



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:02 am GMT

PDB ID : 1UBU  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

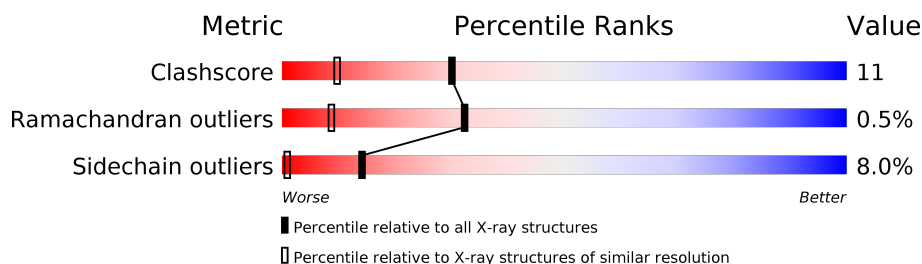
# 1 Overall quality at a glance

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	112137	1063 (1.38-1.34)
Ramachandran outliers	110173	1048 (1.38-1.34)
Sidechain outliers	110143	1048 (1.38-1.34)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	267	 75% 18% 5% •
2	L	534	 79% 15% 5% •

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7157 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			

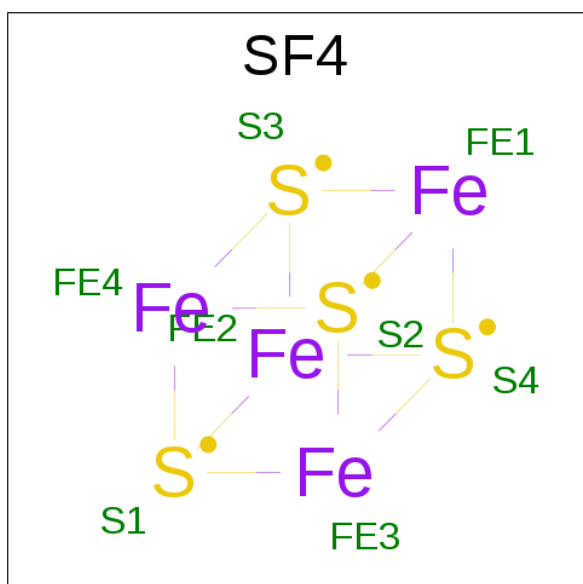
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase Large subunit.

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:

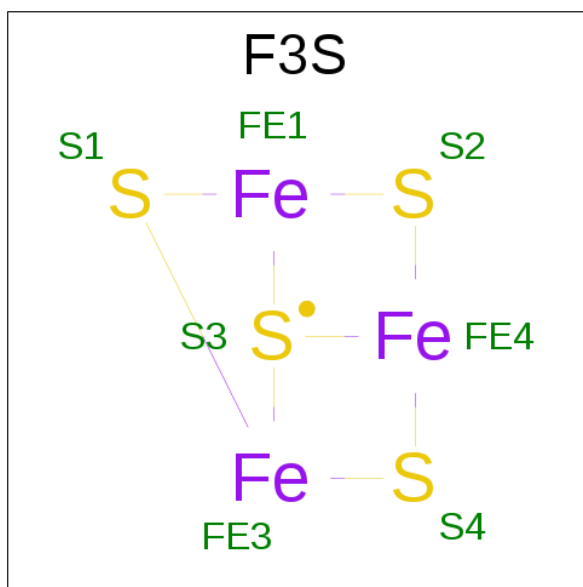
Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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 (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).

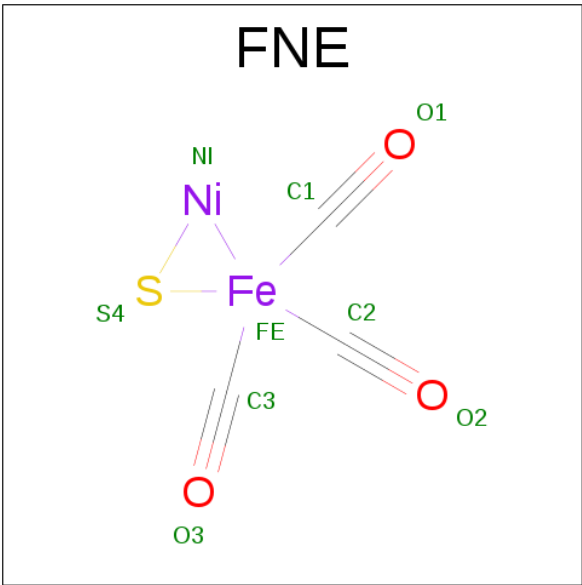


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is (MU-SULPHIDO)-BIS(MU-CYS,S)-[TRICARBONYLIRON-DI-(CYS,S)NIC KEL(II)](FE-NI) (three-letter code: FNE) (formula:  $\text{C}_3\text{FeNiO}_3\text{S}$ ).



