wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 10:14 PM EDT

PDB ID	:	2FRV
Title	:	CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDROGENASE
Authors	:	Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C.
Deposited on	:	1997-06-10
Resolution	:	2.54 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:

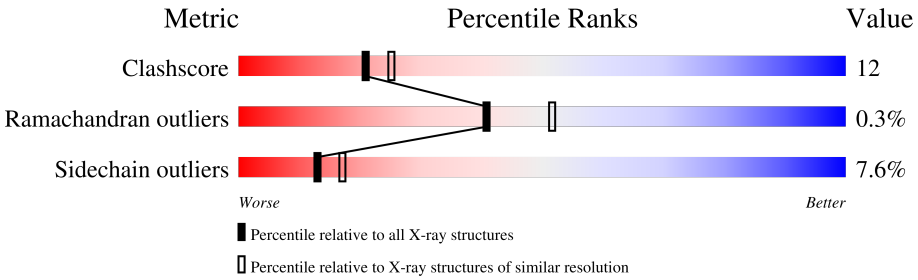
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.54 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	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	69% 26% • •
1	C	264	70% 24% • •
1	E	264	70% 24% 5% •
1	G	264	70% 24% • •
1	I	264	70% 23% 5% •
1	S	264	70% 23% 5% •
2	B	536	63% 31% • ••
2	D	536	63% 30% • ••

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Mol	Chain	Length	Quality of chain
2	F	536	62% 31% 5%
2	H	536	63% 30%
2	J	536	63% 30% 5%
2	L	536	63% 30% 5%

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	B	537	-	-	X	-
7	FCO	D	537	-	-	X	-
7	FCO	F	537	-	-	X	-
7	FCO	H	537	-	-	X	-
7	FCO	J	537	-	-	X	-
7	FCO	L	537	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 38040 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 HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	A	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	C	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	E	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	G	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	I	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	24	VAL	LEU	conflict	UNP P12943
S	89	GLY	ARG	conflict	UNP P12943
A	24	VAL	LEU	conflict	UNP P12943
A	89	GLY	ARG	conflict	UNP P12943
C	24	VAL	LEU	conflict	UNP P12943
C	89	GLY	ARG	conflict	UNP P12943
E	24	VAL	LEU	conflict	UNP P12943
E	89	GLY	ARG	conflict	UNP P12943
G	24	VAL	LEU	conflict	UNP P12943
G	89	GLY	ARG	conflict	UNP P12943
I	24	VAL	LEU	conflict	UNP P12943
I	89	GLY	ARG	conflict	UNP P12943

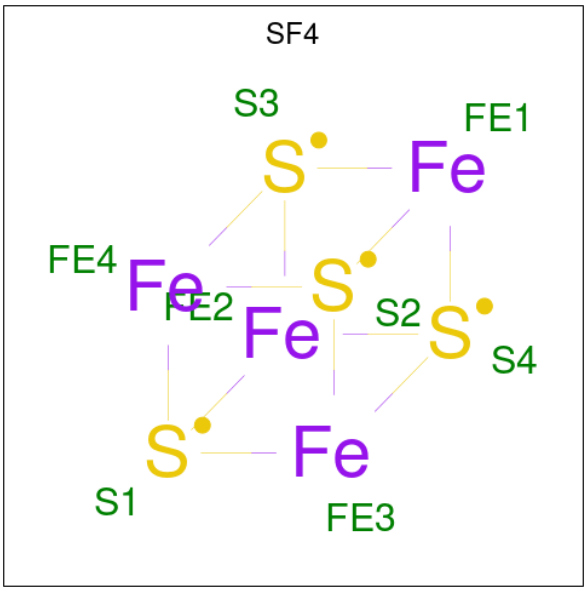
- Molecule 2 is a protein called PERIPLASMIC HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	B	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	D	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	F	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	H	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	J	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			

There are 24 discrepancies between the modelled and reference sequences:

