



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 01:29 PM EDT

PDB ID : 2FRV / pdb_00002frv
Title : CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDRO-
GENASE
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

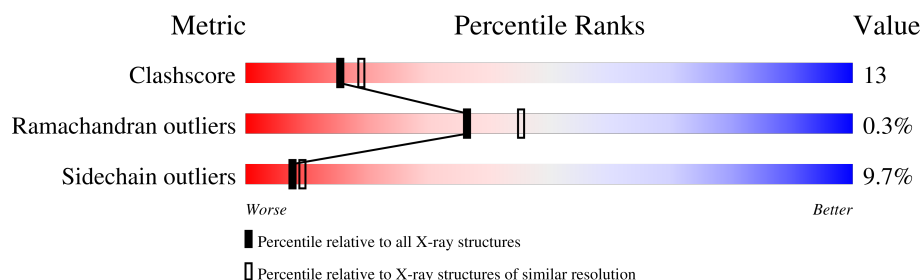
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	56% 31% 11% ..
1	C	264	57% 31% 10% .
1	E	264	56% 32% 10% .
1	G	264	57% 30% 11% .
1	I	264	58% 29% 12% .
1	S	264	56% 32% 10% ..
2	B	536	48% 38% 11% ..
2	D	536	49% 38% 11% ..

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Mol	Chain	Length	Quality of chain
2	F	536	
2	H	536	
2	J	536	
2	L	536	

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

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 1964	C 1249	N 329	O 367	S 19	0	0	0
1	A	261	Total 1964	C 1249	N 329	O 367	S 19	0	0	0
1	C	261	Total 1964	C 1249	N 329	O 367	S 19	0	0	0
1	E	261	Total 1964	C 1249	N 329	O 367	S 19	0	0	0
1	G	261	Total 1964	C 1249	N 329	O 367	S 19	0	0	0
1	I	261	Total 1964	C 1249	N 329	O 367	S 19	0	0	0

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

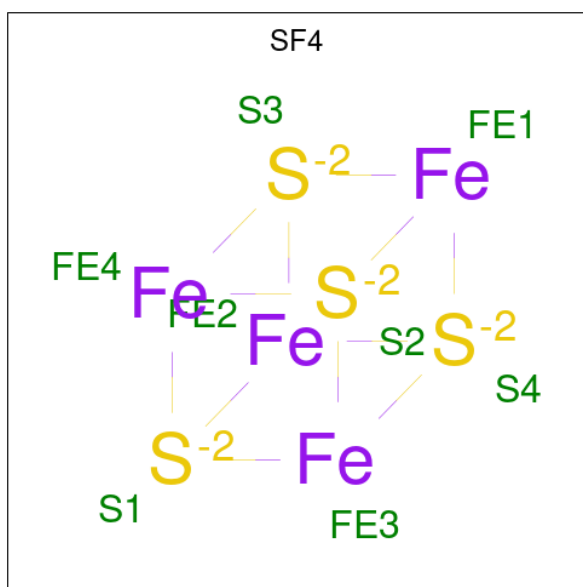
- Molecule 2 is a protein called PERIPLASMIC HYDROGENASE.

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

There are 24 discrepancies between the modelled and reference sequences:

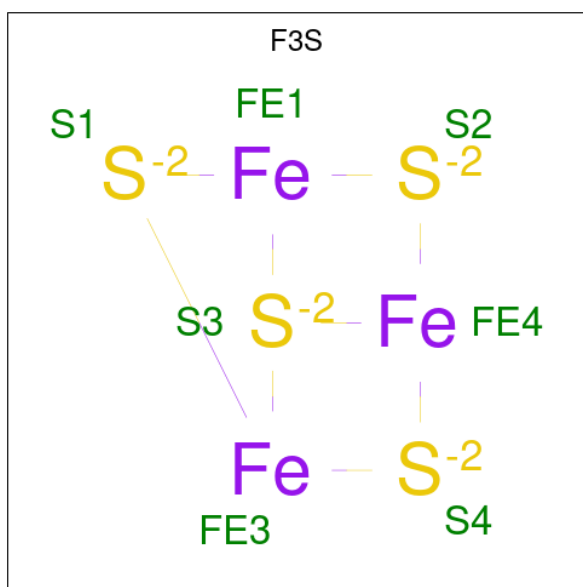
Chain	Residue	Modelled	Actual	Comment	Reference
L	144	LYS	ARG	conflict	UNP P12944
L	332	GLY	ASP	conflict	UNP P12944
L	482	LEU	HIS	conflict	UNP P12944
L	497	GLY	ARG	conflict	UNP P12944
B	144	LYS	ARG	conflict	UNP P12944
B	332	GLY	ASP	conflict	UNP P12944
B	482	LEU	HIS	conflict	UNP P12944
B	497	GLY	ARG	conflict	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 (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