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

- Molecule 7 is water.

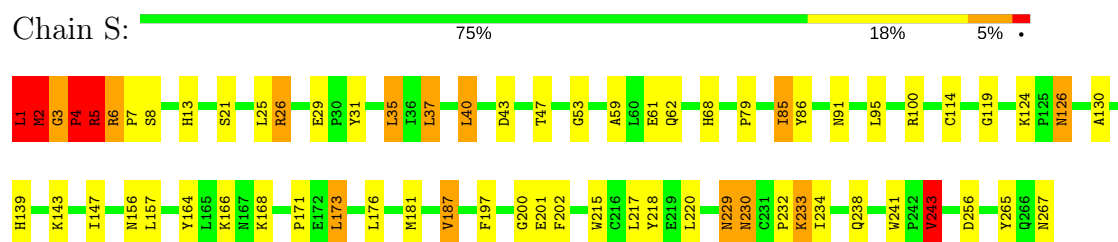
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	S	317	Total	O	0	0
			317	317		
7	L	612	Total	O	0	0
			612	612		

### 3 Residue-property plots

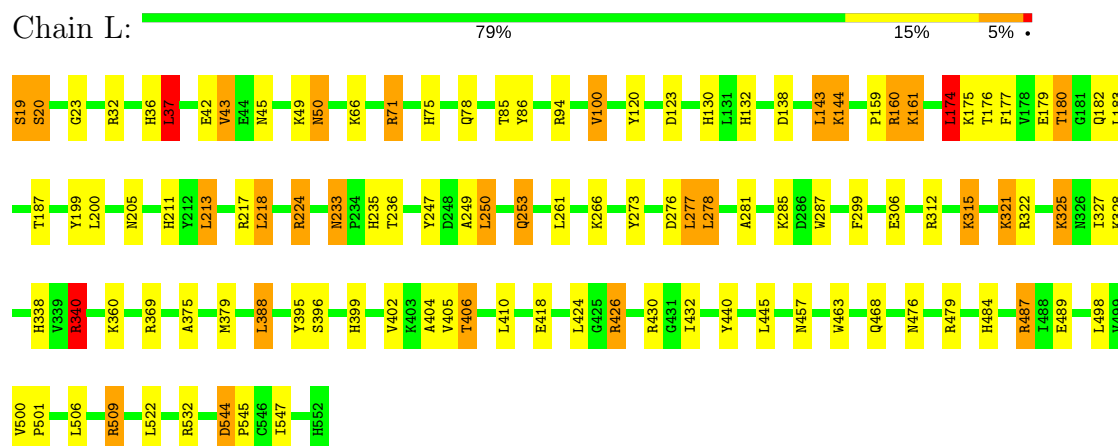
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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, $\alpha$ , $\beta$ , $\gamma$	98.01Å 126.02Å 66.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.35	Depositor
% Data completeness (in resolution range)	91.9 (10.00-1.35)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.121 , 0.186	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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: MG, F3S, FNE, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	S	0.68	1/2075 (0.0%)	1.47	21/2830 (0.7%)
2	L	0.62	0/4288	1.33	45/5831 (0.8%)
All	All	0.64	1/6363 (0.0%)	1.38	66/8661 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	267	ASN	C-O	6.93	1.36	1.23

