



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:56 AM UTC

PDB ID : 1UBK / pdb_00001ubk
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 : 1.18 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

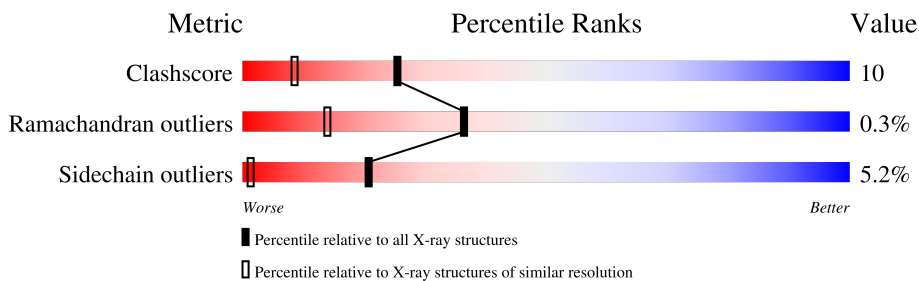
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.18 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	1845 (1.20-1.16)
Ramachandran outliers	187476	1789 (1.20-1.16)
Sidechain outliers	187428	1789 (1.20-1.16)

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 9 unique types of molecules in this entry. The entry contains 7345 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			

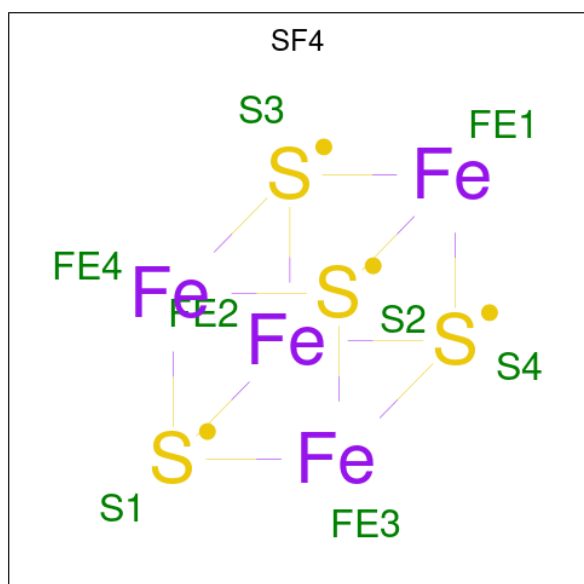
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase Large subunit.

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:

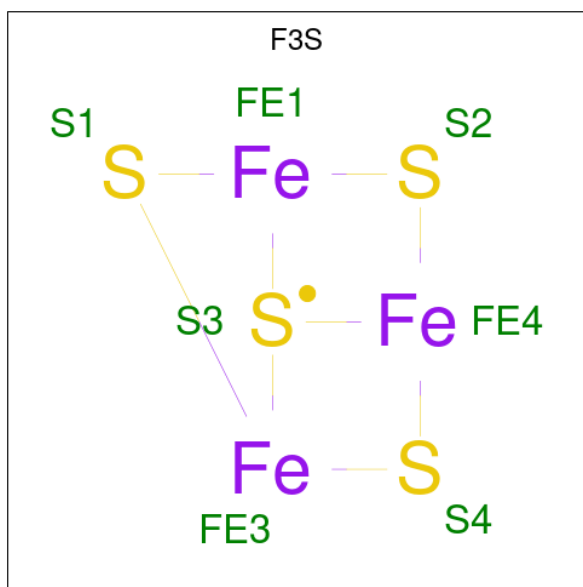
Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

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



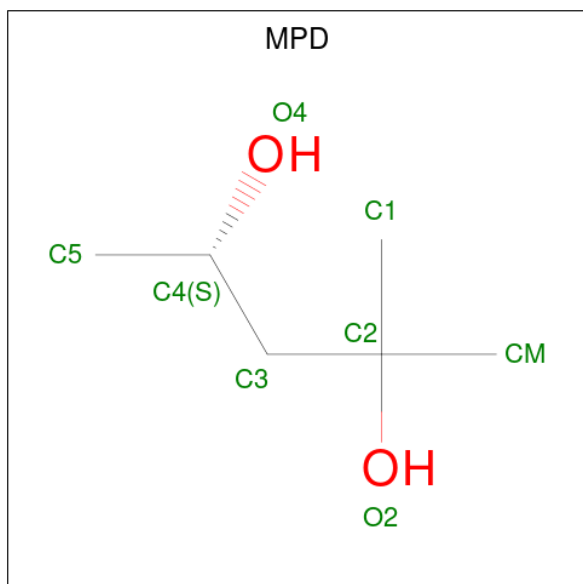
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	S	1	Total	Fe	S	0	0
			8	4	4		