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

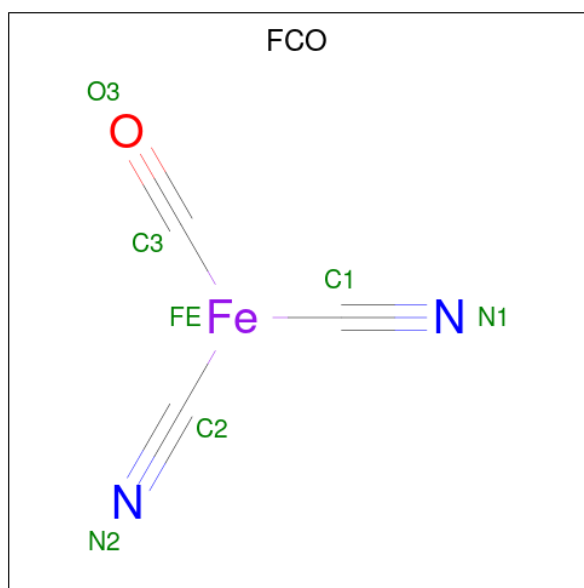
- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	Ni	0	0
			1	1		
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		
5	F	1	Total	Ni	0	0
			1	1		
5	H	1	Total	Ni	0	0
			1	1		
5	J	1	Total	Ni	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		
6	H	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C₃FeN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	D	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	F	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

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

- Molecule 8 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 9 is water.

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

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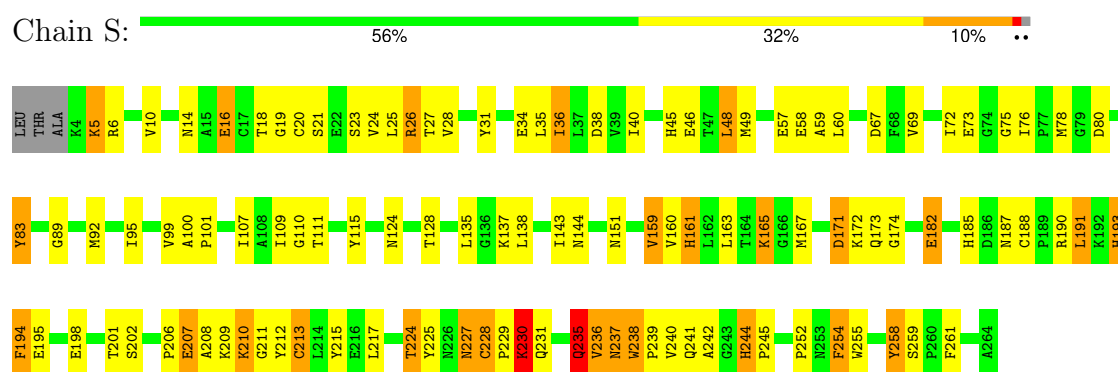
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	112	Total 112	O 112	0	0
9	I	80	Total 80	O 80	0	0
9	J	113	Total 113	O 113	0	0

3 Residue-property plots

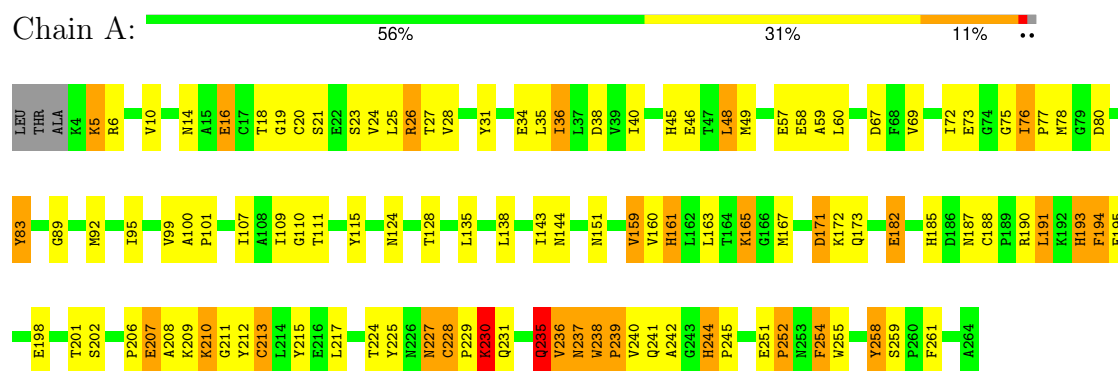
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