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	6	ARG	CD-NE-CZ	27.92	162.69	123.60
1	S	100	ARG	NE-CZ-NH1	14.17	127.38	120.30
1	S	5	ARG	NE-CZ-NH1	-12.47	114.06	120.30
2	L	217	ARG	NE-CZ-NH1	-11.59	114.50	120.30
2	L	273	TYR	CB-CG-CD1	10.67	127.40	121.00
2	L	506	LEU	CA-CB-CG	10.67	139.84	115.30
1	S	2	MET	CA-CB-CG	10.62	131.36	113.30
2	L	340	ARG	NE-CZ-NH2	-10.53	115.03	120.30
2	L	160	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	S	233	LYS	CD-CE-NZ	8.58	131.44	111.70
2	L	430	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	L	426	ARG	NE-CZ-NH1	8.48	124.54	120.30
2	L	487	ARG	CB-CG-CD	8.46	133.61	111.60
1	S	26	ARG	NE-CZ-NH2	-8.43	116.08	120.30
2	L	273	TYR	CG-CD1-CE1	8.11	127.79	121.30
1	S	197	PHE	CB-CG-CD2	-7.88	115.28	120.80
2	L	120	TYR	CB-CG-CD2	-7.84	116.30	121.00
2	L	532	ARG	NE-CZ-NH2	-7.80	116.40	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	71	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	S	218	TYR	CB-CG-CD1	7.56	125.54	121.00
2	L	218	LEU	CA-CB-CG	-7.47	98.12	115.30
2	L	71	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	S	1	LEU	O-C-N	7.01	133.91	122.70
2	L	287	TRP	CA-CB-CG	-6.99	100.41	113.70
2	L	479	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	L	174	LEU	CA-CB-CG	6.61	130.50	115.30
1	S	218	TYR	CB-CG-CD2	-6.51	117.09	121.00
2	L	213	LEU	CA-CB-CG	6.38	129.98	115.30
1	S	26	ARG	CG-CD-NE	-6.29	98.60	111.80
1	S	233	LYS	CA-CB-CG	6.21	127.06	113.40
1	S	26	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	L	509	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	L	247	TYR	CB-CG-CD2	-6.10	117.34	121.00
2	L	224	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	S	100	ARG	CD-NE-CZ	6.10	132.14	123.60
2	L	277	LEU	CA-CB-CG	6.08	129.28	115.30
2	L	430	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	L	100	VAL	CA-CB-CG2	-5.97	101.95	110.90
2	L	273	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	S	243	VAL	CA-CB-CG1	5.89	119.74	110.90
2	L	340	ARG	NH1-CZ-NH2	5.87	125.86	119.40
2	L	250	LEU	CA-CB-CG	5.85	128.76	115.30
1	S	85	ILE	CA-CB-CG1	-5.78	100.02	111.00
2	L	123	ASP	CB-CG-OD2	-5.67	113.19	118.30
2	L	369	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	L	160	ARG	NH1-CZ-NH2	5.57	125.52	119.40
2	L	42	GLU	OE1-CD-OE2	5.52	129.93	123.30
2	L	322	ARG	NE-CZ-NH2	5.47	123.03	120.30
2	L	440	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	S	187	VAL	CA-CB-CG1	5.44	119.06	110.90
2	L	544	ASP	CB-CG-OD1	-5.44	113.41	118.30
2	L	180	THR	CA-CB-CG2	-5.44	104.79	112.40
2	L	487	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	L	199	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	S	5	ARG	CA-C-N	5.21	128.66	117.20
2	L	37	LEU	CA-CB-CG	5.19	127.25	115.30
2	L	120	TYR	CA-CB-CG	5.19	123.26	113.40
1	S	86	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	L	404	ALA	C-N-CA	-5.15	108.83	121.70
1	S	164	TYR	CB-CG-CD2	-5.15	117.91	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	395	TYR	CB-CG-CD2	5.14	124.09	121.00
2	L	94	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	L	426	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	L	273	TYR	CD1-CE1-CZ	-5.07	115.23	119.80
1	S	1	LEU	CA-C-N	-5.04	106.11	117.20
2	L	130	HIS	CA-CB-CG	-5.01	105.08	113.60

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	73	0
2	L	4177	0	4129	78	0
3	S	16	0	0	0	0
4	S	7	0	0	0	0
5	L	1	0	0	0	0
6	L	8	0	0	0	0
7	L	612	0	0	19	0
7	S	317	0	0	9	0
All	All	7157	0	6078	130	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 11.