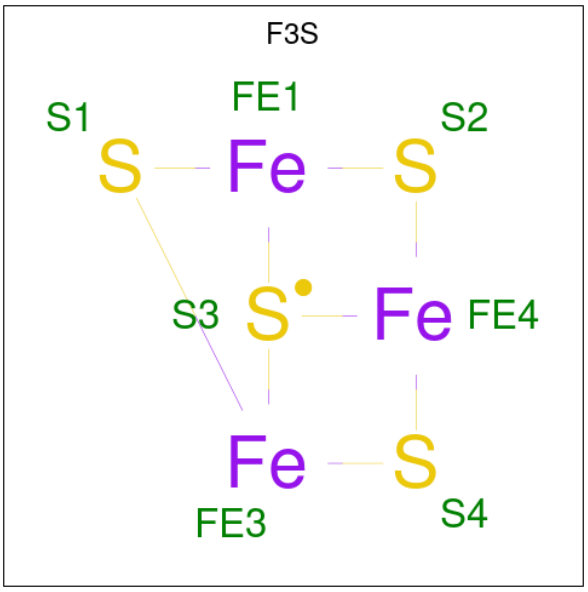
Chain	Residue	Modelled	Actual	Comment	Reference
L	144	LYS	ARG	conflict	UNP P12944
L	332	GLY	ASP	conflict	UNP P12944
L	482	LEU	HIS	conflict	UNP P12944
L	497	GLY	ARG	conflict	UNP P12944
B	144	LYS	ARG	conflict	UNP P12944
B	332	GLY	ASP	conflict	UNP P12944
B	482	LEU	HIS	conflict	UNP P12944
B	497	GLY	ARG	conflict	UNP P12944
D	144	LYS	ARG	conflict	UNP P12944
D	332	GLY	ASP	conflict	UNP P12944
D	482	LEU	HIS	conflict	UNP P12944
D	497	GLY	ARG	conflict	UNP P12944
F	144	LYS	ARG	conflict	UNP P12944
F	332	GLY	ASP	conflict	UNP P12944
F	482	LEU	HIS	conflict	UNP P12944
F	497	GLY	ARG	conflict	UNP P12944
H	144	LYS	ARG	conflict	UNP P12944
H	332	GLY	ASP	conflict	UNP P12944
H	482	LEU	HIS	conflict	UNP P12944
H	497	GLY	ARG	conflict	UNP P12944
J	144	LYS	ARG	conflict	UNP P12944
J	332	GLY	ASP	conflict	UNP P12944
J	482	LEU	HIS	conflict	UNP P12944
J	497	GLY	ARG	conflict	UNP P12944

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	1	Total Fe S 8 4 4	0	0
3	S	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	E	1	Total Fe S 8 4 4	0	0
3	E	1	Total Fe S 8 4 4	0	0
3	G	1	Total Fe S 8 4 4	0	0
3	G	1	Total Fe S 8 4 4	0	0
3	I	1	Total Fe S 8 4 4	0	0
3	I	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	S	1	Total Fe S 7 3 4	0	0
4	A	1	Total Fe S 7 3 4	0	0
4	C	1	Total Fe S 7 3 4	0	0
4	E	1	Total Fe S 7 3 4	0	0
4	G	1	Total Fe S 7 3 4	0	0
4	I	1	Total Fe S 7 3 4	0	0

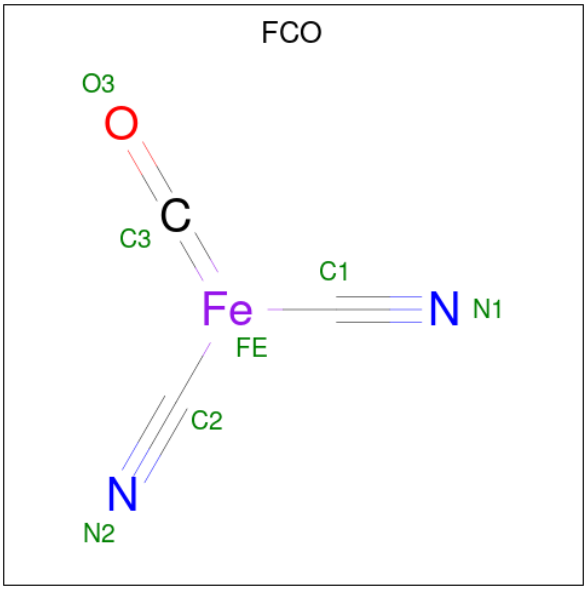
- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Ni 1 1	0	0
5	B	1	Total Ni 1 1	0	0
5	D	1	Total Ni 1 1	0	0
5	F	1	Total Ni 1 1	0	0
5	H	1	Total Ni 1 1	0	0
5	J	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	L	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0
6	H	1	Total Mg 1 1	0	0
6	J	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	L	1	Total C Fe N O 7 3 1 2 1	0	0
7	B	1	Total C Fe N O 7 3 1 2 1	0	0
7	D	1	Total C Fe N O 7 3 1 2 1	0	0
7	F	1	Total C Fe N O 7 3 1 2 1	0	0

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

- Molecule 8 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	O	0	0
			1	1		
8	B	1	Total	O	0	0
			1	1		
8	D	1	Total	O	0	0
			1	1		
8	F	1	Total	O	0	0
			1	1		
8	H	1	Total	O	0	0
			1	1		
8	J	1	Total	O	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	77	Total	O	0	0
			77	77		
9	L	110	Total	O	0	0
			110	110		
9	A	78	Total	O	0	0
			78	78		
9	B	114	Total	O	0	0
			114	114		
9	C	76	Total	O	0	0
			76	76		
9	D	114	Total	O	0	0
			114	114		
9	E	81	Total	O	0	0
			81	81		
9	F	115	Total	O	0	0
			115	115		
9	G	76	Total	O	0	0
			76	76		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	112	Total O 112 112	0	0
9	I	80	Total O 80 80	0	0
9	J	113	Total O 113 113	0	0