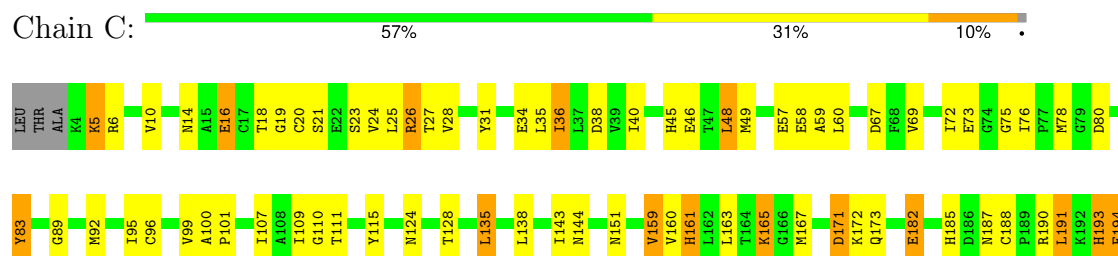
• Molecule 1: PERIPLASMIC HYDROGENASE



• Molecule 1: PERIPLASMIC HYDROGENASE



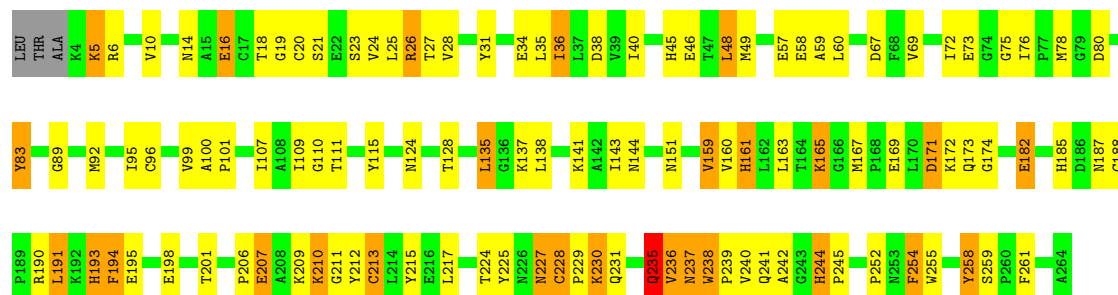
• Molecule 1: PERIPLASMIC HYDROGENASE





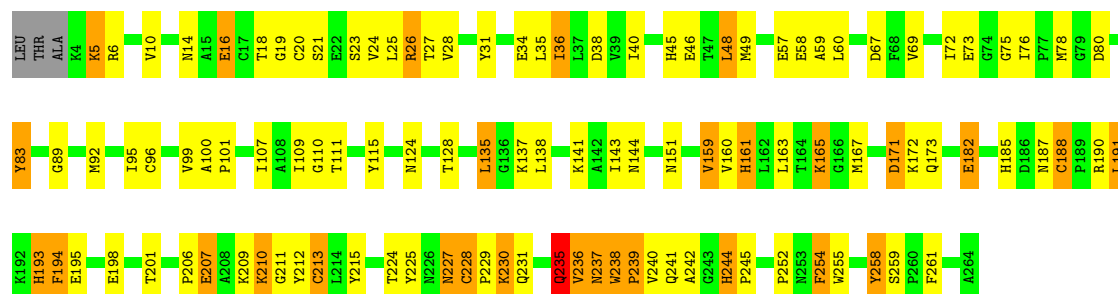
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain E: 56% 32% 10%



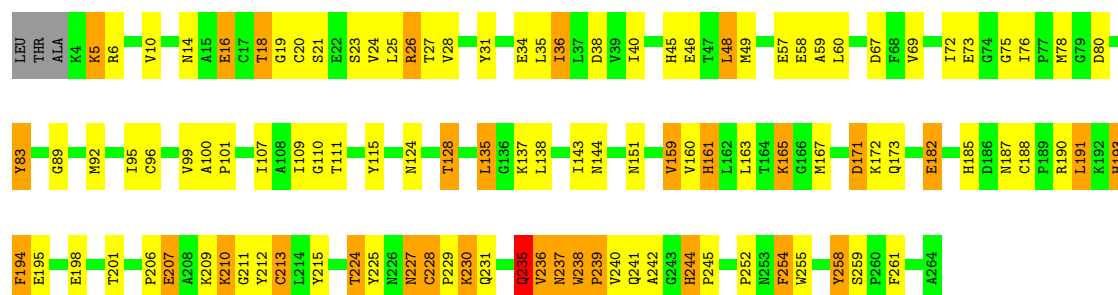
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain G: 57% 30% 11%