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

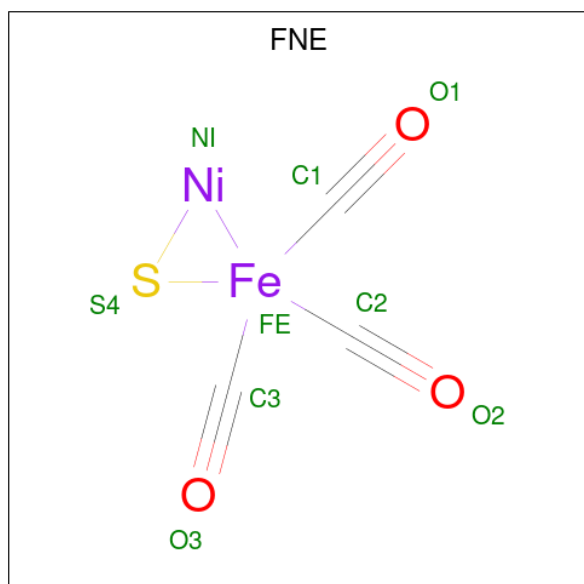


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0

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

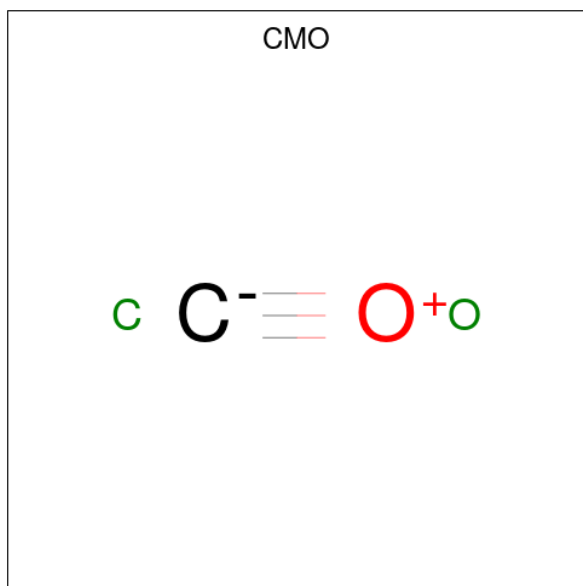
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total Mg 1 1	0	0

- 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 8 3 1 1 3	0	0

- 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.

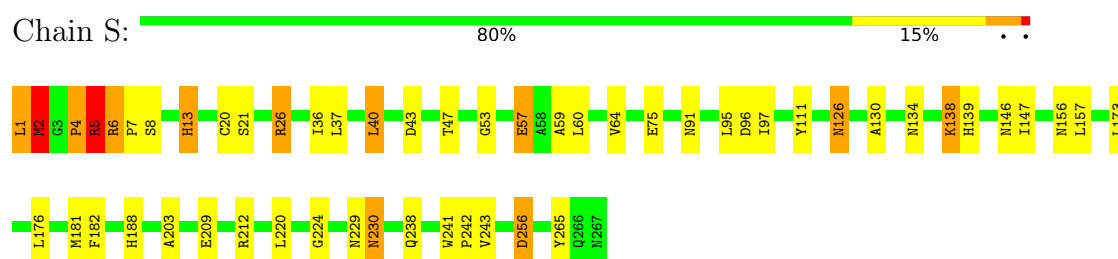
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	371	Total	O	0	0
			371	371		
9	L	688	Total	O	0	0
			688	688		