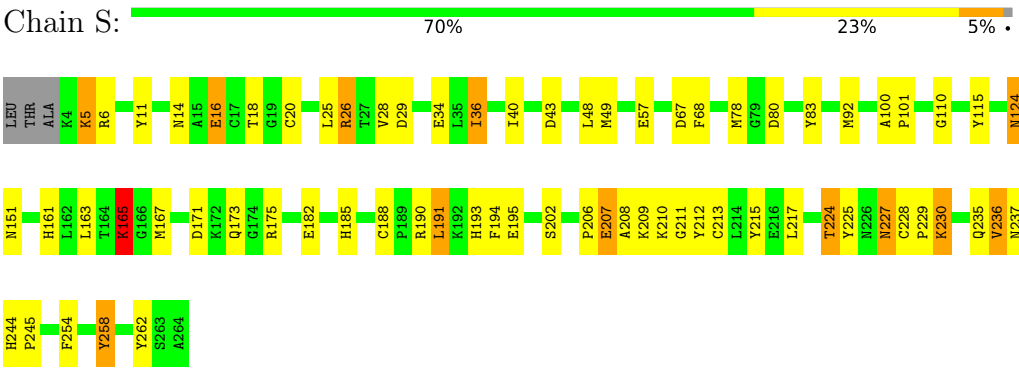
3 Residue-property plots (i)

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. 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.

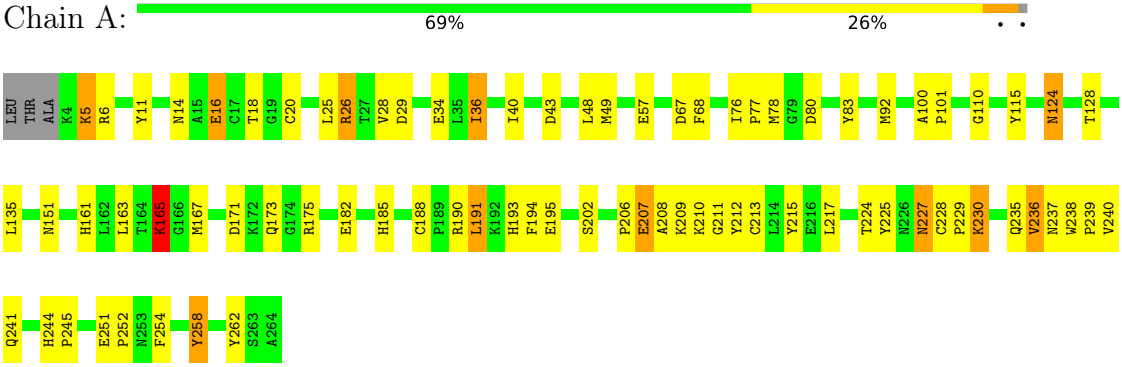
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain S:



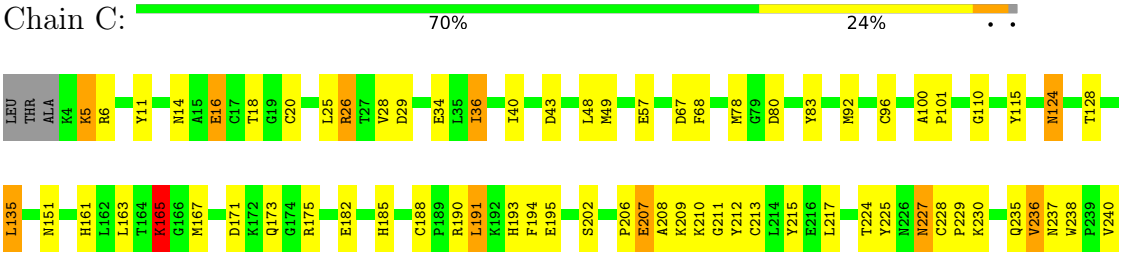
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain A:



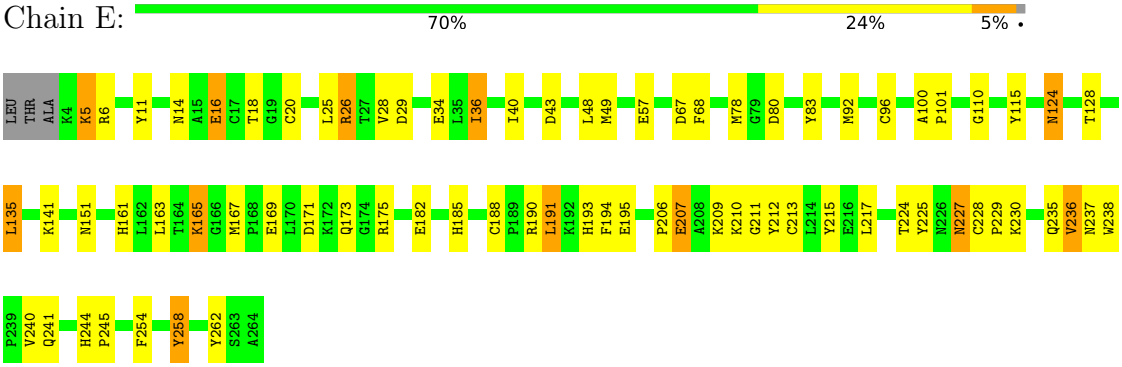
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain C:



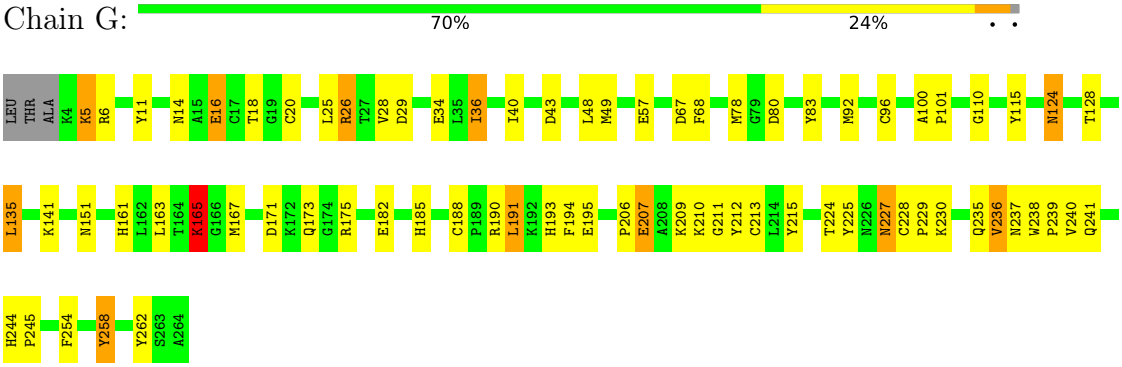
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain E:



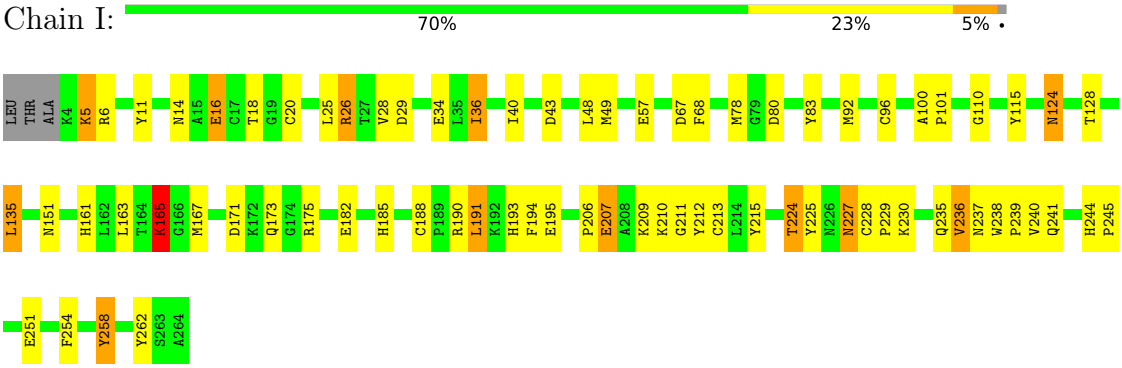
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain G:



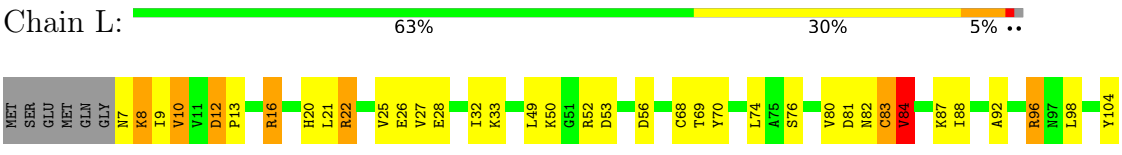
• Molecule 1: PERIPLASMIC HYDROGENASE

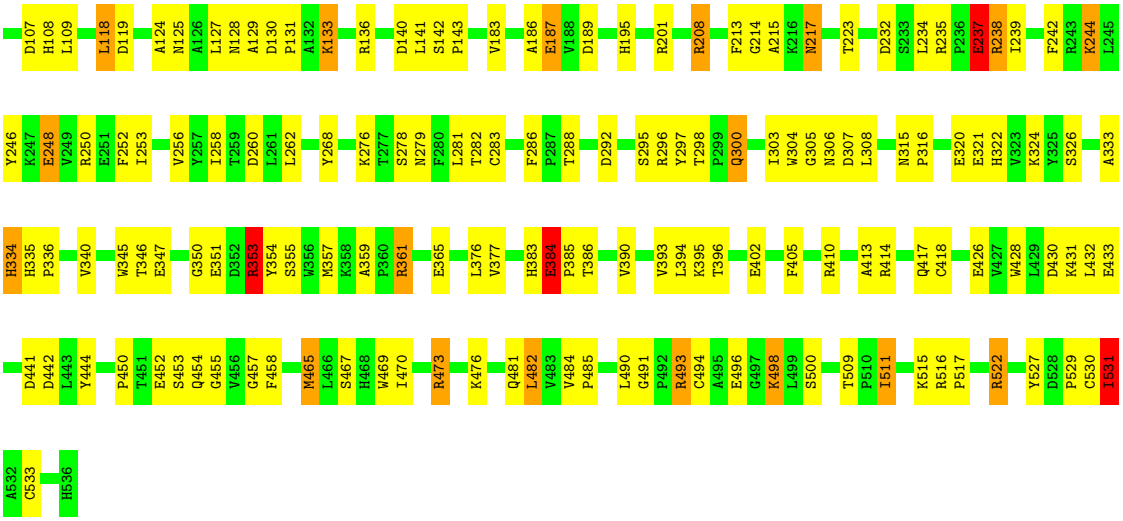
Chain I:



• Molecule 2: PERIPLASMIC HYDROGENASE

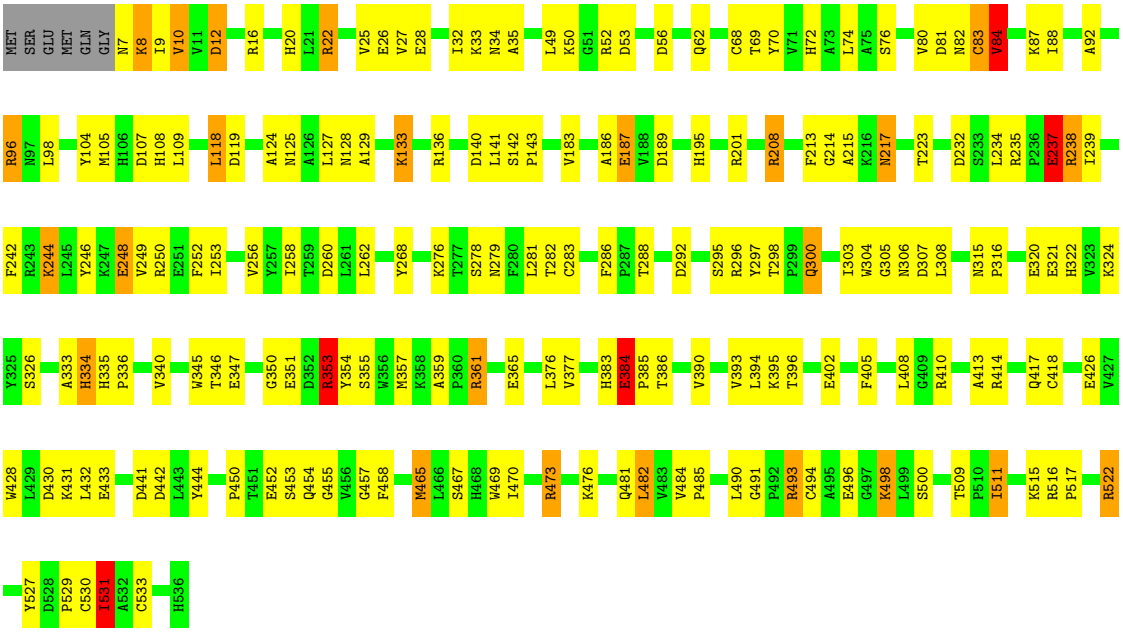
Chain L:





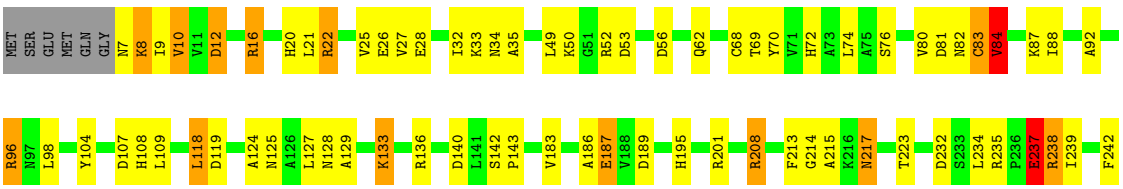
• Molecule 2: PERIPLASMIC HYDROGENASE

Chain B:



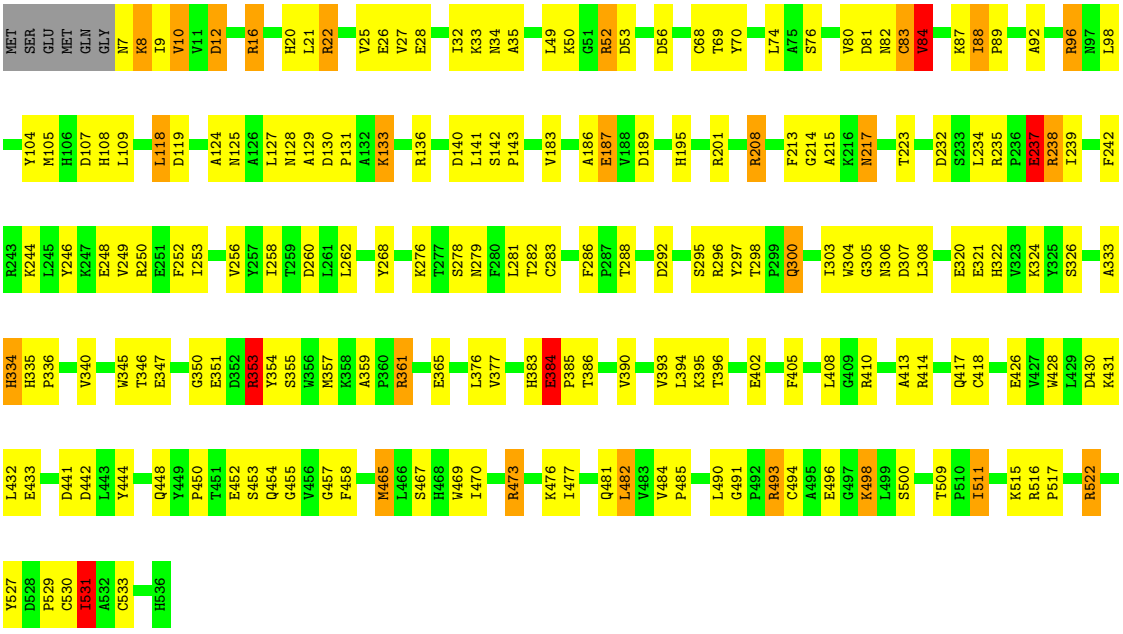
• Molecule 2: PERIPLASMIC HYDROGENASE

Chain D:



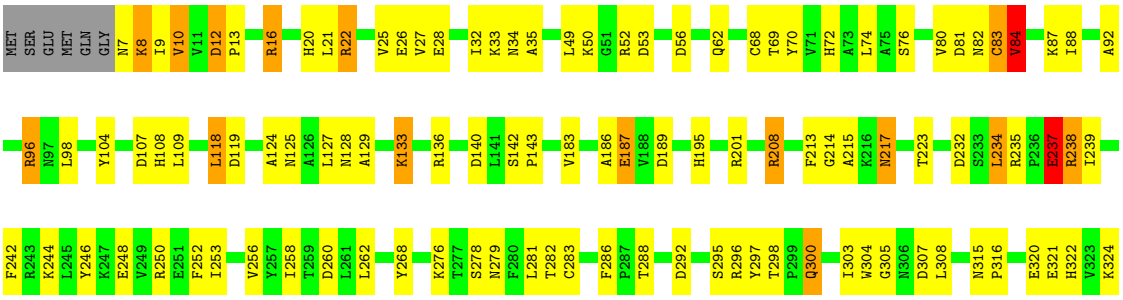
• Molecule 2: PERIPLASMIC HYDROGENASE

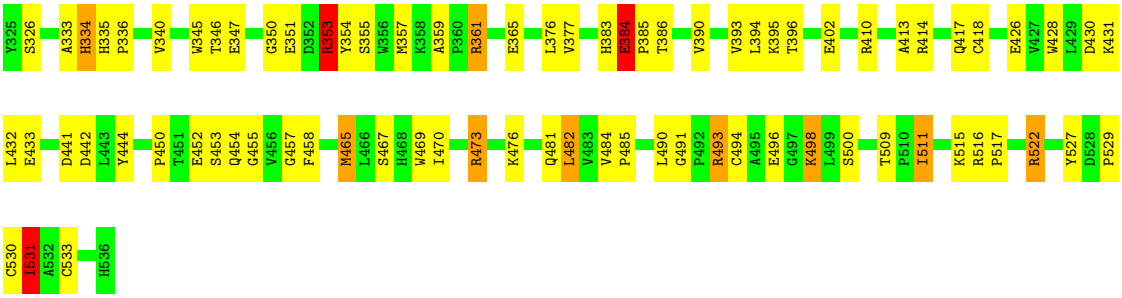
Chain F:



• Molecule 2: PERIPLASMIC HYDROGENASE

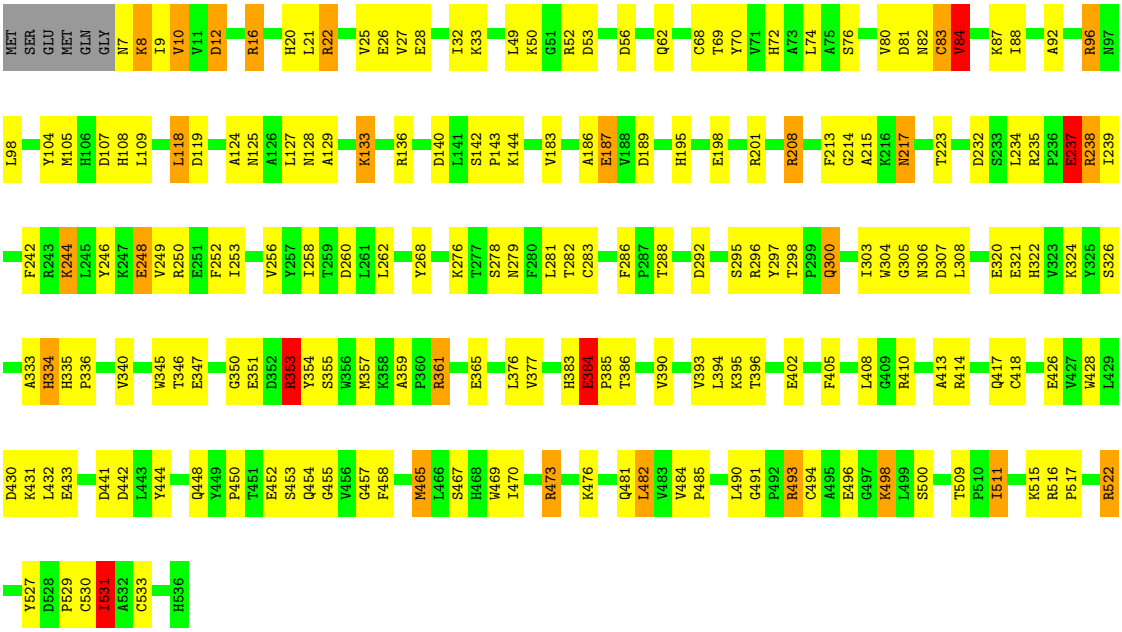
Chain H:





• Molecule 2: PERIPLASMIC HYDROGENASE

Chain J:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	112.78Å 113.16Å 133.91Å 90.03° 90.02° 119.99°	Depositor
Resolution (Å)	8.00 – 2.54	Depositor
% Data completeness (in resolution range)	92.5 (8.00-2.54)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.201 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	38040	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

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: MG, SF4, O, FCO, F3S, NI

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	A	1.02	0/2017	1.83	44/2742 (1.6%)
1	C	1.02	0/2017	1.83	44/2742 (1.6%)
1	E	1.01	0/2017	1.83	43/2742 (1.6%)
1	G	1.02	0/2017	1.83	44/2742 (1.6%)
1	I	1.02	0/2017	1.83	45/2742 (1.6%)
1	S	1.01	0/2017	1.83	44/2742 (1.6%)
2	B	0.96	0/4257	1.90	81/5786 (1.4%)
2	D	0.96	0/4257	1.90	81/5786 (1.4%)
2	F	0.96	0/4257	1.90	81/5786 (1.4%)
2	H	0.96	0/4257	1.90	81/5786 (1.4%)
2	J	0.96	0/4257	1.90	80/5786 (1.4%)
2	L	0.96	0/4257	1.90	81/5786 (1.4%)
All	All	0.98	0/37644	1.88	749/51168 (1.5%)

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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	L	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 749 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	96	ARG	NE-CZ-NH1	22.41	131.51	120.30
2	H	96	ARG	NE-CZ-NH1	22.36	131.48	120.30
2	F	96	ARG	NE-CZ-NH1	22.35	131.47	120.30
2	L	96	ARG	NE-CZ-NH1	22.33	131.46	120.30
2	D	96	ARG	NE-CZ-NH1	22.32	131.46	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	353	ARG	Sidechain
2	D	353	ARG	Sidechain
2	F	353	ARG	Sidechain
2	H	353	ARG	Sidechain
2	L	353	ARG	Sidechain

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	A	1964	0	1895	44	0
1	C	1964	0	1895	38	0
1	E	1964	0	1895	42	0
1	G	1964	0	1895	41	0
1	I	1964	0	1895	40	0
1	S	1964	0	1895	42	0
2	B	4152	0	4114	118	0
2	D	4152	0	4114	114	0
2	F	4152	0	4114	117	0
2	H	4152	0	4114	113	0
2	J	4152	0	4114	117	0
2	L	4152	0	4114	113	0
3	A	16	0	0	0	0
3	C	16	0	0	0	0
3	E	16	0	0	0	0
3	G	16	0	0	0	0
3	I	16	0	0	0	0
3	S	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	7	0	0	0	0
4	C	7	0	0	0	0
4	E	7	0	0	0	0
4	G	7	0	0	0	0
4	I	7	0	0	1	0
4	S	7	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
7	B	7	0	0	2	0
7	D	7	0	0	2	0
7	F	7	0	0	2	0
7	H	7	0	0	2	0
7	J	7	0	0	2	0
7	L	7	0	0	2	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
8	J	1	0	0	0	0
8	L	1	0	0	0	0
9	A	78	0	0	0	2
9	B	114	0	0	0	0
9	C	76	0	0	0	1
9	D	114	0	0	0	0
9	E	81	0	0	0	1
9	F	115	0	0	0	0
9	G	76	0	0	0	0
9	H	112	0	0	0	0
9	I	80	0	0	0	1
9	J	113	0	0	0	0
9	L	110	0	0	0	0
9	S	77	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	38040	0	36054	878	3

