wwPDB X-ray Structure Validation Summary Report (i)

Nov 28, 2023 – 02:36 PM EST

PDB ID	:	1YRQ
Title	:	Structure of the ready oxidized form of [NiFe]-hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Cavazza, C.; Matho, M.; Faber, B.W.; Roseboom, W.; Albracht, S.P.; Garcin, E.; Rousset, M.; Fontecilla-Camps, J.C.
Deposited on	:	2005-02-04
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

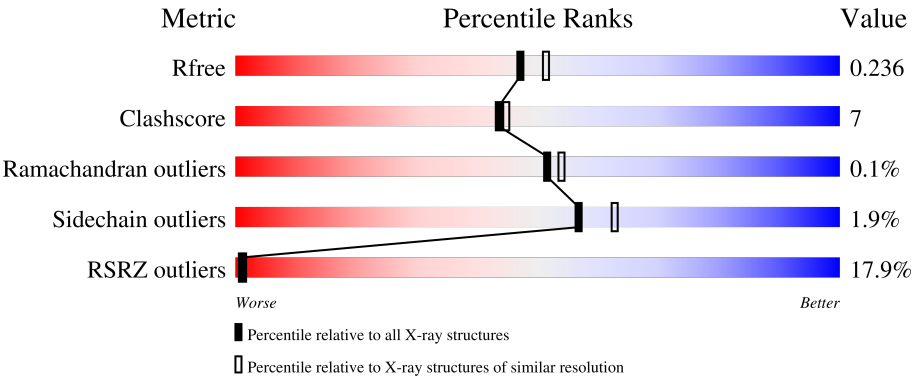
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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.

Mol	Chain	Length	Quality of chain
1	1-A	264	2% 80% 19%
1	1-B	264	15% 83% 16%
1	1-C	264	% 86% 11%
1	1-D	264	% 83% 17%
1	1-F	264	2% 84% 14%

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Mol	Chain	Length	Quality of chain
1	1-G	264	95% 67% 31%
1	2-A	264	2% 81% 19%
1	2-B	264	15% 83% 16%
1	2-C	264	% 86% 11%
1	2-D	264	% 83% 17%
1	2-F	264	2% 83% 15%
1	2-G	264	95% 66% 32%
2	1-H	549	2% 84% 14%
2	1-I	549	5% 85% 14%
2	1-J	549	3% 82% 16%
2	1-K	549	% 83% 15%
2	1-M	549	3% 81% 17%
2	1-N	549	91% 81% 17%
2	2-H	549	2% 84% 14%
2	2-I	549	5% 85% 14%
2	2-J	549	3% 82% 16%
2	2-K	549	% 83% 15%
2	2-M	549	3% 81% 17%
2	2-N	549	91% 81% 16%

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
7	FCO	1-N	550	-	-	X	-
7	FCO	2-N	550	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 77694 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	1-A	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			
1	2-A	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			
1	1-B	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	2-B	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	1-C	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	2-C	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	1-D	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	2-D	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	1-F	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	2-F	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	1-G	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			
1	2-G	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	SER	GLU	conflict	UNP P18187
B	171	SER	GLU	conflict	UNP P18187
C	171	SER	GLU	conflict	UNP P18187
D	171	SER	GLU	conflict	UNP P18187
F	171	SER	GLU	conflict	UNP P18187

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Chain	Residue	Modelled	Actual	Comment	Reference
G	171	SER	GLU	conflict	UNP P18187

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-H	545	Total	C	N	O	S	0	0	0
			4167	2654	725	766	22			
2	2-H	545	Total	C	N	O	S	0	0	0
			4167	2654	725	766	22			
2	1-I	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	2-I	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	1-J	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	2-J	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	1-K	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	2-K	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	1-M	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	2-M	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	1-N	545	Total	C	N	O	S	4	0	0
			4167	2654	725	766	22			
2	2-N	545	Total	C	N	O	S	0	0	0
			4167	2654	725	766	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	198	ASN	ASP	conflict	UNP P18188
H	303	SER	GLU	conflict	UNP P18188
I	198	ASN	ASP	conflict	UNP P18188
I	303	SER	GLU	conflict	UNP P18188
J	198	ASN	ASP	conflict	UNP P18188
J	303	SER	GLU	conflict	UNP P18188
K	198	ASN	ASP	conflict	UNP P18188
K	303	SER	GLU	conflict	UNP P18188
M	198	ASN	ASP	conflict	UNP P18188

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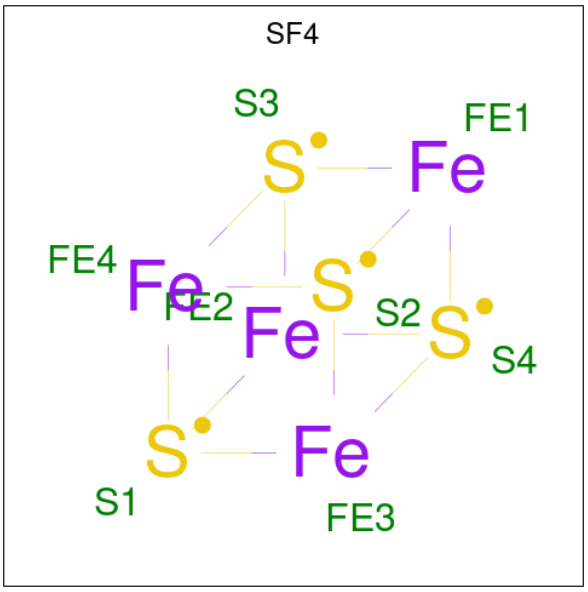
Chain	Residue	Modelled	Actual	Comment	Reference
M	303	SER	GLU	conflict	UNP P18188
N	198	ASN	ASP	conflict	UNP P18188
N	303	SER	GLU	conflict	UNP P18188

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	1	Total Fe S 8 4 4	0	0
3	2-A	1	Total Fe S 8 4 4	0	0
3	1-A	1	Total Fe S 8 4 4	0	0
3	2-A	1	Total Fe S 8 4 4	0	0
3	1-B	1	Total Fe S 8 4 4	0	0
3	2-B	1	Total Fe S 8 4 4	0	0
3	1-B	1	Total Fe S 8 4 4	0	0
3	2-B	1	Total Fe S 8 4 4	0	0
3	1-C	1	Total Fe S 8 4 4	0	0
3	2-C	1	Total Fe S 8 4 4	0	0

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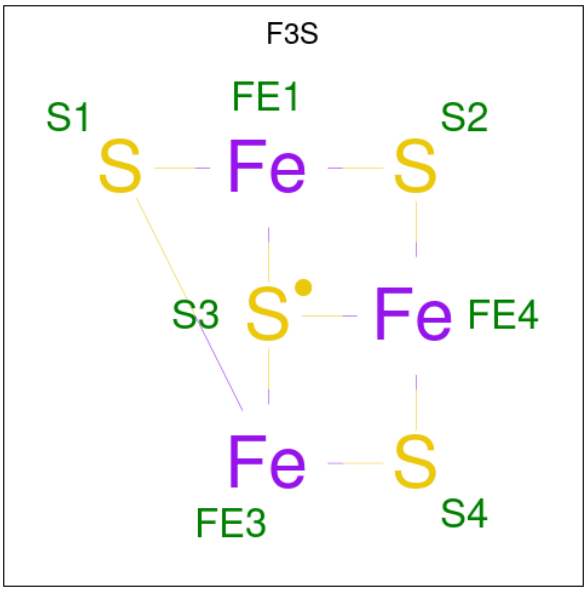
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-C	1	Total Fe S 8 4 4	0	0
3	2-C	1	Total Fe S 8 4 4	0	0
3	1-D	1	Total Fe S 8 4 4	0	0
3	2-D	1	Total Fe S 8 4 4	0	0
3	1-D	1	Total Fe S 8 4 4	0	0
3	2-D	1	Total Fe S 8 4 4	0	0
3	1-F	1	Total Fe S 8 4 4	0	0
3	2-F	1	Total Fe S 8 4 4	0	0
3	1-F	1	Total Fe S 8 4 4	0	0
3	2-F	1	Total Fe S 8 4 4	0	0
3	1-G	1	Total Fe S 8 4 4	0	0
3	2-G	1	Total Fe S 8 4 4	0	0
3	1-G	1	Total Fe S 8 4 4	0	0
3	2-G	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	1	Total Fe S 7 3 4	0	0
4	2-A	1	Total Fe S 7 3 4	0	0
4	1-B	1	Total Fe S 7 3 4	0	0
4	2-B	1	Total Fe S 7 3 4	0	0
4	1-C	1	Total Fe S 7 3 4	0	0
4	2-C	1	Total Fe S 7 3 4	0	0
4	1-D	1	Total Fe S 7 3 4	0	0
4	2-D	1	Total Fe S 7 3 4	0	0
4	1-F	1	Total Fe S 7 3 4	0	0
4	2-F	1	Total Fe S 7 3 4	0	0
4	1-G	1	Total Fe S 7 3 4	0	0
4	2-G	1	Total Fe S 7 3 4	0	0

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-H	1	Total Ni 1 1	0	0
5	2-H	1	Total Ni 1 1	0	0
5	1-I	1	Total Ni 1 1	0	0
5	2-I	1	Total Ni 1 1	0	0
5	1-J	1	Total Ni 1 1	0	0
5	2-J	1	Total Ni 1 1	0	0
5	1-K	1	Total Ni 1 1	0	0
5	2-K	1	Total Ni 1 1	0	0
5	1-M	1	Total Ni 1 1	0	0
5	2-M	1	Total Ni 1 1	0	0
5	1-N	1	Total Ni 1 1	0	0
5	2-N	1	Total Ni 1 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1-H	1	Total Mg 1 1	0	0
6	2-H	1	Total Mg 1 1	0	0
6	1-I	1	Total Mg 1 1	0	0
6	2-I	1	Total Mg 1 1	0	0
6	1-J	1	Total Mg 1 1	0	0
6	2-J	1	Total Mg 1 1	0	0
6	1-K	1	Total Mg 1 1	0	0
6	2-K	1	Total Mg 1 1	0	0