3 Residue-property plots

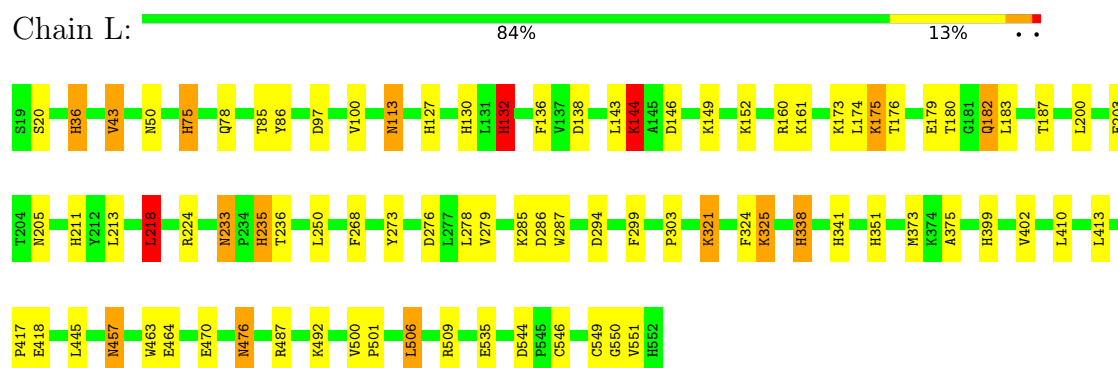
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 2: Periplasmic [NiFe] hydrogenase Large subunit



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	97.60 Å 125.26 Å 66.42 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.18	Depositor
% Data completeness (in resolution range)	82.3 (20.00-1.18)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.110 , 0.151	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7345	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: CMO, FNE, MG, F3S, SF4, MPD

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	0.97	1/2075 (0.0%)	1.43	17/2830 (0.6%)
2	L	0.92	2/4288 (0.0%)	1.44	35/5831 (0.6%)
All	All	0.94	3/6363 (0.0%)	1.43	52/8661 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	126	ASN	C-O	6.58	1.27	1.23
2	L	75	HIS	ND1-CE1	6.25	1.38	1.32
2	L	132	HIS	ND1-CE1	5.40	1.38	1.32

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	182	GLN	OE1-CD-NE2	-14.78	107.82	122.60
2	L	136	PHE	CA-CB-CG	9.48	123.28	113.80
1	S	5	ARG	CD-NE-CZ	-8.95	111.88	124.40
2	L	130	HIS	CA-CB-CG	-8.70	105.10	113.80
2	L	132	HIS	CB-CG-CD2	-8.53	120.11	131.20
2	L	218	LEU	CD1-CG-CD2	7.98	128.36	110.80
2	L	506	LEU	CA-CB-CG	7.71	143.28	116.30
2	L	544	ASP	CA-CB-CG	7.65	120.25	112.60
1	S	13	HIS	CB-CG-CD2	-7.26	121.76	131.20
2	L	36	HIS	CB-CG-ND1	7.15	133.43	122.70
2	L	127	HIS	CA-CB-CG	-6.97	106.83	113.80
2	L	36	HIS	CB-CG-CD2	-6.95	122.17	131.20
2	L	75	HIS	CB-CG-CD2	-6.83	122.32	131.20
2	L	294	ASP	CA-CB-CG	6.79	119.39	112.60
2	L	97	ASP	CA-CB-CG	6.78	119.38	112.60
1	S	212	ARG	NE-CZ-NH2	6.65	125.18	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	235	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	S	138	LYS	CA-CB-CG	6.61	127.32	114.10
2	L	273	TYR	CA-C-N	-6.60	116.08	120.24
2	L	273	TYR	C-N-CA	-6.60	116.08	120.24
2	L	20	SER	CA-C-O	6.40	128.63	121.40
1	S	96	ASP	CA-CB-CG	6.35	118.95	112.60
2	L	324	PHE	CA-CB-CG	-6.29	107.51	113.80
1	S	47	THR	CA-C-N	-6.06	115.41	122.14
1	S	47	THR	C-N-CA	-6.06	115.41	122.14
2	L	43	VAL	CB-CA-C	6.00	120.06	110.82
2	L	132	HIS	CB-CG-ND1	5.91	131.57	122.70
2	L	287	TRP	CA-CB-CG	-5.90	102.38	113.60
2	L	457	ASN	CA-CB-CG	5.84	118.44	112.60
2	L	351	HIS	CA-CB-CG	-5.77	108.03	113.80
2	L	182	GLN	CG-CD-NE2	5.71	124.97	116.40
2	L	75	HIS	CA-CB-CG	-5.66	108.14	113.80
1	S	209	GLU	CB-CG-CD	5.65	122.21	112.60
1	S	6	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	S	138	LYS	CA-C-O	5.53	126.82	120.90
2	L	75	HIS	CB-CG-ND1	5.50	130.96	122.70
1	S	26	ARG	CG-CD-NE	-5.49	99.91	112.00
1	S	256	ASP	CA-CB-CG	-5.46	107.14	112.60
2	L	551	VAL	CB-CA-C	-5.39	105.36	111.55
1	S	13	HIS	CB-CG-ND1	5.37	130.75	122.70
2	L	146	ASP	N-CA-CB	-5.34	103.38	110.17
1	S	57	GLU	CA-CB-CG	5.32	124.75	114.10
1	S	5	ARG	CA-C-O	-5.30	112.93	120.51
2	L	144	LYS	CA-CB-CG	5.29	124.69	114.10
2	L	113	ASN	CA-CB-CG	5.29	117.89	112.60
2	L	338	HIS	CA-CB-CG	-5.21	108.59	113.80
1	S	2	MET	CA-C-N	5.18	130.01	121.87
1	S	2	MET	C-N-CA	5.18	130.01	121.87
2	L	20	SER	O-C-N	-5.18	116.90	123.17
2	L	341	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
2	L	273	TYR	CB-CG-CD1	5.11	128.46	120.80
2	L	476	ASN	CA-CB-CG	-5.05	107.55	112.60

