-	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	2001	MRD	C2-C3-C4-O4
5	S	2001	MRD	CM-C2-C3-C4
5	S	2001	MRD	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	2001	MRD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.