All (130) 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:26:ARG:HH21	2:L:233:ASN:HD21	1.16	0.93
1:S:230:ASN:HB2	1:S:233:LYS:HE2	1.52	0.90
1:S:126:ASN:HD21	1:S:130:ALA:H	1.19	0.84
1:S:2:MET:HA	2:L:182:GLN:HG2	1.61	0.81
1:S:238:GLN:HE21	2:L:224:ARG:HH21	1.29	0.80
2:L:402:VAL:O	2:L:406:THR:HG23	1.84	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:66:LYS:HE2	7:L:3085:HOH:O	1.84	0.77
1:S:1:LEU:HD21	1:S:59:ALA:O	1.84	0.77
1:S:2:MET:HG2	2:L:182:GLN:HE21	1.50	0.76
1:S:6:ARG:HH12	2:L:180:THR:HG21	1.51	0.76
2:L:218:LEU:HG	2:L:218:LEU:O	1.85	0.76
2:L:249:ALA:HB1	7:L:3095:HOH:O	1.83	0.76
2:L:285:LYS:HB2	7:L:3725:HOH:O	1.86	0.74
2:L:78:GLN:HE21	2:L:86:TYR:H	1.32	0.74
1:S:1:LEU:HG	2:L:187:THR:HG21	1.70	0.73
2:L:176:THR:O	2:L:180:THR:HG23	1.89	0.72
1:S:230:ASN:H	1:S:230:ASN:HD22	1.40	0.69
1:S:26:ARG:HH21	2:L:233:ASN:ND2	1.88	0.68
1:S:256:ASP:HB3	7:S:3293:HOH:O	1.92	0.68
1:S:2:MET:HG2	2:L:182:GLN:NE2	2.10	0.67
2:L:325:LYS:HD2	7:L:3772:HOH:O	1.96	0.65
2:L:306:GLU:HB2	7:L:3612:HOH:O	1.96	0.65
2:L:484:HIS:CD2	2:L:498:LEU:HD22	2.32	0.65
2:L:406:THR:HG22	2:L:432:ILE:HG21	1.78	0.64
1:S:2:MET:HG3	1:S:8:SER:HB2	1.78	0.63
1:S:2:MET:HB3	7:S:3088:HOH:O	1.98	0.63
1:S:6:ARG:NH1	2:L:180:THR:HG21	2.15	0.61
2:L:321:LYS:HD3	2:L:321:LYS:N	2.14	0.61
2:L:281:ALA:HB1	2:L:424:LEU:HD21	1.82	0.61
1:S:256:ASP:HB3	7:S:3294:HOH:O	1.99	0.60
2:L:321:LYS:HE2	7:L:3488:HOH:O	2.01	0.60
1:S:13:HIS:HD2	7:S:3020:HOH:O	1.83	0.59
1:S:53:GLY:HA3	7:L:3878:HOH:O	2.02	0.59
2:L:211:HIS:HE1	7:L:3172:HOH:O	1.86	0.58
2:L:405:VAL:HG22	2:L:432:ILE:HG23	1.86	0.58
1:S:126:ASN:HD21	1:S:130:ALA:N	1.97	0.58
2:L:37:LEU:HG	2:L:547:ILE:HD11	1.86	0.58
1:S:2:MET:HA	2:L:182:GLN:CG	2.34	0.58
1:S:1:LEU:HD11	1:S:62:GLN:HG2	1.86	0.57
1:S:233:LYS:HE3	1:S:234:ILE:HD11	1.86	0.57
1:S:2:MET:HE1	1:S:3:GLY:O	2.03	0.57
1:S:2:MET:SD	1:S:8:SER:HB2	2.45	0.57
1:S:1:LEU:HD13	7:S:3088:HOH:O	2.03	0.57
1:S:233:LYS:HE3	1:S:234:ILE:CD1	2.36	0.56
2:L:281:ALA:CB	2:L:424:LEU:HD21	2.36	0.56
2:L:75:HIS:HD2	7:L:3017:HOH:O	1.89	0.55
1:S:156:ASN:HD21	1:S:230:ASN:HD21	1.53	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1:LEU:HB3	2:L:187:THR:OG1	2.06	0.55
1:S:6:ARG:HH12	2:L:180:THR:CG2	2.20	0.55
2:L:253:GLN:NE2	2:L:253:GLN:H	2.05	0.55
1:S:2:MET:HG3	1:S:43:ASP:OD1	2.08	0.54
2:L:299:PHE:H	2:L:476:ASN:ND2	2.05	0.54
1:S:1:LEU:HD12	1:S:1:LEU:H3	1.71	0.54
1:S:217:LEU:HD12	1:S:243:VAL:HB	1.90	0.54
2:L:36:HIS:HD2	7:L:3047:HOH:O	1.91	0.53
2:L:379:MET:HE1	7:L:3728:HOH:O	2.08	0.53
1:S:1:LEU:HA	2:L:187:THR:OG1	2.09	0.53
2:L:211:HIS:HD2	2:L:276:ASP:OD2	1.92	0.53
1:S:31:TYR:O	1:S:35:LEU:HD22	2.09	0.53
1:S:1:LEU:CG	2:L:187:THR:HG21	2.39	0.52
2:L:19:SER:HB3	2:L:45:ASN:OD1	2.08	0.52
2:L:261:LEU:HD11	7:L:3921:HOH:O	2.08	0.52
1:S:7:PRO:HG2	1:S:40:LEU:HD12	1.92	0.52
1:S:229:ASN:HD22	1:S:230:ASN:H	1.57	0.52
1:S:2:MET:CG	1:S:8:SER:HB2	2.39	0.52
2:L:388:LEU:HG	2:L:426:ARG:HA	1.90	0.52
2:L:175:LYS:HG2	2:L:179:GLU:OE1	2.11	0.52
