



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:57 PM GMT

PDB ID : 4UCX
Title : Structure of the T18G small subunit mutant of D. fructosovorans NiFe- hydrogenase
Authors : Abou-Hamdan, A.; Ceccaldi, P.; Lebrette, H.; Gutierrez-Sanz, O.; Richaud, P.; Cournac, L.; Guigliarelli, B.; deLacey, A.L.; Leger, C.; Volbeda, A.; Burlat, B.; Dementin, S.
Deposited on : 2014-12-05
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

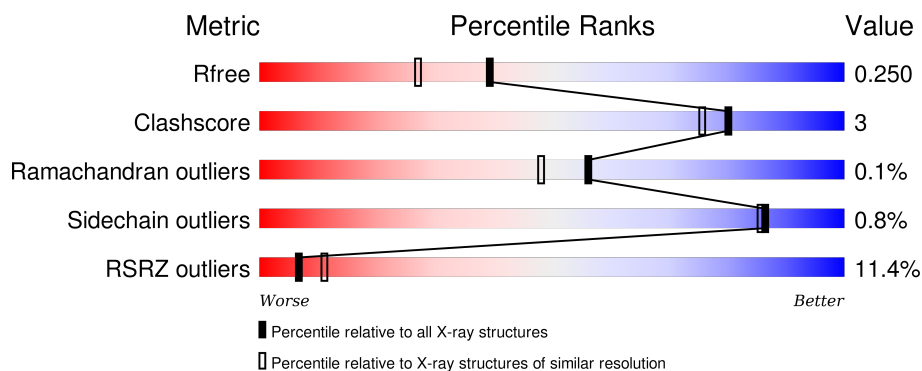
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	264	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	B	264	<div> <div>37%</div> <div>88%</div> <div>12%</div> </div>
1	C	264	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
2	Q	563	<div> <div>4%</div> <div>90%</div> <div>6%</div> </div>
2	R	563	<div> <div>17%</div> <div>88%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	S	563	

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
5	GOL	A	1271	-	-	-	X
5	GOL	A	1272	-	-	X	X
5	GOL	Q	1562	-	-	-	X
5	GOL	Q	1563	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19169 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 HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1968	1253	329	371	15			
1	B	262	Total	C	N	O	S	0	2	0
			1968	1254	325	374	15			
1	C	260	Total	C	N	O	S	0	0	0
			1954	1244	326	369	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	THR	ENGINEERED MUTATION	UNP P18187
B	18	GLY	THR	ENGINEERED MUTATION	UNP P18187
C	18	GLY	THR	ENGINEERED MUTATION	UNP P18187

- Molecule 2 is a protein called NICKEL-DEPENDENT HYDROGENASE LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	7	0
			4185	2670	722	771	22			
2	R	545	Total	C	N	O	S	0	3	0
			4178	2664	724	768	22			
2	S	544	Total	C	N	O	S	0	2	0
			4159	2650	718	769	22			

There are 45 discrepancies between the modelled and reference sequences:

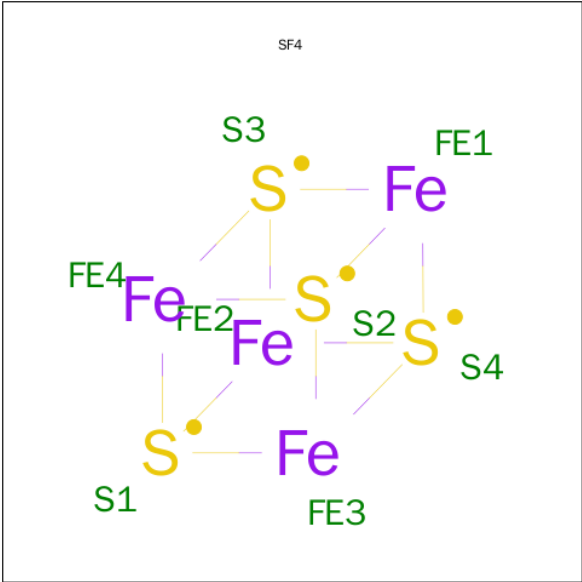
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	EXPRESSION TAG	UNP P18188
Q	-12	SER	-	EXPRESSION TAG	UNP P18188
Q	-11	TRP	-	EXPRESSION TAG	UNP P18188
Q	-10	SER	-	EXPRESSION TAG	UNP P18188