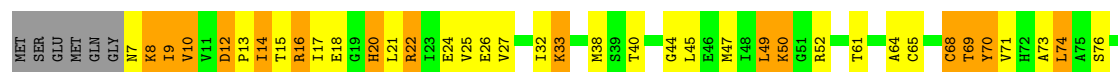
• Molecule 1: PERIPLASMIC HYDROGENASE

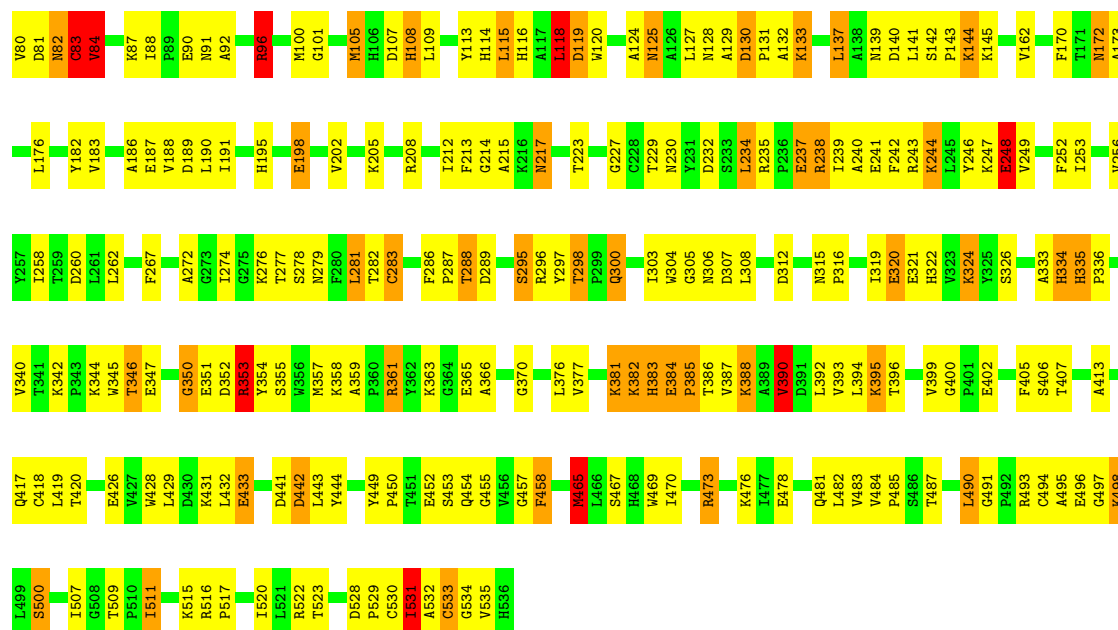
Chain I: 58% 29% 12%



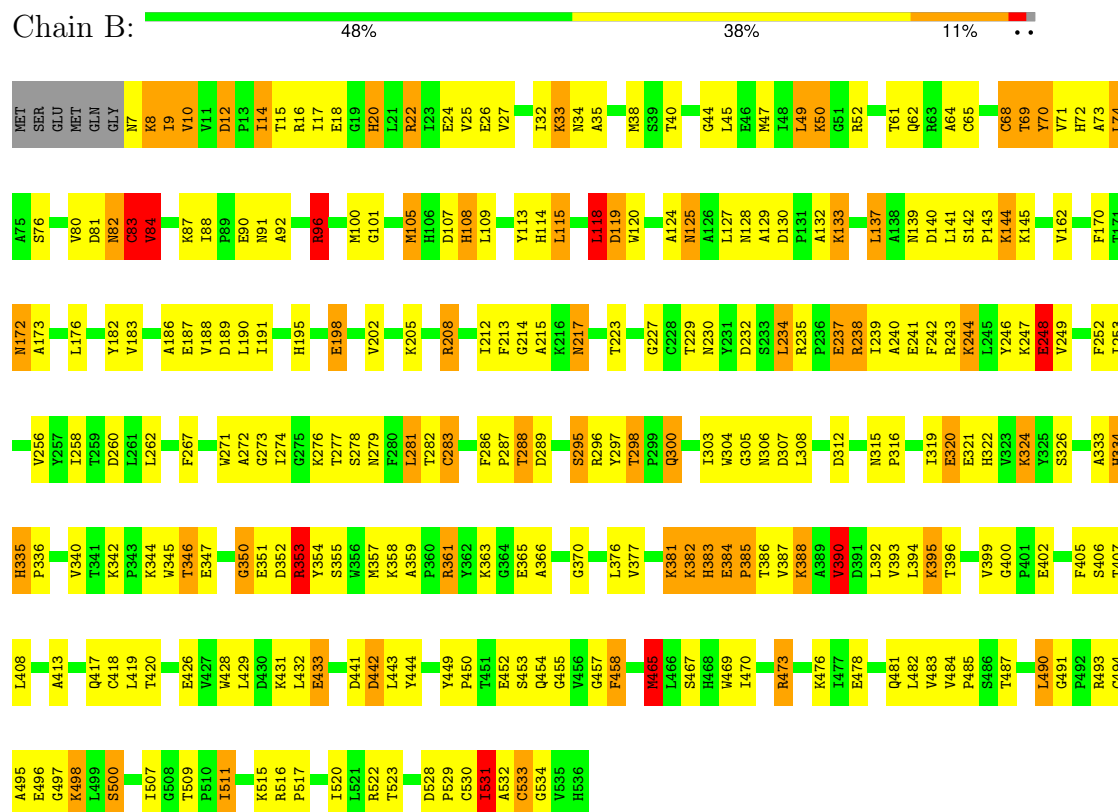
• Molecule 2: PERIPLASMIC HYDROGENASE

Chain L: 49% 37% 11%



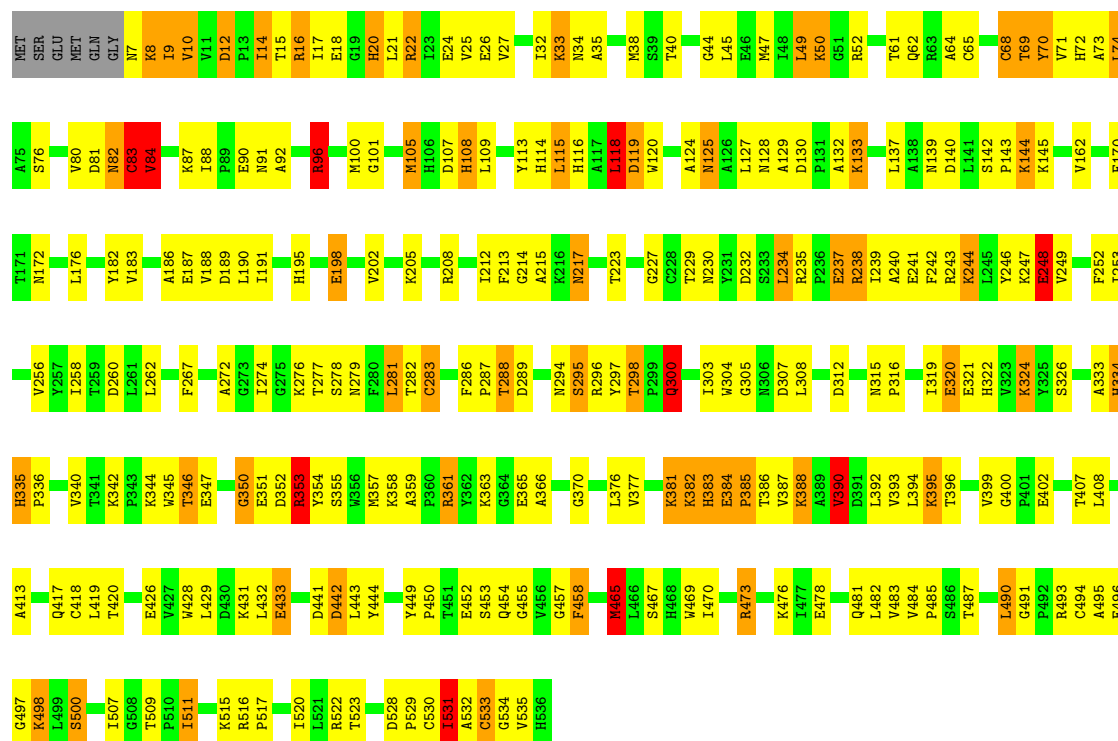


• Molecule 2: PERIPLASMIC HYDROGENASE



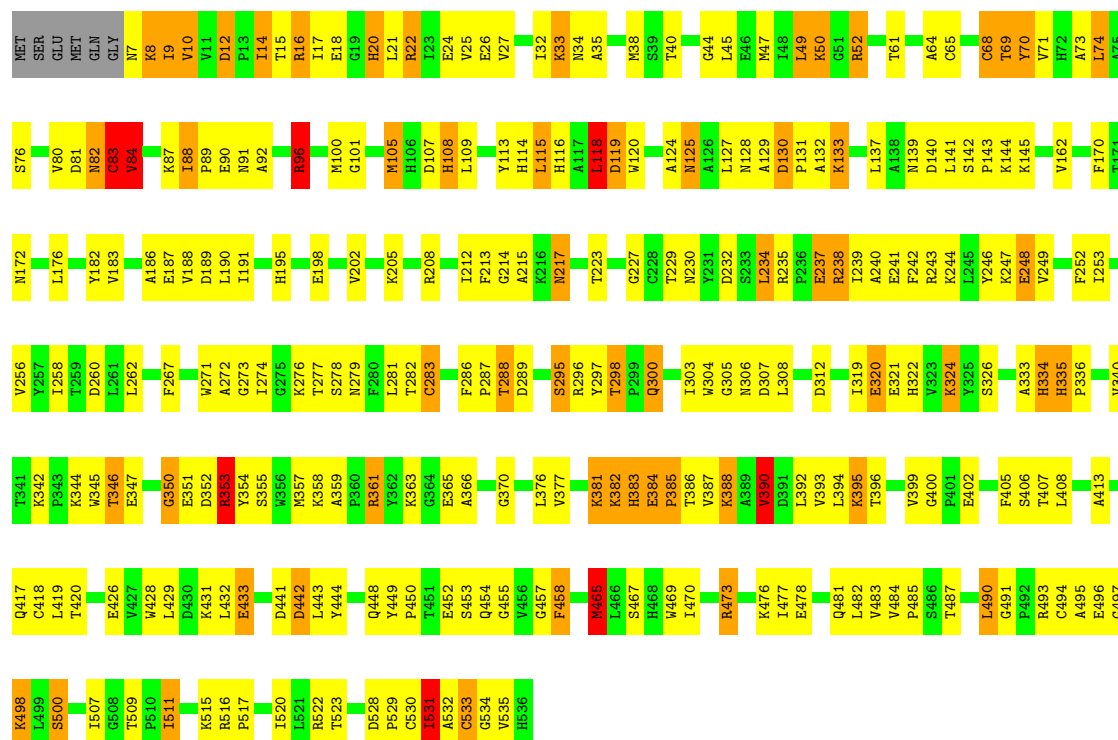
• Molecule 2: PERIPLASMIC HYDROGENASE





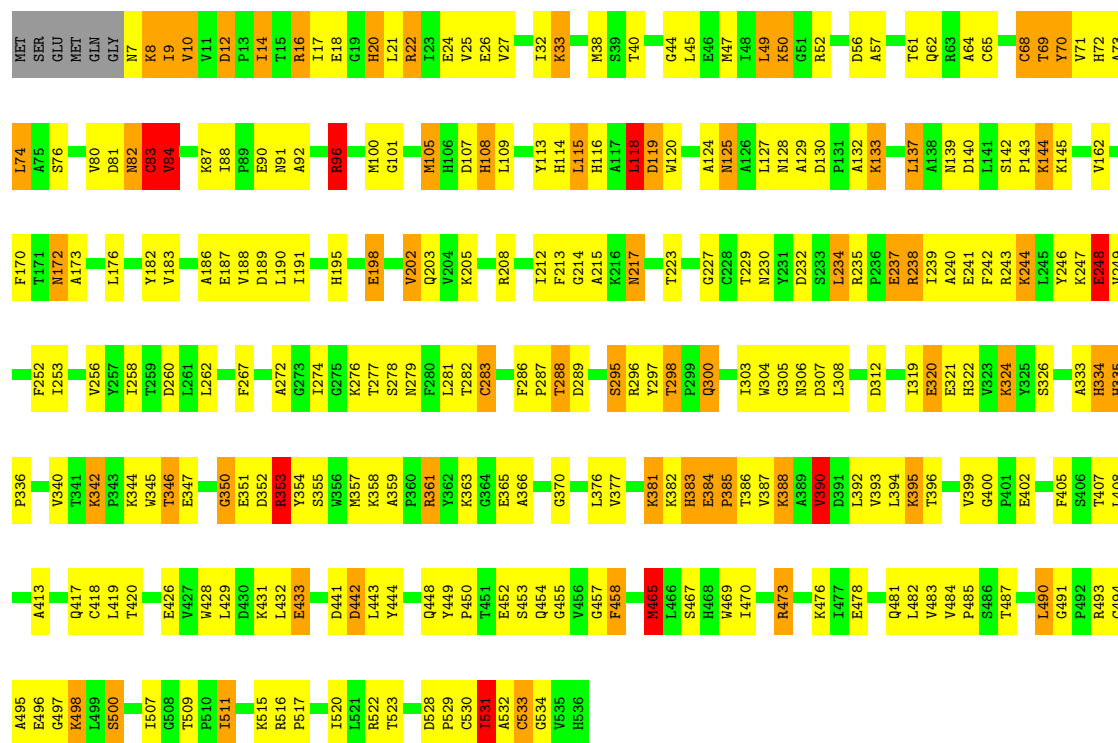
• Molecule 2: PERIPLASMIC HYDROGENASE

Chain F: 48% 39% 11% ..



• Molecule 2: PERIPLASMIC HYDROGENASE

E496	A413	A333	V249	V162	H72	MET
G497	A417	H334	F252	F170	A73	SER
K498	Q417	H335	I253	N171	L74	GLU
L499	L419	P336	V256	A173	A75	MET
S500	T420	V340	V257	L176	S76	GLN