2:L:50:ASN:HD21	2:L:509:ARG:NH2	2.07	0.51
1:S:21:SER:O	1:S:25:LEU:HD13	2.10	0.51
1:S:238:GLN:NE2	2:L:224:ARG:HH21	2.02	0.50
1:S:230:ASN:N	1:S:230:ASN:HD22	2.04	0.50
2:L:159:PRO:O	2:L:161:LYS:HE2	2.12	0.49
2:L:23:GLY:O	2:L:43:VAL:HG13	2.12	0.49
2:L:143:LEU:HD13	2:L:174:LEU:HD13	1.95	0.49
1:S:13:HIS:HE1	1:S:21:SER:OG	1.95	0.48
2:L:328:LYS:HE3	7:L:3881:HOH:O	2.12	0.48
1:S:5:ARG:NH1	1:S:5:ARG:HB3	2.28	0.48
2:L:399:HIS:HD2	2:L:402:VAL:H	1.60	0.48
1:S:265:TYR:OH	2:L:75:HIS:HE1	1.97	0.48
2:L:327:ILE:HD11	2:L:396:SER:HB2	1.96	0.47
1:S:139:HIS:CD2	1:S:139:HIS:H	2.31	0.47
1:S:29:GLU:OE1	1:S:31:TYR:HE1	1.96	0.47
1:S:26:ARG:NH2	2:L:233:ASN:HD21	1.98	0.47
1:S:1:LEU:N	1:S:1:LEU:HD12	2.30	0.46
1:S:1:LEU:HD22	1:S:43:ASP:HB3	1.96	0.46
2:L:143:LEU:HD13	2:L:174:LEU:CD1	2.46	0.46
1:S:200:GLY:HA2	1:S:202:PHE:CE2	2.51	0.46
1:S:230:ASN:H	1:S:230:ASN:ND2	2.10	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:338:HIS:HB2	2:L:375:ALA:HB3	1.98	0.46
1:S:265:TYR:HB3	7:L:3888:HOH:O	2.16	0.46
1:S:181:MET:HE3	7:S:3654:HOH:O	2.15	0.45
2:L:78:GLN:HE22	2:L:236:THR:H	1.64	0.45
2:L:489:GLU:HG2	7:L:3862:HOH:O	2.15	0.45
2:L:138:ASP:H	2:L:205:ASN:ND2	2.14	0.45
1:S:126:ASN:ND2	1:S:130:ALA:H	2.00	0.45
1:S:2:MET:HE1	1:S:68:HIS:HB2	1.99	0.45
1:S:3:GLY:HA3	1:S:4:PRO:HD3	1.88	0.45
1:S:2:MET:CG	2:L:182:GLN:HE21	2.25	0.45
2:L:487:ARG:NH2	7:L:3311:HOH:O	2.49	0.45
2:L:71:ARG:NH1	7:L:3888:HOH:O	2.49	0.44
2:L:487:ARG:HB2	7:L:3131:HOH:O	2.17	0.44
2:L:266:LYS:NZ	7:L:3874:HOH:O	2.51	0.44
2:L:468:GLN:HB2	2:L:468:GLN:HE21	1.52	0.43
1:S:143:LYS:HD3	7:S:3222:HOH:O	2.19	0.43
1:S:5:ARG:CZ	1:S:5:ARG:HB3	2.48	0.43
2:L:100:VAL:HG11	2:L:463:TRP:CE3	2.53	0.43
2:L:50:ASN:HD21	2:L:509:ARG:HH22	1.67	0.43
1:S:166:LYS:NZ	7:S:3502:HOH:O	2.49	0.43
2:L:500:VAL:CG1	2:L:501:PRO:HD2	2.49	0.42
1:S:171:PRO:O	1:S:173:LEU:HD13	2.20	0.42
2:L:312:ARG:O	2:L:315:LYS:HD2	2.19	0.42
2:L:85:THR:OG1	2:L:235:HIS:HD2	2.02	0.42
2:L:144:LYS:HE2	2:L:144:LYS:HB2	1.44	0.42
1:S:6:ARG:HH12	2:L:180:THR:CB	2.33	0.42
2:L:340:ARG:HD3	2:L:340:ARG:O	2.19	0.42
1:S:6:ARG:NH2	7:S:3175:HOH:O	2.46	0.42
2:L:78:GLN:NE2	2:L:235:HIS:HA	2.35	0.42
2:L:544:ASP:N	2:L:545:PRO:HD3	2.34	0.42
1:S:232:PRO:HG3	1:S:241:TRP:CH2	2.55	0.42
1:S:124:LYS:HB3	1:S:124:LYS:NZ	2.35	0.41
1:S:37:LEU:HD12	2:L:177:PHE:CD2	2.56	0.41
1:S:47:THR:O	2:L:32:ARG:HA	2.20	0.41
2:L:484:HIS:CG	2:L:498:LEU:HD22	2.55	0.41
2:L:278:LEU:HA	2:L:278:LEU:HD12	1.78	0.41
1:S:147:ILE:HD13	1:S:157:LEU:HA	2.03	0.41
1:S:156:ASN:HD21	1:S:230:ASN:ND2	2.16	0.41
1:S:114:CYS:HA	1:S:119:GLY:HA3	2.03	0.40
1:S:201:GLU:HB3	1:S:215:TRP:CE3	2.56	0.40
2:L:160:ARG:C	2:L:161:LYS:HE2	2.41	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:230:ASN:N	1:S:230:ASN:ND2	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	5 (2%)	3 (1%)	17	2
2	L	532/534 (100%)	518 (97%)	13 (2%)	1 (0%)	51	19
All	All	797/801 (100%)	775 (97%)	18 (2%)	4 (0%)	32	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	4	PRO
2	L	20	SER
1	S	5	ARG
1	S	3	GLY