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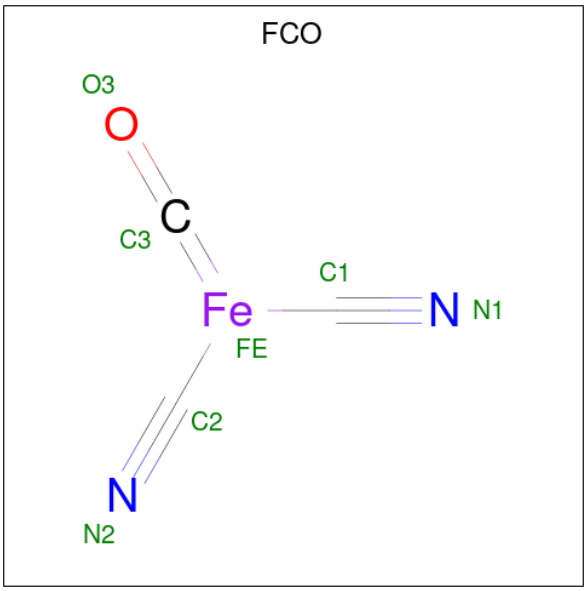
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1-M	1	Total Mg 1 1	0	0
6	2-M	1	Total Mg 1 1	0	0
6	1-N	1	Total Mg 1 1	0	0
6	2-N	1	Total Mg 1 1	0	0

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	1-H	1	Total C Fe N O 7 3 1 2 1	0	0
7	2-H	1	Total C Fe N O 7 3 1 2 1	0	0
7	1-I	1	Total C Fe N O 7 3 1 2 1	0	0
7	2-I	1	Total C Fe N O 7 3 1 2 1	0	0
7	1-J	1	Total C Fe N O 7 3 1 2 1	0	0
7	2-J	1	Total C Fe N O 7 3 1 2 1	0	0
7	1-K	1	Total C Fe N O 7 3 1 2 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	2-K	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	1-M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	1-N	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-N	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	1-A	122	Total	O	0	0
			122	122		
8	2-A	122	Total	O	0	0
			122	122		
8	1-H	245	Total	O	0	0
			245	245		
8	2-H	245	Total	O	0	0
			245	245		
8	1-B	83	Total	O	0	0
			83	83		
8	2-B	84	Total	O	0	0
			84	84		
8	1-I	218	Total	O	0	0
			218	218		
8	2-I	218	Total	O	0	0
			218	218		
8	1-C	120	Total	O	0	0
			120	120		
8	2-C	120	Total	O	0	0
			120	120		
8	1-J	208	Total	O	0	0
			208	208		
8	2-J	208	Total	O	0	0
			208	208		
8	1-D	149	Total	O	0	0
			149	149		
8	2-D	148	Total	O	0	0
			148	148		

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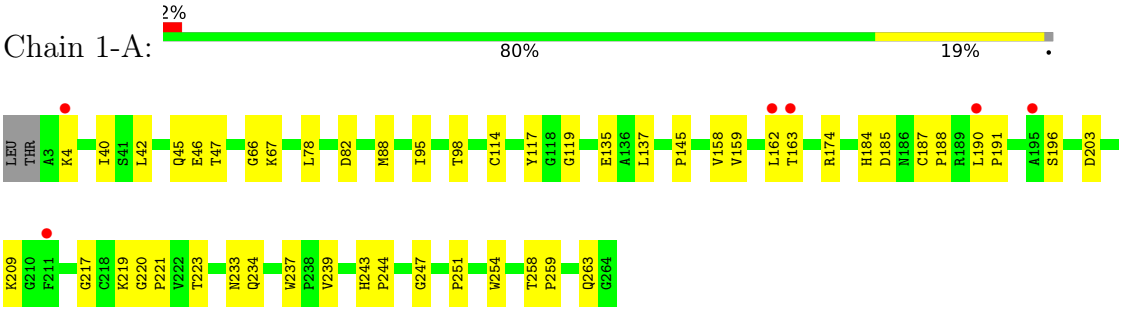
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	1-K	253	Total O 253 253	0	0
8	2-K	253	Total O 253 253	0	0
8	1-F	108	Total O 108 108	0	0
8	2-F	109	Total O 109 109	0	0
8	1-M	183	Total O 183 183	0	0
8	2-M	183	Total O 183 183	0	0
8	1-G	59	Total O 59 59	0	0
8	2-G	58	Total O 58 58	0	0
8	1-N	138	Total O 138 138	0	0
8	2-N	124	Total O 124 124	0	0

3 Residue-property plots (i)

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 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.

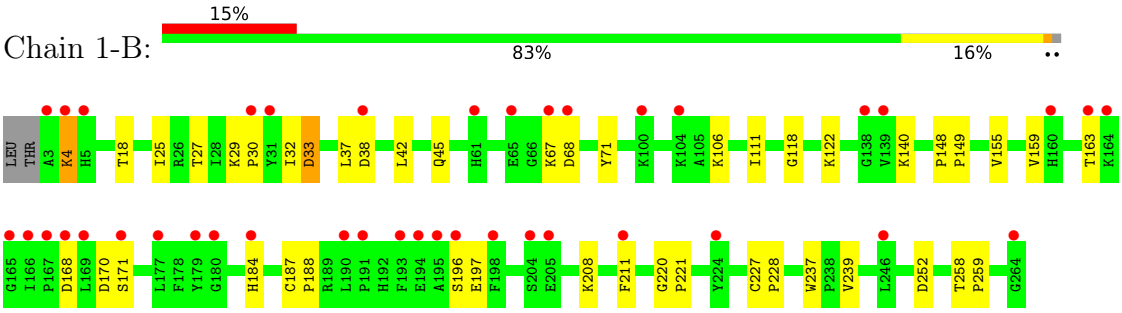
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-A:



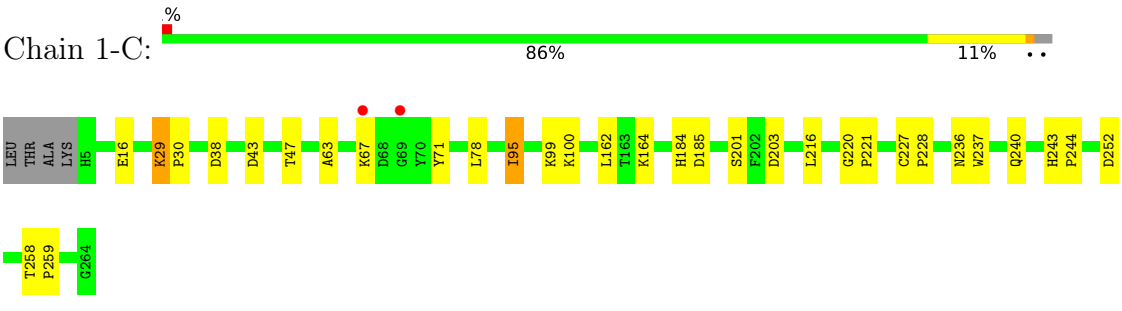
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-B:



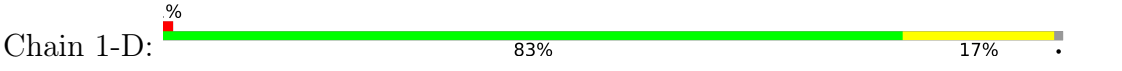
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

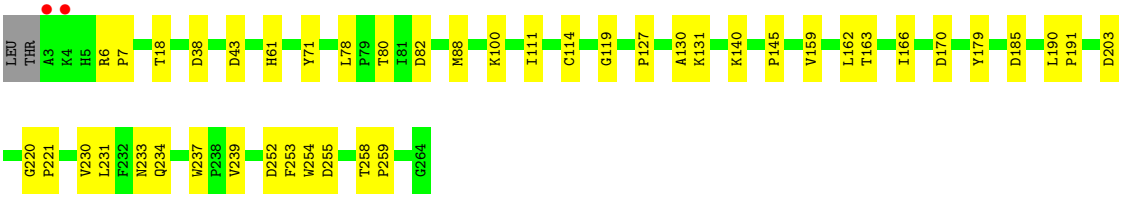
Chain 1-C:



• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

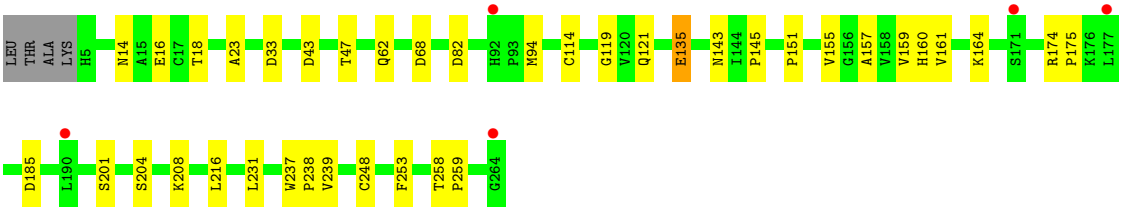
Chain 1-D:





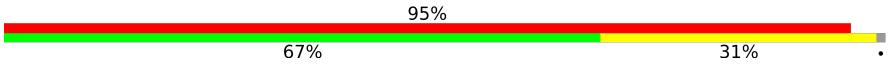
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