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	63	0
2	L	4177	0	4129	69	0
3	S	16	0	0	0	0
4	S	7	0	0	0	0
5	L	32	0	56	7	0
5	S	24	0	42	5	0
6	L	1	0	0	0	0
7	L	8	0	0	0	0
8	L	2	0	0	0	0
9	L	688	0	0	18	0
9	S	371	0	0	11	0
All	All	7345	0	6176	119	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 10.

All (119) 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	1.25	1.00
1:S:238:GLN:HE21	2:L:224:ARG:HH21	1.22	0.87
1:S:26:ARG:HH21	2:L:233:ASN:HD21	1.21	0.86
1:S:126:ASN:HD21	1:S:130:ALA:H	1.21	0.85
2:L:470:GLU:HG2	2:L:487:ARG:HD3	1.59	0.84
1:S:176:LEU:HD13	9:S:3183:HOH:O	1.80	0.82
2:L:487:ARG:HB3	9:L:4011:HOH:O	1.84	0.77
5:L:2011:MPD:HM1	9:L:3322:HOH:O	1.84	0.76
2:L:78:GLN:HE21	2:L:86:TYR:H	1.31	0.75
1:S:6:ARG:H	2:L:182:GLN:HE22	1.32	0.75
2:L:173:LYS:HB2	5:L:2012:MPD:H11	1.69	0.75
1:S:256:ASP:HB3	9:S:3425:HOH:O	1.85	0.73
2:L:175:LYS:O	2:L:179:GLU:HG3	1.89	0.73
1:S:2:MET:HA	2:L:182:GLN:HG2	1.72	0.72
5:L:2010:MPD:HM3	9:L:3337:HOH:O	1.91	0.71
1:S:1:LEU:HB3	2:L:187:THR:OG1	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1:LEU:HD21	1:S:59:ALA:O	1.90	0.71
1:S:2:MET:SD	1:S:8:SER:HB2	2.34	0.68
1:S:6:ARG:H	2:L:182:GLN:NE2	1.90	0.68
1:S:146:ASN:ND2	5:S:2004:MPD:H13	2.05	0.68
1:S:134:ASN:HB2	5:S:2004:MPD:H12	1.75	0.68
2:L:176:THR:O	2:L:180:THR:HG23	1.95	0.67
1:S:2:MET:HE2	2:L:182:GLN:HG2	1.78	0.63
1:S:2:MET:HG2	1:S:8:SER:HB2	1.81	0.61
1:S:1:LEU:HG	2:L:187:THR:HG21	1.81	0.61
1:S:5:ARG:HB2	9:L:3193:HOH:O	2.02	0.60
1:S:6:ARG:HB2	2:L:182:GLN:NE2	2.15	0.60
2:L:211:HIS:HE1	9:L:3221:HOH:O	1.84	0.60
1:S:13:HIS:HD2	9:S:3034:HOH:O	1.84	0.60
2:L:173:LYS:CB	5:L:2012:MPD:H11	2.33	0.59
1:S:6:ARG:HB2	2:L:182:GLN:HE22	1.68	0.58
2:L:50:ASN:HD21	2:L:509:ARG:NH2	2.01	0.58
1:S:7:PRO:HG2	1:S:40:LEU:HD12	1.86	0.57
2:L:36:HIS:HD2	9:L:3070:HOH:O	1.86	0.57
1:S:238:GLN:NE2	2:L:224:ARG:HH21	1.98	0.57