### 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%)	192 (90%)	21 (10%)	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	438/438 (100%)	407 (93%)	31 (7%)	17 1
All	All	651/651 (100%)	599 (92%)	52 (8%)	14 1

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	1	LEU
1	S	2	MET
1	S	4	PRO
1	S	5	ARG
1	S	35	LEU
1	S	37	LEU
1	S	40	LEU
1	S	61	GLU
1	S	79	PRO
1	S	85	ILE
1	S	91	ASN
1	S	95	LEU
1	S	126	ASN
1	S	168	LYS
1	S	173	LEU
1	S	176	LEU
1	S	187	VAL
1	S	220	LEU
1	S	229	ASN
1	S	230	ASN
1	S	243	VAL
2	L	19	SER
2	L	20	SER
2	L	37	LEU
2	L	43	VAL
2	L	49	LYS
2	L	50	ASN
2	L	132	HIS
2	L	143	LEU
2	L	144	LYS
2	L	161	LYS
2	L	174	LEU
2	L	183	LEU
2	L	200	LEU
2	L	213	LEU
2	L	233	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	250	LEU
2	L	253	GLN
2	L	277	LEU
2	L	278	LEU
2	L	315	LYS
2	L	321	LYS
2	L	325	LYS
2	L	340	ARG
2	L	360	LYS
2	L	388	LEU
2	L	406	THR
2	L	410	LEU
2	L	418	GLU
2	L	445	LEU
2	L	457	ASN
2	L	522	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	13	HIS
1	S	91	ASN
1	S	126	ASN
1	S	139	HIS
1	S	190	GLN
1	S	229	ASN
1	S	230	ASN
1	S	238	GLN
1	S	266	GLN
1	S	267	ASN
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	253	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	L	310	ASN
2	L	334	GLN
2	L	399	HIS
2	L	446	GLN
2	L	451	ASN
2	L	457	ASN
2	L	468	GLN
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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z  > 2$
6	FNE	L	1004	2	3,7,9	2.32	1 (33%)	0,9,15	0.00	-
3	SF4	S	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	S	1002	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	S	1003	1	0,9,9	0.00	-	0,15,15	0.00	-

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
6	FNE	L	1004	2	-	0/0/9/18	0/0/0/1
3	SF4	S	1001	1	-	0/0/48/48	0/6/5/5
3	SF4	S	1002	1	-	0/0/48/48	0/6/5/5
4	F3S	S	1003	1	-	0/0/24/24	0/0/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1004	FNE	O2-C2	-3.70	1.10	1.17

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.