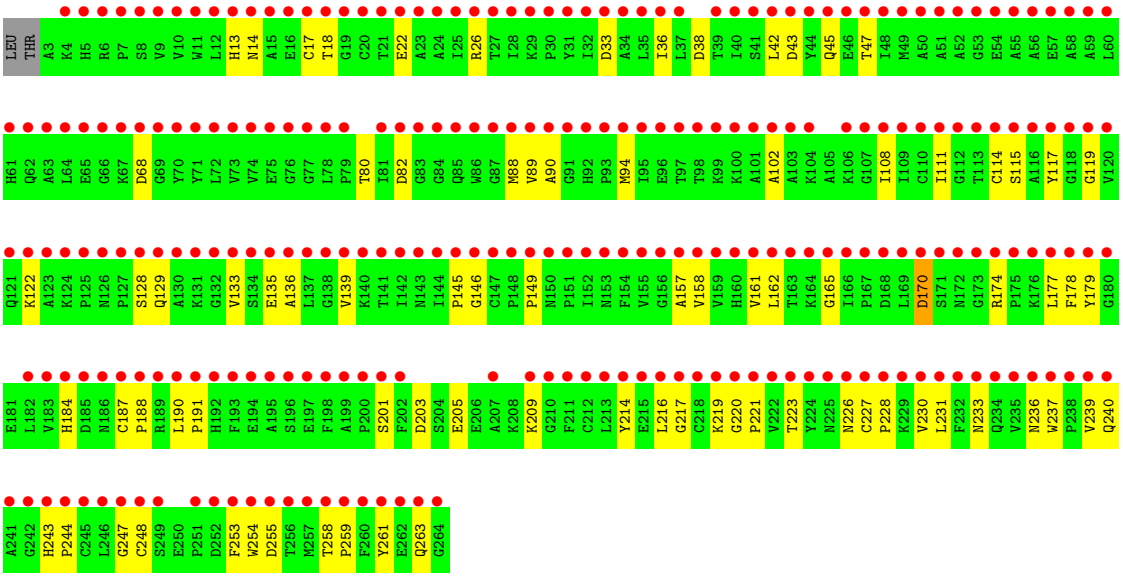
Chain 1-F:



• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

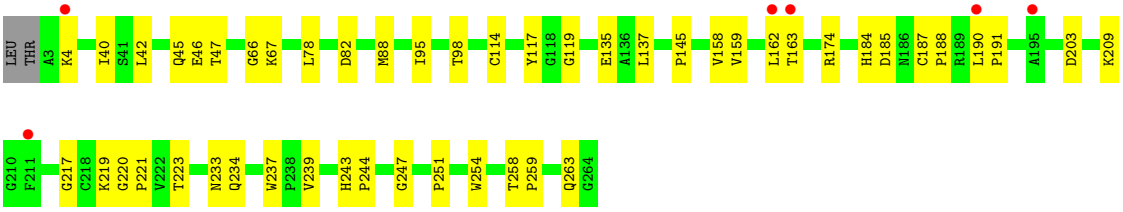
Chain 1-G:





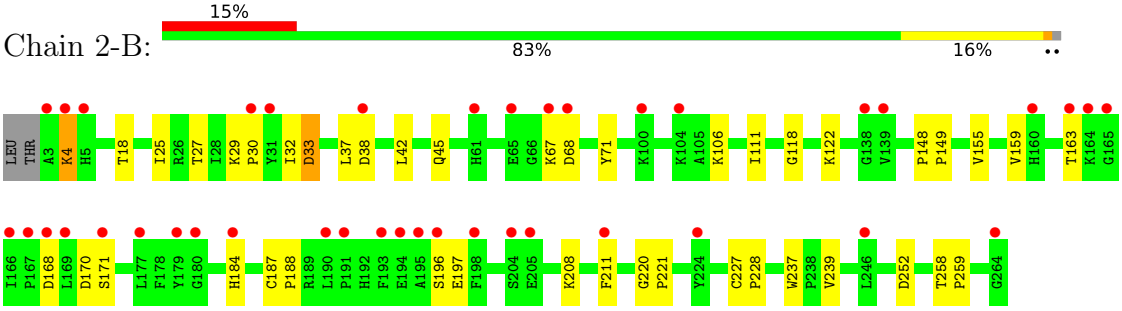
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-A:



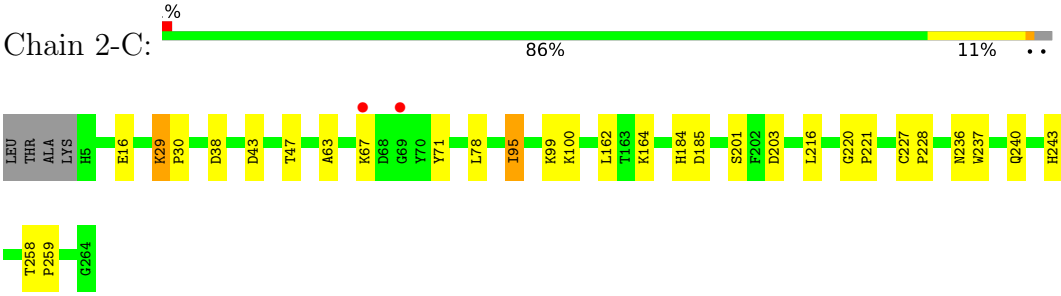
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-B:



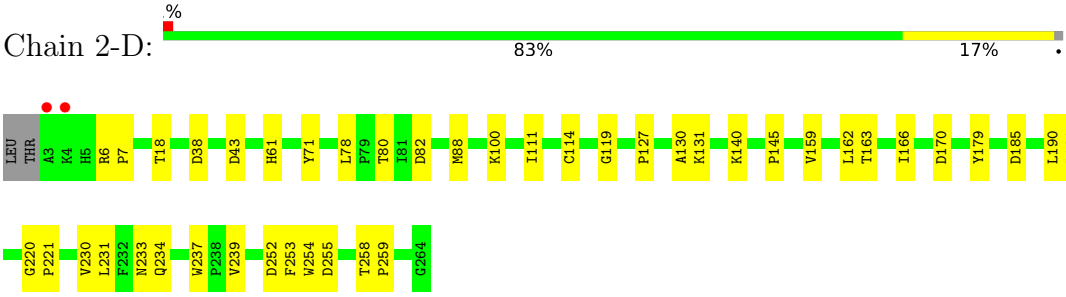
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-C:



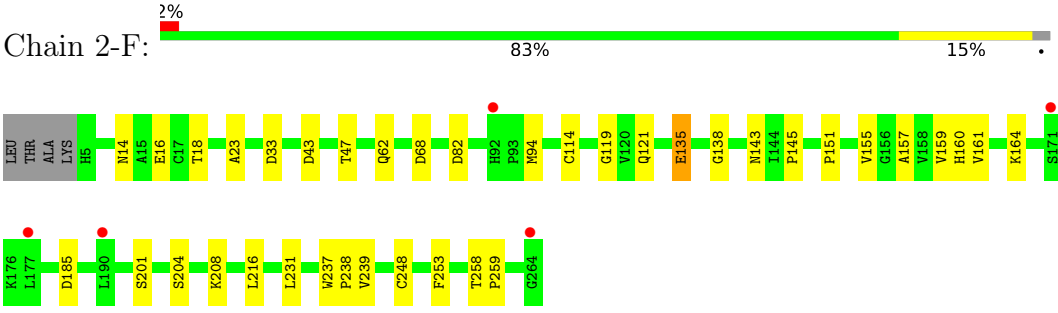
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-D:



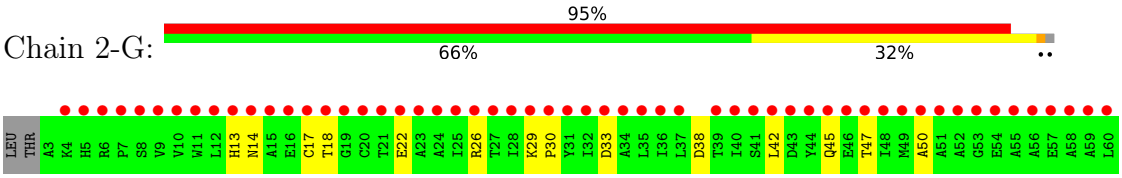
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

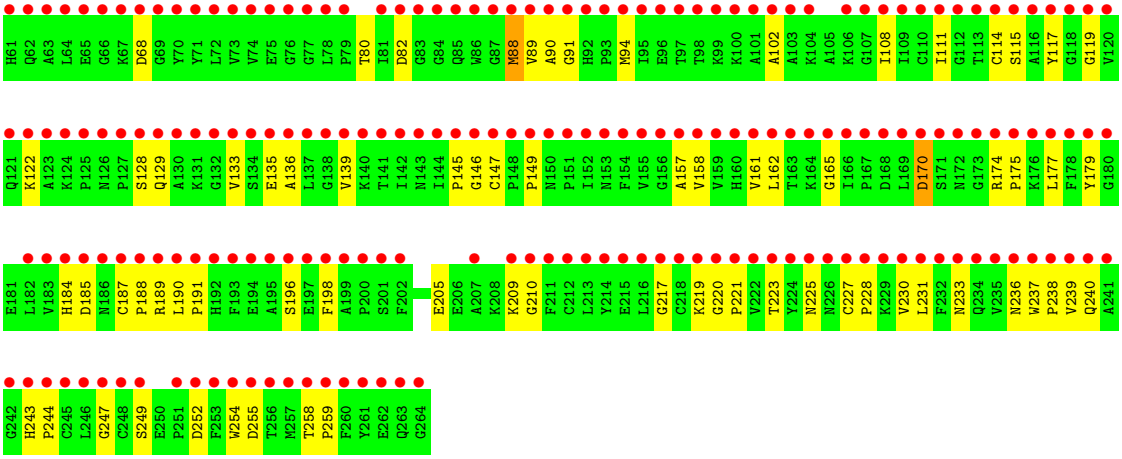
Chain 2-F:



• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

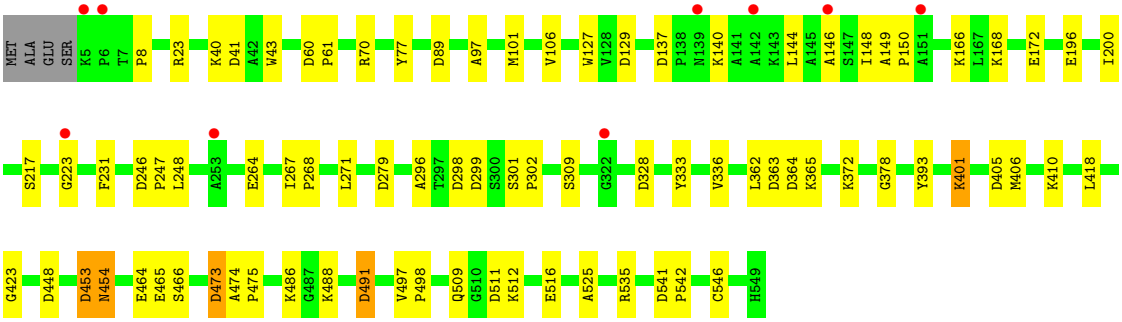
Chain 2-G:





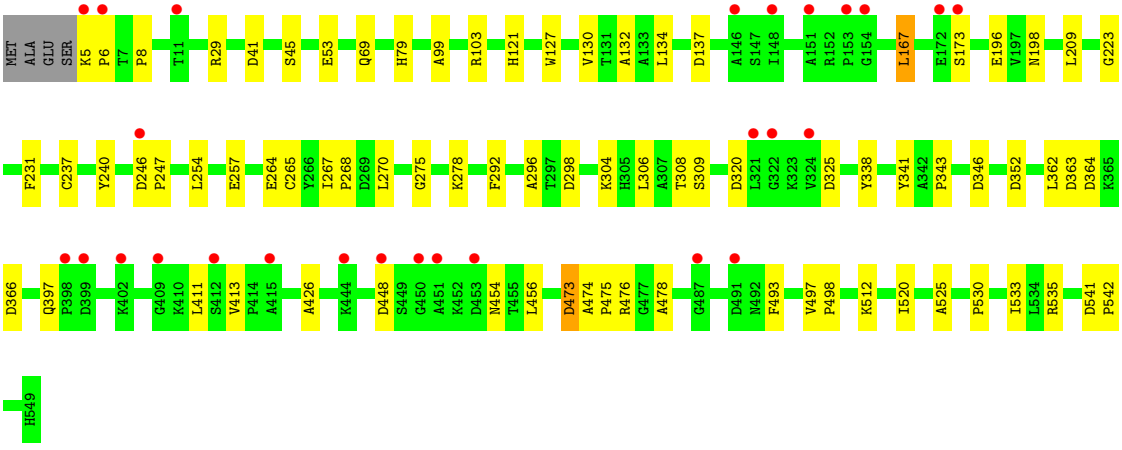
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-H:



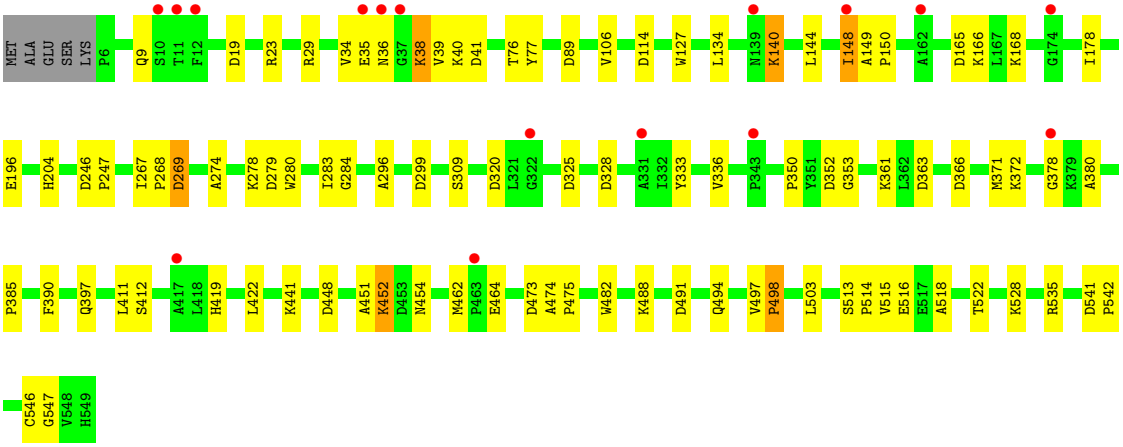
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-I:



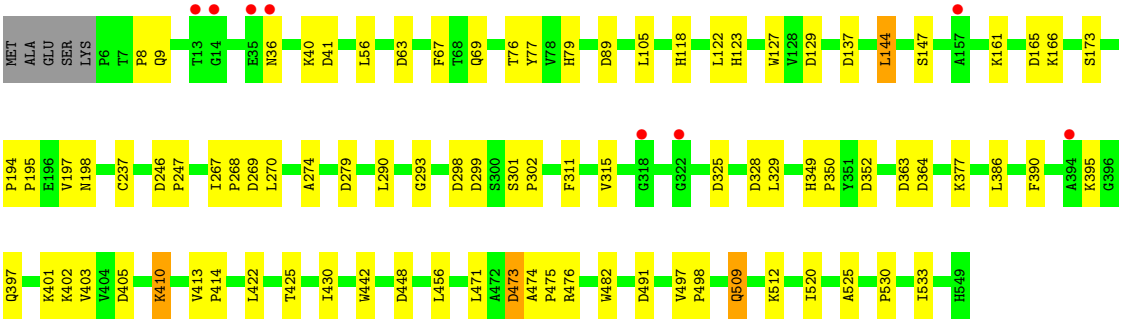
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-J:



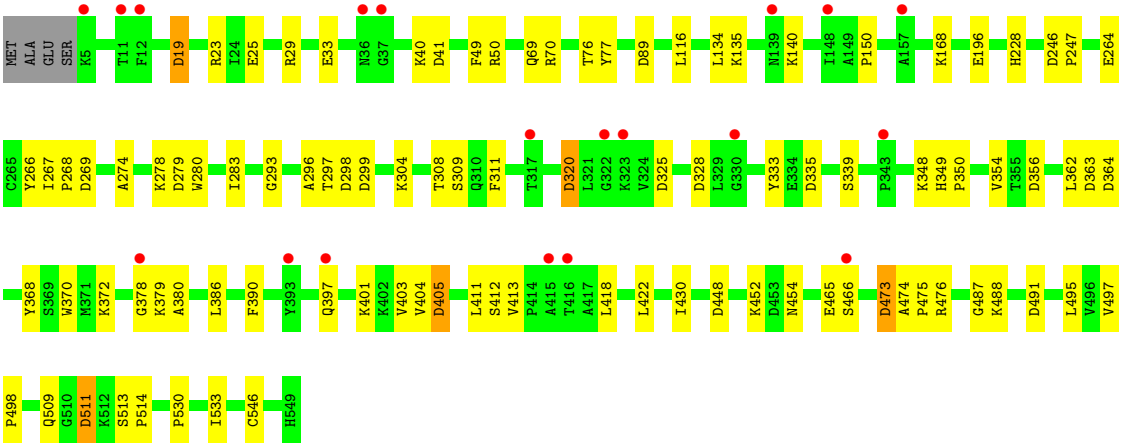
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-K:



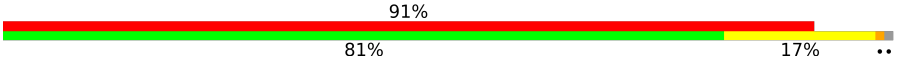
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

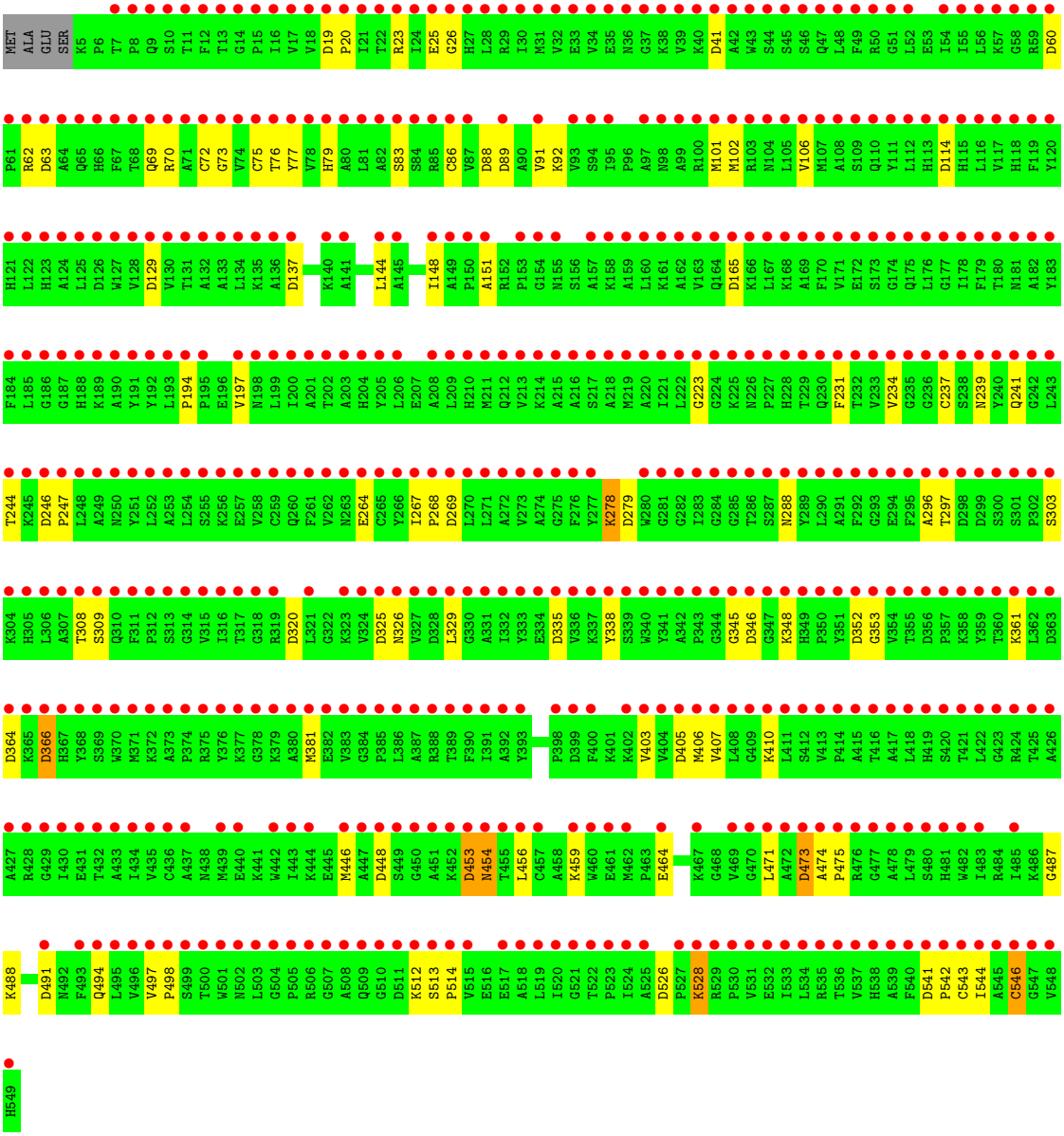
Chain 1-M:



• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

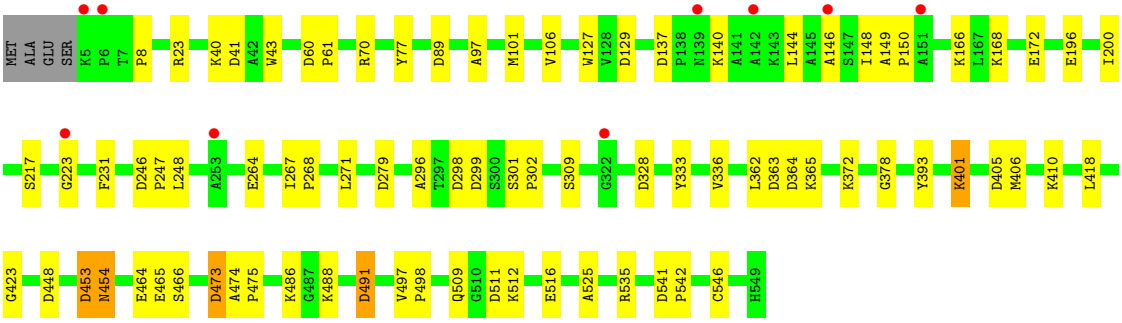
Chain 1-N:





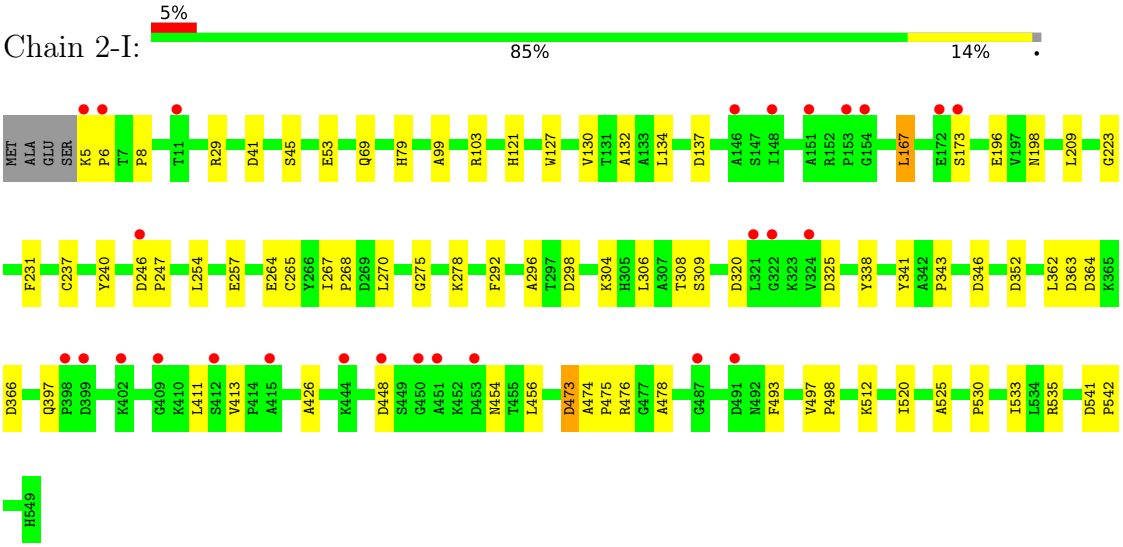
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-H:



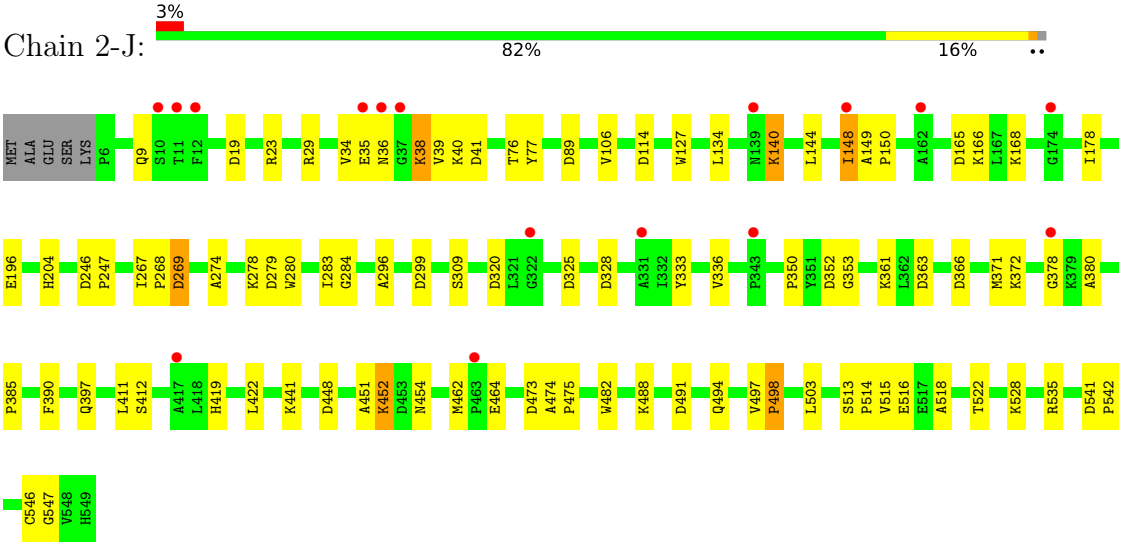
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-I:



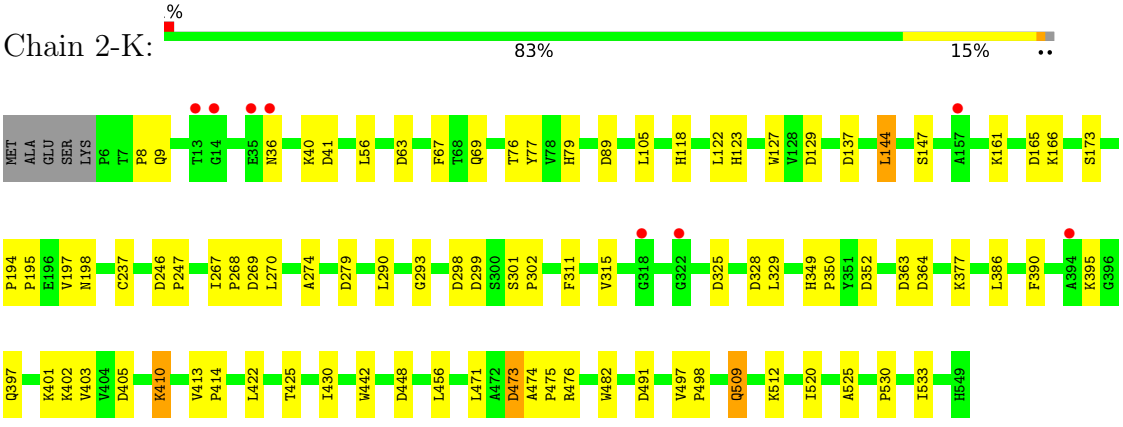
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-J:



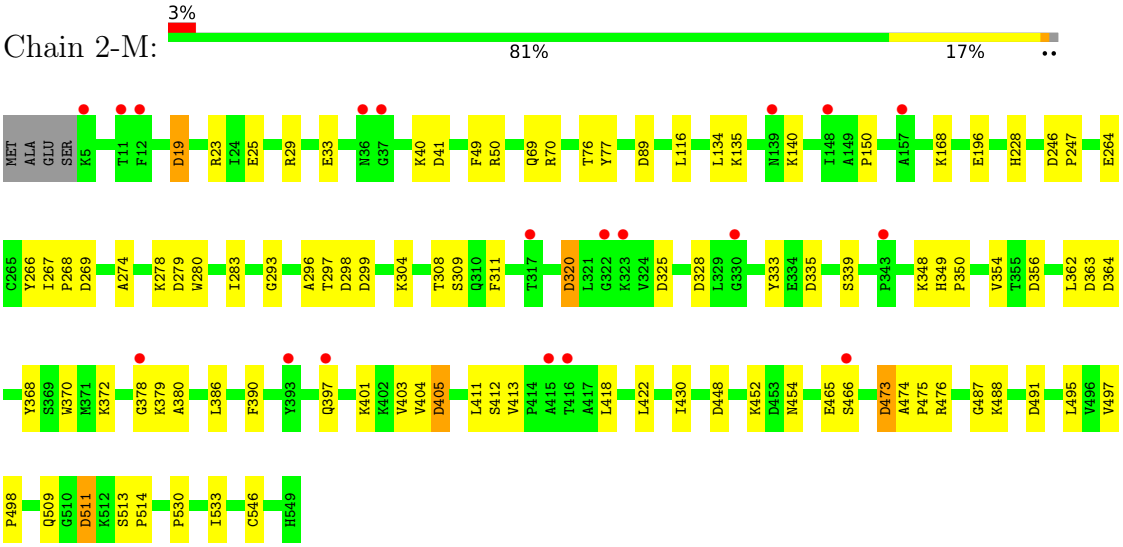
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-K:



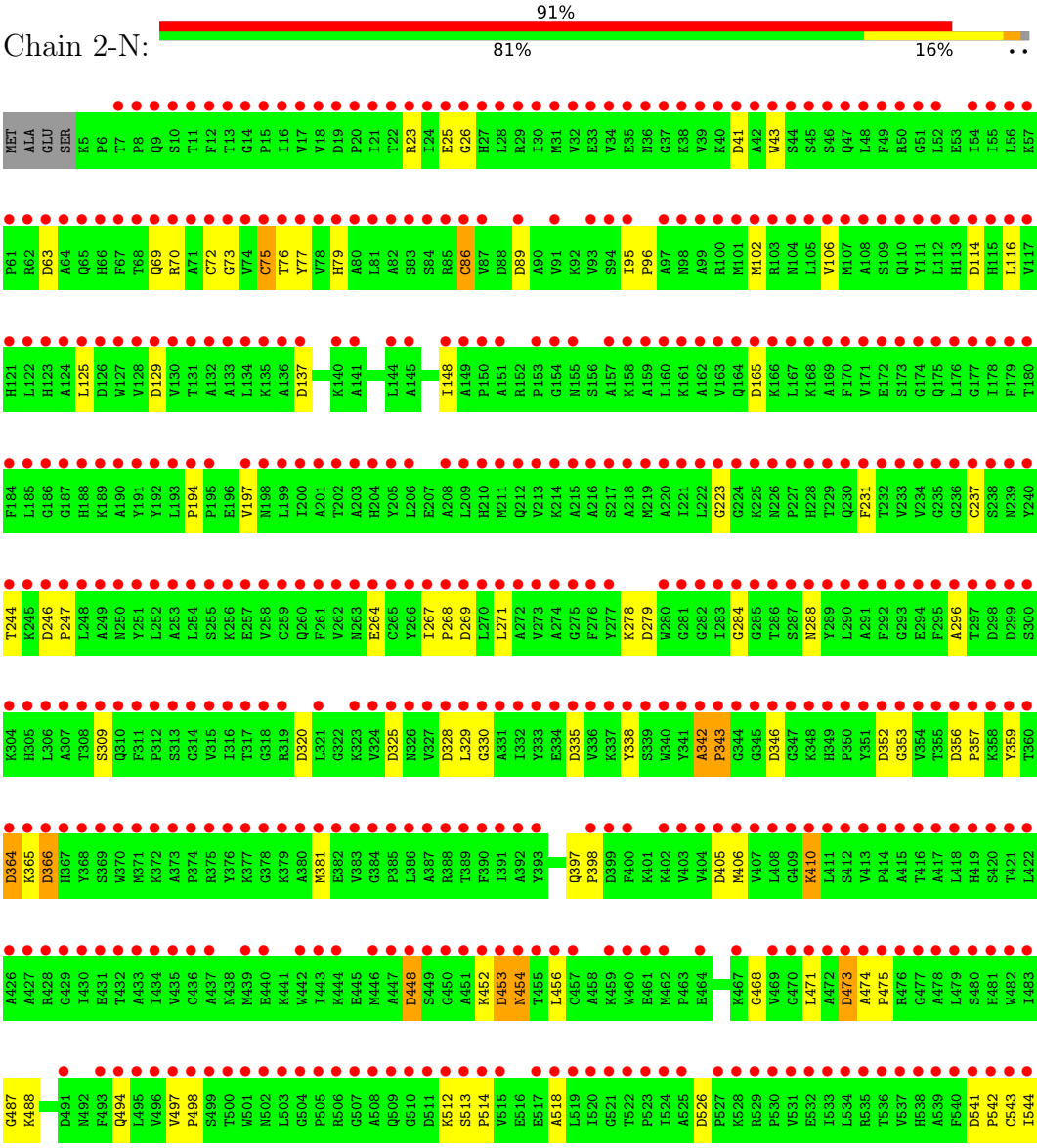
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-M:



• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-N:




V548
H549

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.50Å 99.70Å 183.20Å 90.00° 91.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 29.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.6 (20.00-2.10) 87.7 (29.51-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.171 , 0.220 0.192 , 0.236	Depositor DCC
R_{free} test set	11812 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.59 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	77694	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3614e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FCO, MG, NI, F3S, 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	1-A	0.58	0/2024	0.76	3/2755 (0.1%)
1	1-B	0.46	0/2025	0.70	6/2757 (0.2%)
1	1-C	0.52	0/2005	0.73	5/2731 (0.2%)
1	1-D	0.63	0/2025	0.78	8/2757 (0.3%)
1	1-F	0.52	0/2005	0.73	4/2731 (0.1%)
1	1-G	0.31	0/2024	0.63	8/2755 (0.3%)
1	2-A	0.58	0/2024	0.76	3/2755 (0.1%)
1	2-B	0.46	0/2025	0.70	6/2757 (0.2%)
1	2-C	0.52	0/2005	0.73	5/2731 (0.2%)
1	2-D	0.63	0/2025	0.78	8/2757 (0.3%)
1	2-F	0.52	0/2005	0.73	4/2731 (0.1%)
1	2-G	0.27	0/2024	0.61	8/2755 (0.3%)
2	1-H	0.57	0/4272	0.81	16/5800 (0.3%)
2	1-I	0.53	0/4271	0.78	11/5798 (0.2%)
2	1-J	0.51	0/4267	0.78	13/5792 (0.2%)
2	1-K	0.56	0/4267	0.81	19/5792 (0.3%)
2	1-M	0.50	0/4271	0.77	18/5798 (0.3%)
2	1-N	0.39	2/4272 (0.0%)	0.69	25/5800 (0.4%)
2	2-H	0.57	0/4272	0.81	16/5800 (0.3%)
2	2-I	0.53	0/4271	0.78	11/5798 (0.2%)
2	2-J	0.51	0/4267	0.78	13/5792 (0.2%)
2	2-K	0.56	0/4267	0.81	19/5792 (0.3%)
2	2-M	0.50	0/4271	0.77	18/5798 (0.3%)
2	2-N	0.30	1/4272 (0.0%)	0.68	22/5800 (0.4%)
All	All	0.51	3/75456 (0.0%)	0.76	269/102532 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-N	361	LYS	CB-CG	10.38	1.80	1.52
2	1-N	459	LYS	C-O	5.89	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-N	75	CYS	CB-SG	5.08	1.90	1.82

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	185	ASP	CB-CG-OD2	8.28	125.75	118.30
1	2-A	185	ASP	CB-CG-OD2	8.28	125.75	118.30
2	1-H	279	ASP	CB-CG-OD2	8.05	125.54	118.30
2	2-H	279	ASP	CB-CG-OD2	8.05	125.54	118.30
2	1-K	129	ASP	CB-CG-OD2	8.00	125.50	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1970	0	1910	30	1
1	1-B	1971	0	1914	22	0
1	1-C	1952	0	1891	14	0
1	1-D	1971	0	1914	26	0
1	1-F	1952	0	1891	25	0
1	1-G	1970	0	1910	62	0
1	2-A	1970	0	1910	30	0
1	2-B	1971	0	1914	21	0
1	2-C	1952	0	1891	14	0
1	2-D	1971	0	1914	26	0
1	2-F	1952	0	1891	28	0
1	2-G	1970	0	1910	67	0
2	1-H	4167	0	4140	52	0
2	1-I	4166	0	4139	45	0
2	1-J	4162	0	4139	57	0
2	1-K	4162	0	4139	52	0
2	1-M	4166	0	4139	57	0
2	1-N	4167	0	4140	60	1
2	2-H	4167	0	4140	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2-I	4166	0	4139	45	0
2	2-J	4162	0	4139	57	0
2	2-K	4162	0	4139	52	0
2	2-M	4166	0	4139	57	0
2	2-N	4167	0	4140	80	0
3	1-A	16	0	0	0	0
3	1-B	16	0	0	0	0
3	1-C	16	0	0	0	0
3	1-D	16	0	0	0	0
3	1-F	16	0	0	0	0
3	1-G	16	0	0	0	0
3	2-A	16	0	0	0	0
3	2-B	16	0	0	0	0
3	2-C	16	0	0	0	0
3	2-D	16	0	0	0	0
3	2-F	16	0	0	0	0
3	2-G	16	0	0	1	0
4	1-A	7	0	0	0	0
4	1-B	7	0	0	0	0
4	1-C	7	0	0	0	0
4	1-D	7	0	0	0	0
4	1-F	7	0	0	0	0
4	1-G	7	0	0	0	0
4	2-A	7	0	0	0	0
4	2-B	7	0	0	0	0
4	2-C	7	0	0	0	0
4	2-D	7	0	0	0	0
4	2-F	7	0	0	0	0
4	2-G	7	0	0	0	0
5	1-H	1	0	0	0	0
5	1-I	1	0	0	0	0
5	1-J	1	0	0	0	0
5	1-K	1	0	0	0	0
5	1-M	1	0	0	0	0
5	1-N	1	0	0	0	0
5	2-H	1	0	0	0	0
5	2-I	1	0	0	0	0
5	2-J	1	0	0	0	0
5	2-K	1	0	0	0	0
5	2-M	1	0	0	0	0
5	2-N	1	0	0	0	0
6	1-H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	1-I	1	0	0	0	0
6	1-J	1	0	0	0	0
6	1-K	1	0	0	0	0
6	1-M	1	0	0	0	0
6	1-N	1	0	0	0	0
6	2-H	1	0	0	0	0
6	2-I	1	0	0	0	0
6	2-J	1	0	0	0	0
6	2-K	1	0	0	0	0
6	2-M	1	0	0	0	0
6	2-N	1	0	0	0	0
7	1-H	7	0	0	0	0
7	1-I	7	0	0	0	0
7	1-J	7	0	0	0	0
7	1-K	7	0	0	0	0
7	1-M	7	0	0	1	0
7	1-N	7	0	0	2	0
7	2-H	7	0	0	0	0
7	2-I	7	0	0	0	0
7	2-J	7	0	0	0	0
7	2-K	7	0	0	0	0
7	2-M	7	0	0	1	0
7	2-N	7	0	0	3	0
8	1-A	122	0	0	3	0
8	1-B	83	0	0	1	0
8	1-C	120	0	0	1	0
8	1-D	149	0	0	4	0
8	1-F	108	0	0	2	0
8	1-G	59	0	0	10	0
8	1-H	245	0	0	2	0
8	1-I	218	0	0	3	0
8	1-J	208	0	0	3	0
8	1-K	253	0	0	6	0
8	1-M	183	0	0	2	0
8	1-N	138	0	0	1	0
8	2-A	122	0	0	3	0
8	2-B	84	0	0	1	0
8	2-C	120	0	0	1	0
8	2-D	148	0	0	4	0
8	2-F	109	0	0	2	0
8	2-G	58	0	0	8	0
8	2-H	245	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2-I	218	0	0	3	0
8	2-J	208	0	0	3	0
8	2-K	253	0	0	6	0
8	2-M	183	0	0	2	0
8	2-N	124	0	0	2	0
All	All	77694	0	72532	977	1

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.