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 12.

The worst 5 of 878 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:I:235:GLN:NE2	2:J:208:ARG:HH21	1.56	1.03
1:E:235:GLN:NE2	2:F:208:ARG:HH21	1.56	1.03
1:C:235:GLN:NE2	2:D:208:ARG:HH21	1.56	1.02
1:A:235:GLN:NE2	2:B:208:ARG:HH21	1.56	1.02
1:G:235:GLN:NE2	2:H:208:ARG:HH21	1.56	1.02

All (3) 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)
9:A:340:HOH:O	9:I:1015:HOH:O[1_445]	1.32	0.88
9:A:341:HOH:O	9:C:450:HOH:O[1_444]	1.34	0.86
9:S:338:HOH:O	9:E:639:HOH:O[1_556]	1.41	0.79

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	A	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	C	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	E	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	G	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	S	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
2	B	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	D	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	F	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	H	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	J	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	L	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
All	All	4722/4800 (98%)	4500 (95%)	210 (4%)	12 (0%)	41	51

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	5	LYS
2	L	118	LEU
1	A	5	LYS
2	B	118	LEU
1	C	5	LYS

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	A	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	C	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	E	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	G	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	I	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	S	208/210 (99%)	194 (93%)	14 (7%)	16	21
2	B	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	D	434/439 (99%)	399 (92%)	35 (8%)	11	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	H	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	J	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	L	434/439 (99%)	399 (92%)	35 (8%)	11	14
All	All	3852/3894 (99%)	3558 (92%)	294 (8%)	13	17

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	361	ARG
2	J	476	LYS
2	H	482	LEU
2	J	8	LYS
2	B	531	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	124	ASN
1	I	124	ASN
1	G	161	HIS
2	H	217	ASN
1	I	231	GLN

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 42 ligands modelled in this entry, 18 are monoatomic - leaving 24 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	I	267	1	0,12,12	-	-	-		
4	F3S	S	266	1	0,9,9	-	-	-		
3	SF4	S	267	1	0,12,12	-	-	-		
4	F3S	G	266	1	0,9,9	-	-	-		
7	FCO	F	537	8,2	0,6,6	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
4	F3S	I	266	1	0,9,9	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
7	FCO	L	537	8,2	0,6,6	-	-	-		
7	FCO	J	537	8,2	0,6,6	-	-	-		
7	FCO	H	537	8,2	0,6,6	-	-	-		
4	F3S	E	266	1	0,9,9	-	-	-		
7	FCO	B	537	8,2	0,6,6	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
3	SF4	S	265	1	0,12,12	-	-	-		
3	SF4	G	265	1	0,12,12	-	-	-		
7	FCO	D	537	8,2	0,6,6	-	-	-		
3	SF4	G	267	1	0,12,12	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
3	SF4	E	265	1	0,12,12	-	-	-		
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	I	265	1	0,12,12	-	-	-		
3	SF4	E	267	1	0,12,12	-	-	-		
4	F3S	A	266	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
3	SF4	E	265	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	267	1	-	-	0/6/5/5
3	SF4	I	265	1	-	-	0/6/5/5
3	SF4	I	267	1	-	-	0/6/5/5
3	SF4	S	265	1	-	-	0/6/5/5
4	F3S	S	266	1	-	-	0/3/3/3
3	SF4	E	267	1	-	-	0/6/5/5
4	F3S	C	266	1	-	-	0/3/3/3
3	SF4	S	267	1	-	-	0/6/5/5
3	SF4	G	265	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
4	F3S	E	266	1	-	-	0/3/3/3
4	F3S	G	266	1	-	-	0/3/3/3
3	SF4	C	267	1	-	-	0/6/5/5
4	F3S	I	266	1	-	-	0/3/3/3
3	SF4	G	267	1	-	-	0/6/5/5
3	SF4	A	265	1	-	-	0/6/5/5
3	SF4	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.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	266	F3S	1	0
7	F	537	FCO	2	0
4	I	266	F3S	1	0
7	L	537	FCO	2	0
7	J	537	FCO	2	0
7	H	537	FCO	2	0
7	B	537	FCO	2	0
7	D	537	FCO	2	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.