I507	E426	K342	T258	L178	N82	GLY
G508	V427	P343	T259	Y182	C83	K8
T509	K428	K344	L261	V183	V84	I9
P510	L429	W345	L262	A186	K87	V10
I511	D430	T346	F267	A187	E188	D12
K515	K431	E347	G350	A272	E189	P13
R516	L432	E433	E351	G273	N90	T15
P517	K433	D441	D352	L274	N91	R16
R522	E433	D442	R353	K275	A92	E18
T523	D443	L443	Y354	G276	R96	G19
D528	Y444	S453	S355	T277	H20	H20
P529	Y449	K455	K357	N279	L21	L21
C530	P450	E456	K358	F280	E198	R22
I531	L451	P360	E359	L281	G101	T23
A532	E452	E453	E454	K205	M105	E24
C533	S453	Q454	Y362	C283	D107	V25
G534	K455	K363	G364	F286	H108	V27
V535	L456	E365	E366	T287	L109	
H536	F458	E366	D288	G213	Y113	T32
				A215	H114	K33
				E216	L115	N34
				N217	A117	A35
				L118	S39	M38
				D119	T40	S39
				W120	G44	T40
				G227	L45	G44
				C228	E46	L45
				T229	M47	E46
				N230	A126	M47
				L127	L49	I48
				N128	K50	L49
				S233	A129	L49
				D130	R52	G51
				P131	G51	R52
				R235	A132	
				P236	E56	D56
				E237	K133	A57
				N125	L137	A57
				A240	Q62	T61
				E241	R63	Q62
				F242	D140	R63
				L141	C65	A64
				K244	S142	C65
				L245	P143	
				Y246	T69	C68
				Y247	Y70	T69
				E248	K145	Y70
				E249	E249	V71



4 Data and refinement statistics

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, FCO, MG, SF4, O, F3S

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.28	3/2017 (0.1%)	2.30	108/2742 (3.9%)
1	C	1.28	3/2017 (0.1%)	2.30	109/2742 (4.0%)
1	E	1.28	3/2017 (0.1%)	2.30	111/2742 (4.0%)
1	G	1.28	3/2017 (0.1%)	2.30	111/2742 (4.0%)
1	I	1.28	3/2017 (0.1%)	2.30	112/2742 (4.1%)
1	S	1.28	3/2017 (0.1%)	2.30	111/2742 (4.0%)
2	B	1.23	5/4257 (0.1%)	2.33	231/5786 (4.0%)
2	D	1.23	5/4257 (0.1%)	2.33	232/5786 (4.0%)
2	F	1.23	5/4257 (0.1%)	2.33	233/5786 (4.0%)
2	H	1.23	5/4257 (0.1%)	2.33	230/5786 (4.0%)
2	J	1.23	5/4257 (0.1%)	2.33	229/5786 (4.0%)
2	L	1.23	5/4257 (0.1%)	2.33	233/5786 (4.0%)
All	All	1.25	48/37644 (0.1%)	2.32	2050/51168 (4.0%)

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

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	528	ASP	C-O	10.80	1.29	1.23
2	D	528	ASP	C-O	10.72	1.28	1.23
2	L	528	ASP	C-O	10.69	1.28	1.23
2	J	528	ASP	C-O	10.69	1.28	1.23
2	H	528	ASP	C-O	10.66	1.28	1.23