The worst 5 of 977 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)
2:N:342:ALA:HB1	2:N:343:PRO:CD	1.55	1.33
1:G:177:LEU:HD23	1:G:178:PHE:CE2	1.78	1.17
1:G:177:LEU:HD23	1:G:178:PHE:CZ	1.79	1.16
2:N:342:ALA:CB	2:N:343:PRO:HD2	1.79	1.12
2:N:43:TRP:CZ2	2:N:365:LYS:HE2	1.84	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:OG	2:N:528:LYS:NZ[2_656]	1.95	0.25

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	1-A	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	1-B	260/264 (98%)	250 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-C	258/264 (98%)	247 (96%)	11 (4%)	0	100	100
1	1-D	260/264 (98%)	251 (96%)	9 (4%)	0	100	100
1	1-F	258/264 (98%)	245 (95%)	12 (5%)	1 (0%)	34	32
1	1-G	260/264 (98%)	250 (96%)	10 (4%)	0	100	100
1	2-A	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	2-B	260/264 (98%)	250 (96%)	10 (4%)	0	100	100
1	2-C	258/264 (98%)	247 (96%)	11 (4%)	0	100	100
1	2-D	260/264 (98%)	251 (96%)	9 (4%)	0	100	100
1	2-F	258/264 (98%)	245 (95%)	12 (5%)	1 (0%)	34	32
1	2-G	260/264 (98%)	249 (96%)	11 (4%)	0	100	100
2	1-H	543/549 (99%)	527 (97%)	16 (3%)	0	100	100
2	1-I	543/549 (99%)	526 (97%)	17 (3%)	0	100	100
2	1-J	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
2	1-K	542/549 (99%)	530 (98%)	12 (2%)	0	100	100
2	1-M	543/549 (99%)	523 (96%)	20 (4%)	0	100	100
2	1-N	543/549 (99%)	524 (96%)	18 (3%)	1 (0%)	47	49
2	2-H	543/549 (99%)	527 (97%)	16 (3%)	0	100	100
2	2-I	543/549 (99%)	526 (97%)	17 (3%)	0	100	100
2	2-J	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
2	2-K	542/549 (99%)	530 (98%)	12 (2%)	0	100	100
2	2-M	543/549 (99%)	523 (96%)	20 (4%)	0	100	100
2	2-N	543/549 (99%)	521 (96%)	19 (4%)	3 (1%)	25	21
All	All	9624/9756 (99%)	9300 (97%)	318 (3%)	6 (0%)	51	54

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2-N	343	PRO
2	2-N	342	ALA
1	1-F	231	LEU
1	2-F	231	LEU
2	1-N	148	ILE

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	1-A	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	1-B	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	1-C	206/210 (98%)	200 (97%)	6 (3%)	42	46
1	1-D	208/210 (99%)	206 (99%)	2 (1%)	76	82
1	1-F	206/210 (98%)	203 (98%)	3 (2%)	65	71
1	1-G	208/210 (99%)	207 (100%)	1 (0%)	88	92
1	2-A	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	2-B	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	2-C	206/210 (98%)	200 (97%)	6 (3%)	42	46
1	2-D	208/210 (99%)	206 (99%)	2 (1%)	76	82
1	2-F	206/210 (98%)	203 (98%)	3 (2%)	65	71
1	2-G	208/210 (99%)	206 (99%)	2 (1%)	76	82
2	1-H	435/439 (99%)	429 (99%)	6 (1%)	67	73
2	1-I	435/439 (99%)	431 (99%)	4 (1%)	78	84
2	1-J	435/439 (99%)	424 (98%)	11 (2%)	47	52
2	1-K	435/439 (99%)	428 (98%)	7 (2%)	62	69
2	1-M	435/439 (99%)	421 (97%)	14 (3%)	39	41
2	1-N	435/439 (99%)	426 (98%)	9 (2%)	53	59
2	2-H	435/439 (99%)	429 (99%)	6 (1%)	67	73
2	2-I	435/439 (99%)	431 (99%)	4 (1%)	78	84
2	2-J	435/439 (99%)	424 (98%)	11 (2%)	47	52
2	2-K	435/439 (99%)	428 (98%)	7 (2%)	62	69
2	2-M	435/439 (99%)	421 (97%)	14 (3%)	39	41
2	2-N	435/439 (99%)	426 (98%)	9 (2%)	53	59
All	All	7708/7788 (99%)	7565 (98%)	143 (2%)	57	63

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2-F	16	GLU
2	2-M	135	LYS
2	2-M	473	ASP
2	1-M	135	LYS
2	1-M	33	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
2	2-H	454	ASN
1	2-C	172	ASN
2	2-H	509	GLN
1	2-B	172	ASN
1	2-D	14	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 72 ligands modelled in this entry, 24 are monoatomic - leaving 48 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	1-F	267	1	0,12,12	-	-	-		
3	SF4	1-D	265	1	0,12,12	-	-	-		
4	F3S	1-A	266	1	0,9,9	-	-	-		
7	FCO	1-K	550	8,2	0,6,6	-	-	-		
3	SF4	1-F	265	1	0,12,12	-	-	-		
7	FCO	1-N	550	8,2	0,6,6	-	-	-		
4	F3S	2-D	266	1	0,9,9	-	-	-		
4	F3S	1-D	266	1	0,9,9	-	-	-		
3	SF4	2-F	265	1	0,12,12	-	-	-		
3	SF4	1-C	267	1	0,12,12	-	-	-		
7	FCO	2-M	550	8,2	0,6,6	-	-	-		
3	SF4	2-B	267	1	0,12,12	-	-	-		
4	F3S	2-A	266	1	0,9,9	-	-	-		
7	FCO	1-I	550	8,2	0,6,6	-	-	-		
4	F3S	1-B	266	1	0,9,9	-	-	-		
3	SF4	2-B	265	1	0,12,12	-	-	-		
4	F3S	1-C	266	1	0,9,9	-	-	-		
4	F3S	1-G	266	1	0,9,9	-	-	-		
4	F3S	2-B	266	1	0,9,9	-	-	-		
3	SF4	2-A	267	1	0,12,12	-	-	-		
4	F3S	1-F	266	1	0,9,9	-	-	-		
3	SF4	2-A	265	1	0,12,12	-	-	-		
3	SF4	1-B	267	1	0,12,12	-	-	-		
4	F3S	2-C	266	1	0,9,9	-	-	-		
4	F3S	2-G	266	1	0,9,9	-	-	-		
3	SF4	1-G	267	1	0,12,12	-	-	-		
3	SF4	2-D	267	1	0,12,12	-	-	-		
7	FCO	2-N	550	8,2	0,6,6	-	-	-		
7	FCO	2-K	550	8,2	0,6,6	-	-	-		
7	FCO	2-I	550	8,2	0,6,6	-	-	-		
3	SF4	2-F	267	1	0,12,12	-	-	-		
7	FCO	1-J	550	8,2	0,6,6	-	-	-		
7	FCO	2-J	550	8,2	0,6,6	-	-	-		
3	SF4	1-B	265	1	0,12,12	-	-	-		
3	SF4	2-G	267	1	0,12,12	-	-	-		
3	SF4	1-A	267	1	0,12,12	-	-	-		
3	SF4	1-G	265	1	0,12,12	-	-	-		
7	FCO	1-M	550	8,2	0,6,6	-	-	-		
3	SF4	1-D	267	1	0,12,12	-	-	-		
3	SF4	1-C	265	1	0,12,12	-	-	-		
3	SF4	1-A	265	1	0,12,12	-	-	-		
4	F3S	2-F	266	1	0,9,9	-	-	-		
3	SF4	2-G	265	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SF4	2-D	265	1	0,12,12	-	-	-		
3	SF4	2-C	267	1	0,12,12	-	-	-		
7	FCO	1-H	550	8,2	0,6,6	-	-	-		
7	FCO	2-H	550	8,2	0,6,6	-	-	-		
3	SF4	2-C	265	1	0,12,12	-	-	-		