2:L:211:HIS:HD2	2:L:276:ASP:OD2	1.88	0.56
1:S:156:ASN:HD21	1:S:230:ASN:HD21	1.52	0.56
1:S:230:ASN:HD22	1:S:230:ASN:H	1.54	0.56
2:L:321:LYS:N	2:L:321:LYS:HD3	2.21	0.56
2:L:535:GLU:HB2	9:L:3816:HOH:O	2.06	0.55
1:S:1:LEU:HD22	1:S:43:ASP:HB3	1.88	0.55
1:S:53:GLY:HA3	9:L:4004:HOH:O	2.07	0.55
1:S:2:MET:HG2	1:S:43:ASP:OD1	2.07	0.55
1:S:1:LEU:HD12	1:S:1:LEU:H3	1.71	0.55
2:L:100:VAL:HG11	2:L:463:TRP:CE3	2.42	0.55
1:S:1:LEU:HD13	9:S:3300:HOH:O	2.07	0.55
2:L:492:LYS:HD2	9:L:3436:HOH:O	2.06	0.55
2:L:233:ASN:C	2:L:233:ASN:HD22	2.16	0.54
2:L:299:PHE:H	2:L:476:ASN:ND2	2.06	0.53
1:S:265:TYR:OH	2:L:75:HIS:HE1	1.90	0.53
1:S:134:ASN:HD22	5:S:2004:MPD:H12	1.74	0.53
1:S:2:MET:HA	2:L:182:GLN:CG	2.38	0.53
2:L:399:HIS:HD2	2:L:402:VAL:H	1.56	0.53
1:S:1:LEU:CG	2:L:187:THR:HG21	2.39	0.52
2:L:470:GLU:HG2	2:L:487:ARG:CD	2.36	0.52
1:S:2:MET:CG	1:S:8:SER:HB2	2.39	0.52
2:L:75:HIS:HD2	9:L:3074:HOH:O	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:138:ASP:H	2:L:205:ASN:ND2	2.08	0.51
1:S:1:LEU:HD12	1:S:1:LEU:N	2.26	0.51
1:S:241:TRP:CH2	1:S:243:VAL:HB	2.45	0.51
1:S:139:HIS:H	1:S:139:HIS:CD2	2.29	0.51
1:S:229:ASN:HD22	1:S:230:ASN:H	1.60	0.50
5:L:2012:MPD:O4	5:L:2012:MPD:O2	2.29	0.50
1:S:5:ARG:HB3	2:L:182:GLN:OE1	2.12	0.50
1:S:13:HIS:HE1	1:S:21:SER:OG	1.93	0.49
2:L:78:GLN:HE22	2:L:236:THR:H	1.60	0.49
2:L:160:ARG:HB3	9:L:4000:HOH:O	2.11	0.49
2:L:285:LYS:HE2	2:L:413:LEU:O	2.13	0.49
2:L:399:HIS:CD2	2:L:402:VAL:H	2.30	0.49
1:S:2:MET:HB3	1:S:43:ASP:OD1	2.11	0.48
1:S:26:ARG:HH21	2:L:233:ASN:ND2	2.00	0.48
1:S:203:ALA:O	1:S:220:LEU:HD13	2.14	0.48
2:L:325:LYS:HD2	2:L:325:LYS:N	2.29	0.48
1:S:2:MET:HE1	1:S:6:ARG:O	2.14	0.48
2:L:50:ASN:HD21	2:L:509:ARG:HH22	1.61	0.48
2:L:487:ARG:HD2	9:L:4011:HOH:O	2.14	0.47
1:S:5:ARG:HD3	9:S:3903:HOH:O	2.14	0.46
2:L:218:LEU:HD13	2:L:268:PHE:CD2	2.50	0.46
1:S:2:MET:HG3	9:S:3300:HOH:O	2.15	0.46
2:L:175:LYS:NZ	9:L:3656:HOH:O	2.49	0.46