The worst 5 of 2050 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	353	ARG	CD-NE-CZ	16.53	147.54	124.40
2	F	353	ARG	CD-NE-CZ	16.53	147.54	124.40
2	D	353	ARG	CD-NE-CZ	16.52	147.52	124.40
2	B	353	ARG	CD-NE-CZ	16.50	147.50	124.40
2	J	353	ARG	CD-NE-CZ	16.50	147.50	124.40

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	46	0
1	C	1964	0	1895	40	0
1	E	1964	0	1895	44	0
1	G	1964	0	1895	43	0
1	I	1964	0	1895	41	0
1	S	1964	0	1895	43	0
2	B	4152	0	4114	132	0
2	D	4152	0	4114	125	0
2	F	4152	0	4114	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	4152	0	4114	128	0
2	J	4152	0	4114	129	0
2	L	4152	0	4114	127	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	38040	0	36054	964	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 13.

The worst 5 of 964 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%)	30	39
1	C	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	E	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	G	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	I	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	S	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
2	B	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	D	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	F	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	H	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	J	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	L	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
All	All	4722/4800 (98%)	4500 (95%)	210 (4%)	12 (0%)	36	45

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 ⓘ

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%)	189 (91%)	19 (9%)	9	11
1	C	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	E	208/210 (99%)	189 (91%)	19 (9%)	9	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	I	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	S	208/210 (99%)	189 (91%)	19 (9%)	9	11
2	B	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	D	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	F	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	H	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	J	434/439 (99%)	390 (90%)	44 (10%)	7	8
2	L	434/439 (99%)	391 (90%)	43 (10%)	7	9
All	All	3852/3894 (99%)	3479 (90%)	373 (10%)	8	9

5 of 373 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	381	LYS
2	H	234	LEU
2	F	465	MET
1	G	191	LEU
2	H	465	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	124	ASN
2	J	417	GLN
2	F	335	HIS
2	J	383	HIS
1	I	231	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	G	267	1	0,12,12	-	-	-		
7	FCO	J	537	2,8	3,6,6	2.36	1 (33%)	-		
7	FCO	D	537	2,8	3,6,6	2.37	1 (33%)	-		
3	SF4	S	267	1	0,12,12	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
3	SF4	E	265	1	0,12,12	-	-	-		
7	FCO	L	537	2,8	3,6,6	2.36	1 (33%)	-		
4	F3S	G	266	1	0,9,9	-	-	-		
7	FCO	H	537	2,8	3,6,6	2.34	1 (33%)	-		
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	I	267	1	0,12,12	-	-	-		
3	SF4	I	265	1	0,12,12	-	-	-		
3	SF4	G	265	1	0,12,12	-	-	-		
3	SF4	S	265	1	0,12,12	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
7	FCO	B	537	2,8	3,6,6	2.36	1 (33%)	-		
7	FCO	F	537	2,8	3,6,6	2.36	1 (33%)	-		
4	F3S	E	266	1	0,9,9	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	I	266	1	0,9,9	-	-	-		
3	SF4	E	267	1	0,12,12	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
4	F3S	S	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
4	F3S	C	266	1	-	-	0/3/3/3
3	SF4	G	265	1	-	-	0/6/5/5
3	SF4	G	267	1	-	-	0/6/5/5
4	F3S	G	266	1	-	-	0/3/3/3
4	F3S	I	266	1	-	-	0/3/3/3
3	SF4	S	265	1	-	-	0/6/5/5
3	SF4	A	265	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
3	SF4	E	267	1	-	-	0/6/5/5
3	SF4	I	267	1	-	-	0/6/5/5
3	SF4	C	265	1	-	-	0/6/5/5
3	SF4	C	267	1	-	-	0/6/5/5
4	F3S	S	266	1	-	-	0/3/3/3
3	SF4	S	267	1	-	-	0/6/5/5
3	SF4	I	265	1	-	-	0/6/5/5
4	F3S	E	266	1	-	-	0/3/3/3
3	SF4	A	267	1	-	-	0/6/5/5
3	SF4	E	265	1	-	-	0/6/5/5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	537	FCO	C1-N1	3.90	1.20	1.15
7	L	537	FCO	C1-N1	3.87	1.20	1.15
7	J	537	FCO	C1-N1	3.87	1.20	1.15
7	B	537	FCO	C1-N1	3.87	1.20	1.15
7	F	537	FCO	C1-N1	3.87	1.20	1.15

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
7	J	537	FCO	2	0
7	D	537	FCO	2	0
7	L	537	FCO	2	0

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.