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	1-F	267	1	-	-	0/6/5/5
3	SF4	1-D	265	1	-	-	0/6/5/5
4	F3S	1-A	266	1	-	-	0/3/3/3
3	SF4	1-F	265	1	-	-	0/6/5/5
4	F3S	2-D	266	1	-	-	0/3/3/3
4	F3S	1-D	266	1	-	-	0/3/3/3
3	SF4	2-F	265	1	-	-	0/6/5/5
3	SF4	1-C	267	1	-	-	0/6/5/5
3	SF4	2-B	267	1	-	-	0/6/5/5
4	F3S	2-A	266	1	-	-	0/3/3/3
4	F3S	1-B	266	1	-	-	0/3/3/3
3	SF4	2-B	265	1	-	-	0/6/5/5
4	F3S	1-C	266	1	-	-	0/3/3/3
4	F3S	1-G	266	1	-	-	0/3/3/3
4	F3S	2-B	266	1	-	-	0/3/3/3
3	SF4	2-A	267	1	-	-	0/6/5/5
4	F3S	1-F	266	1	-	-	0/3/3/3
3	SF4	2-A	265	1	-	-	0/6/5/5
3	SF4	1-B	267	1	-	-	0/6/5/5
4	F3S	2-C	266	1	-	-	0/3/3/3
4	F3S	2-G	266	1	-	-	0/3/3/3
3	SF4	1-G	267	1	-	-	0/6/5/5
3	SF4	2-D	267	1	-	-	0/6/5/5
3	SF4	2-F	267	1	-	-	0/6/5/5
3	SF4	1-B	265	1	-	-	0/6/5/5
3	SF4	2-G	267	1	-	-	0/6/5/5
3	SF4	1-A	267	1	-	-	0/6/5/5
3	SF4	1-G	265	1	-	-	0/6/5/5
3	SF4	1-D	267	1	-	-	0/6/5/5
3	SF4	1-C	265	1	-	-	0/6/5/5
3	SF4	1-A	265	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F3S	2-F	266	1	-	-	0/3/3/3
3	SF4	2-G	265	1	-	-	0/6/5/5
3	SF4	2-D	265	1	-	-	0/6/5/5
3	SF4	2-C	267	1	-	-	0/6/5/5
3	SF4	2-C	265	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1-N	550	FCO	2	0
7	2-M	550	FCO	1	0
7	2-N	550	FCO	3	0
7	1-M	550	FCO	1	0
3	2-G	265	SF4	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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1-A	262/264 (99%)	-0.24	6 (2%) 60 65	5, 9, 18, 28	8 (3%)
1	1-B	262/264 (99%)	0.57	40 (15%) 2 3	4, 10, 18, 25	6 (2%)
1	1-C	260/264 (98%)	-0.36	2 (0%) 86 88	4, 9, 16, 23	6 (2%)
1	1-D	262/264 (99%)	-0.48	2 (0%) 86 88	3, 9, 16, 30	5 (1%)
1	1-F	260/264 (98%)	-0.14	5 (1%) 66 71	4, 10, 17, 24	6 (2%)
1	1-G	262/264 (99%)	5.25	251 (95%) 0 0	6, 10, 10, 11	262 (100%)
1	2-A	262/264 (99%)	-0.24	6 (2%) 60 65	5, 9, 18, 28	8 (3%)
1	2-B	262/264 (99%)	0.57	40 (15%) 2 3	4, 10, 18, 25	6 (2%)
1	2-C	260/264 (98%)	-0.36	2 (0%) 86 88	4, 9, 16, 23	6 (2%)
1	2-D	262/264 (99%)	-0.48	2 (0%) 86 88	3, 9, 16, 30	5 (1%)
1	2-F	260/264 (98%)	-0.14	5 (1%) 66 71	4, 10, 17, 24	6 (2%)
1	2-G	262/264 (99%)	5.25	251 (95%) 0 0	6, 10, 10, 11	262 (100%)
2	1-H	545/549 (99%)	-0.25	9 (1%) 70 74	4, 9, 16, 27	11 (2%)
2	1-I	545/549 (99%)	-0.01	27 (4%) 28 34	3, 9, 16, 24	6 (1%)
2	1-J	544/549 (99%)	-0.11	16 (2%) 51 57	4, 9, 17, 23	12 (2%)
2	1-K	544/549 (99%)	-0.23	8 (1%) 73 77	3, 9, 17, 24	12 (2%)
2	1-M	545/549 (99%)	0.03	19 (3%) 44 50	3, 10, 16, 31	12 (2%)
2	1-N	545/549 (99%)	4.35	502 (92%) 0 0	6, 10, 11, 12	545 (100%)
2	2-H	545/549 (99%)	-0.25	9 (1%) 70 74	4, 9, 16, 27	11 (2%)
2	2-I	545/549 (99%)	-0.01	27 (4%) 28 34	3, 9, 16, 24	6 (1%)
2	2-J	544/549 (99%)	-0.11	16 (2%) 51 57	4, 9, 17, 23	12 (2%)
2	2-K	544/549 (99%)	-0.23	8 (1%) 73 77	3, 9, 17, 24	12 (2%)
2	2-M	545/549 (99%)	0.03	19 (3%) 44 50	3, 10, 16, 31	12 (2%)
2	2-N	545/549 (99%)	4.35	502 (92%) 0 0	6, 10, 11, 12	545 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	9672/9756 (99%)	0.67	1774 (18%)	1	1	3, 9, 16, 31	1782 (18%)

The worst 5 of 1774 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-N	171	VAL	15.6
2	2-N	171	VAL	15.6
2	1-N	186	GLY	15.1
2	2-N	186	GLY	15.1
1	1-G	137	LEU	13.5

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SF4	1-G	265	8/8	0.85	0.32	4,6,7,8	8
3	SF4	2-G	265	8/8	0.85	0.32	8,10,11,12	8
6	MG	1-N	553	1/1	0.86	0.27	8,8,8,8	1
6	MG	2-N	553	1/1	0.86	0.27	8,8,8,8	1
4	F3S	1-G	266	7/7	0.92	0.36	8,9,11,11	7
4	F3S	2-G	266	7/7	0.92	0.36	10,10,11,11	7
6	MG	1-M	553	1/1	0.95	0.13	8,8,8,8	0
6	MG	2-M	553	1/1	0.95	0.13	8,8,8,8	0
3	SF4	1-G	267	8/8	0.96	0.41	7,10,10,12	8
3	SF4	2-G	267	8/8	0.96	0.41	7,10,10,12	8
6	MG	1-H	553	1/1	0.96	0.06	8,8,8,8	0
6	MG	2-H	553	1/1	0.96	0.06	8,8,8,8	0
6	MG	1-K	553	1/1	0.97	0.07	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	2-K	553	1/1	0.97	0.07	3,3,3,3	0
3	SF4	1-A	265	8/8	0.97	0.05	7,9,10,12	0
3	SF4	2-A	265	8/8	0.97	0.05	7,9,10,12	0
6	MG	1-J	553	1/1	0.97	0.09	5,5,5,5	0
6	MG	2-J	553	1/1	0.97	0.09	5,5,5,5	0
7	FCO	1-N	550	7/7	0.97	0.37	5,6,7,9	7
7	FCO	2-N	550	7/7	0.97	0.37	5,6,7,9	7
4	F3S	1-D	266	7/7	0.98	0.04	7,8,10,10	0
4	F3S	2-D	266	7/7	0.98	0.04	7,8,10,10	0
4	F3S	1-F	266	7/7	0.98	0.05	7,9,12,12	0
4	F3S	2-F	266	7/7	0.98	0.05	7,9,12,12	0
3	SF4	1-B	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	2-B	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	1-F	265	8/8	0.98	0.06	6,7,10,10	0
3	SF4	2-F	265	8/8	0.98	0.06	6,7,10,10	0
3	SF4	1-F	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	2-F	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	1-A	267	8/8	0.98	0.05	7,8,10,11	0
3	SF4	2-A	267	8/8	0.98	0.05	7,8,10,11	0
3	SF4	1-B	265	8/8	0.98	0.09	5,6,9,9	0
3	SF4	2-B	265	8/8	0.98	0.09	5,6,9,9	0
4	F3S	1-A	266	7/7	0.98	0.05	6,7,10,13	0
4	F3S	2-A	266	7/7	0.98	0.05	6,7,10,13	0
4	F3S	1-B	266	7/7	0.98	0.06	9,10,10,10	0
4	F3S	2-B	266	7/7	0.98	0.06	9,10,10,10	0
5	NI	1-N	551	1/1	0.99	0.32	13,13,13,13	1
5	NI	2-N	551	1/1	0.99	0.32	12,12,12,12	1
3	SF4	1-C	267	8/8	0.99	0.04	5,9,10,10	0
3	SF4	2-C	267	8/8	0.99	0.04	5,9,10,10	0
6	MG	1-I	553	1/1	0.99	0.07	6,6,6,6	0
6	MG	2-I	553	1/1	0.99	0.07	6,6,6,6	0
4	F3S	1-C	266	7/7	0.99	0.04	9,10,11,12	0
4	F3S	2-C	266	7/7	0.99	0.04	9,10,11,12	0
3	SF4	1-D	265	8/8	0.99	0.03	6,8,9,9	0
3	SF4	2-D	265	8/8	0.99	0.03	6,8,9,9	0
3	SF4	1-D	267	8/8	0.99	0.04	3,7,9,9	0
3	SF4	2-D	267	8/8	0.99	0.04	3,7,9,9	0
3	SF4	1-C	265	8/8	0.99	0.04	6,6,8,9	0
3	SF4	2-C	265	8/8	0.99	0.04	6,6,8,9	0
7	FCO	1-H	550	7/7	0.99	0.06	8,9,11,13	0
7	FCO	2-H	550	7/7	0.99	0.06	8,9,11,13	0
7	FCO	1-K	550	7/7	0.99	0.07	6,8,10,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	FCO	2-K	550	7/7	0.99	0.07	6,8,10,12	0
7	FCO	1-M	550	7/7	0.99	0.10	4,6,7,12	0
7	FCO	2-M	550	7/7	0.99	0.10	4,6,7,12	0
5	NI	1-I	551	1/1	0.99	0.03	10,10,10,10	0
5	NI	2-I	551	1/1	0.99	0.03	10,10,10,10	0
5	NI	1-M	551	1/1	1.00	0.06	8,8,8,8	0
5	NI	2-M	551	1/1	1.00	0.06	8,8,8,8	0
7	FCO	1-I	550	7/7	1.00	0.06	3,5,8,9	0
7	FCO	2-I	550	7/7	1.00	0.06	3,5,8,9	0
7	FCO	1-J	550	7/7	1.00	0.08	7,7,11,12	0
7	FCO	2-J	550	7/7	1.00	0.08	7,7,11,12	0
5	NI	1-H	551	1/1	1.00	0.02	9,9,9,9	0
5	NI	2-H	551	1/1	1.00	0.02	9,9,9,9	0
5	NI	1-J	551	1/1	1.00	0.05	9,9,9,9	0
5	NI	2-J	551	1/1	1.00	0.05	9,9,9,9	0
5	NI	1-K	551	1/1	1.00	0.04	11,11,11,11	0
5	NI	2-K	551	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.