1:S:2:MET:HE1	1:S:4:PRO:O	2.16	0.45
9:S:3617:HOH:O	5:L:2012:MPD:H52	2.15	0.45
2:L:175:LYS:NZ	9:L:3578:HOH:O	2.49	0.45
1:S:134:ASN:CB	5:S:2004:MPD:H12	2.43	0.45
2:L:500:VAL:CG1	2:L:501:PRO:HD2	2.47	0.45
1:S:5:ARG:HA	9:S:3903:HOH:O	2.17	0.45
1:S:6:ARG:N	2:L:182:GLN:HE22	2.08	0.45
2:L:160:ARG:HD2	9:L:3759:HOH:O	2.16	0.45
1:S:126:ASN:HD21	1:S:130:ALA:N	2.00	0.44
2:L:535:GLU:N	9:L:3816:HOH:O	2.49	0.44
1:S:188:HIS:HB2	1:S:224:GLY:C	2.43	0.44
1:S:126:ASN:ND2	1:S:130:ALA:H	2.03	0.44
2:L:149:LYS:HD3	2:L:203:GLU:HG2	1.98	0.44
2:L:299:PHE:H	2:L:476:ASN:HD22	1.65	0.44
2:L:338:HIS:HB2	2:L:375:ALA:HB3	2.00	0.43
2:L:78:GLN:NE2	2:L:235:HIS:HA	2.33	0.43
2:L:175:LYS:HE2	2:L:175:LYS:HB3	1.54	0.43
2:L:417:PRO:HD2	2:L:418:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:100:VAL:HG13	2:L:464:GLU:O	2.18	0.43
2:L:113:ASN:HD21	2:L:303:PRO:HD2	1.83	0.43
2:L:173:LYS:HG2	5:L:2012:MPD:H31	2.00	0.43
2:L:321:LYS:HD3	2:L:321:LYS:H	1.83	0.43
1:S:5:ARG:NH1	9:S:3903:HOH:O	2.52	0.43
1:S:60:LEU:O	1:S:64:VAL:HG22	2.19	0.42
1:S:111:TYR:CE1	1:S:157:LEU:HB2	2.54	0.42
2:L:85:THR:OG1	2:L:235:HIS:HD2	2.03	0.42
1:S:97:ILE:HD11	9:S:3968:HOH:O	2.19	0.41
2:L:144:LYS:NZ	9:L:4040:HOH:O	2.49	0.41
2:L:286:ASP:OD2	2:L:286:ASP:N	2.53	0.41
1:S:5:ARG:HD3	1:S:5:ARG:HA	1.33	0.41
1:S:147:ILE:HD13	1:S:157:LEU:HA	2.02	0.41
1:S:181:MET:HE3	1:S:182:PHE:CE2	2.55	0.41
2:L:373:MET:HE2	2:L:550:GLY:HA3	2.02	0.41
2:L:132:HIS:HD2	9:L:3113:HOH:O	2.03	0.41
2:L:218:LEU:CD1	2:L:268:PHE:HB2	2.51	0.41
1:S:20:CYS:HB2	1:S:75:GLU:CD	2.46	0.40
1:S:57:GLU:HG2	9:S:3826:HOH:O	2.22	0.40
2:L:100:VAL:HG11	2:L:463:TRP:HE3	1.84	0.40
2:L:546:CYS:SG	2:L:549:CYS:HB2	2.62	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%)	256 (97%)	7 (3%)	2 (1%)	16	2
2	L	532/534 (100%)	519 (98%)	13 (2%)	0	100	100
All	All	797/801 (100%)	775 (97%)	20 (2%)	2 (0%)	36	14

All (2) Ramachandran outliers are listed below:

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

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%)	201 (94%)	12 (6%)	19	1
2	L	438/438 (100%)	416 (95%)	22 (5%)	22	1
All	All	651/651 (100%)	617 (95%)	34 (5%)	21	1

All (34) 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	37	LEU
1	S	40	LEU
1	S	91	ASN
1	S	95	LEU
1	S	138	LYS
1	S	173	LEU
1	S	230	ASN
1	S	242	PRO
2	L	43	VAL
2	L	132	HIS
2	L	143	LEU
2	L	144	LYS
2	L	152	LYS
2	L	161	LYS
2	L	174	LEU
2	L	175	LYS
2	L	183	LEU

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Mol	Chain	Res	Type
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	445	LEU
2	L	457	ASN
2	L	506	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	13	HIS
1	S	68	HIS
1	S	91	ASN
1	S	126	ASN
1	S	139	HIS
1	S	146	ASN
1	S	190	GLN
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	171	GLN
2	L	182	GLN
2	L	188	ASN
2	L	205	ASN
2	L	211	HIS
2	L	233	ASN
2	L	235	HIS
2	L	310	ASN

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Mol	Chain	Res	Type
2	L	334	GLN
2	L	399	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
5	MPD	S	2004	-	7,7,7	0.85	0	9,10,10	0.95	1 (11%)
3	SF4	S	1002	1	0,12,12	-	-	-		
5	MPD	S	2007	-	7,7,7	0.56	0	9,10,10	1.03	0
5	MPD	L	2006	-	7,7,7	0.48	0	9,10,10	0.47	0
5	MPD	L	2010	-	7,7,7	0.50	0	9,10,10	0.87	0
5	MPD	L	2011	-	7,7,7	0.47	0	9,10,10	0.73	0
5	MPD	S	2001	-	7,7,7	0.62	0	9,10,10	1.45	2 (22%)
5	MPD	L	2012	-	7,7,7	0.50	0	9,10,10	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CMO	L	1006	7	0,1,1	-	-	-		
3	SF4	S	1001	1	0,12,12	-	-	-		
7	FNE	L	1004	8,2	3,7,9	1.03	0	-		
4	F3S	S	1003	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
5	MPD	S	2007	-	-	1/5/5/5	-
5	MPD	S	2004	-	-	0/5/5/5	-
3	SF4	S	1002	1	-	-	0/6/5/5
5	MPD	L	2006	-	-	4/5/5/5	-
3	SF4	S	1001	1	-	-	0/6/5/5
5	MPD	L	2010	-	-	3/5/5/5	-
5	MPD	S	2001	-	-	1/5/5/5	-
5	MPD	L	2012	-	-	3/5/5/5	-
5	MPD	L	2011	-	-	3/5/5/5	-
4	F3S	S	1003	1	-	-	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2001	MPD	CM-C2-C1	2.87	117.05	110.63
5	S	2004	MPD	O2-C2-CM	2.13	114.63	107.99
5	S	2001	MPD	O2-C2-C3	-2.03	101.67	109.27

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	2011	MPD	C2-C3-C4-O4
5	L	2011	MPD	C2-C3-C4-C5
5	S	2001	MPD	C1-C2-C3-C4
5	S	2007	MPD	C1-C2-C3-C4
5	L	2006	MPD	CM-C2-C3-C4
5	L	2010	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	L	2012	MPD	C1-C2-C3-C4
5	L	2012	MPD	CM-C2-C3-C4
5	L	2006	MPD	O2-C2-C3-C4
5	L	2010	MPD	O2-C2-C3-C4
5	L	2012	MPD	O2-C2-C3-C4
5	L	2006	MPD	C2-C3-C4-O4
5	L	2006	MPD	C1-C2-C3-C4
5	L	2010	MPD	C1-C2-C3-C4
5	L	2011	MPD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	2004	MPD	5	0
5	L	2010	MPD	1	0
5	L	2011	MPD	1	0
5	L	2012	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.