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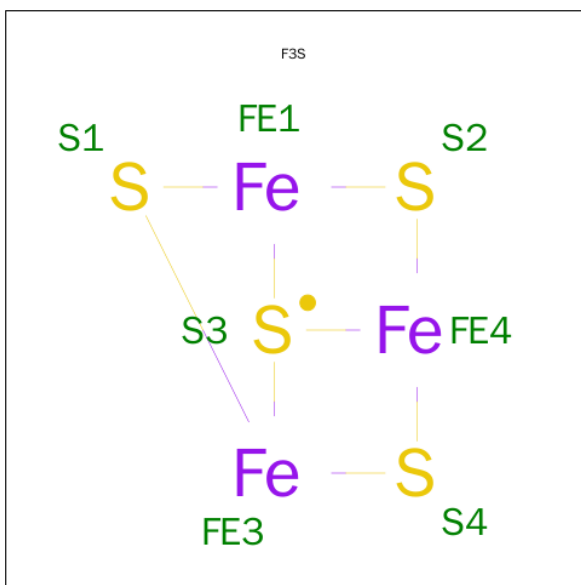
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-9	HIS	-	EXPRESSION TAG	UNP P18188
Q	-8	PRO	-	EXPRESSION TAG	UNP P18188
Q	-7	GLN	-	EXPRESSION TAG	UNP P18188
Q	-6	PHE	-	EXPRESSION TAG	UNP P18188
Q	-5	GLU	-	EXPRESSION TAG	UNP P18188
Q	-4	LYS	-	EXPRESSION TAG	UNP P18188
Q	-3	GLY	-	EXPRESSION TAG	UNP P18188
Q	-2	ALA	-	EXPRESSION TAG	UNP P18188
Q	-1	SER	-	EXPRESSION TAG	UNP P18188
Q	0	GLY	-	EXPRESSION TAG	UNP P18188
Q	1	ALA	-	EXPRESSION TAG	UNP P18188
R	-13	ALA	-	EXPRESSION TAG	UNP P18188
R	-12	SER	-	EXPRESSION TAG	UNP P18188
R	-11	TRP	-	EXPRESSION TAG	UNP P18188
R	-10	SER	-	EXPRESSION TAG	UNP P18188
R	-9	HIS	-	EXPRESSION TAG	UNP P18188
R	-8	PRO	-	EXPRESSION TAG	UNP P18188
R	-7	GLN	-	EXPRESSION TAG	UNP P18188
R	-6	PHE	-	EXPRESSION TAG	UNP P18188
R	-5	GLU	-	EXPRESSION TAG	UNP P18188
R	-4	LYS	-	EXPRESSION TAG	UNP P18188
R	-3	GLY	-	EXPRESSION TAG	UNP P18188
R	-2	ALA	-	EXPRESSION TAG	UNP P18188
R	-1	SER	-	EXPRESSION TAG	UNP P18188
R	0	GLY	-	EXPRESSION TAG	UNP P18188
R	1	ALA	-	EXPRESSION TAG	UNP P18188
S	-13	ALA	-	EXPRESSION TAG	UNP P18188
S	-12	SER	-	EXPRESSION TAG	UNP P18188
S	-11	TRP	-	EXPRESSION TAG	UNP P18188
S	-10	SER	-	EXPRESSION TAG	UNP P18188
S	-9	HIS	-	EXPRESSION TAG	UNP P18188
S	-8	PRO	-	EXPRESSION TAG	UNP P18188
S	-7	GLN	-	EXPRESSION TAG	UNP P18188
S	-6	PHE	-	EXPRESSION TAG	UNP P18188
S	-5	GLU	-	EXPRESSION TAG	UNP P18188
S	-4	LYS	-	EXPRESSION TAG	UNP P18188
S	-3	GLY	-	EXPRESSION TAG	UNP P18188
S	-2	ALA	-	EXPRESSION TAG	UNP P18188
S	-1	SER	-	EXPRESSION TAG	UNP P18188
S	0	GLY	-	EXPRESSION TAG	UNP P18188
S	1	ALA	-	EXPRESSION TAG	UNP P18188

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



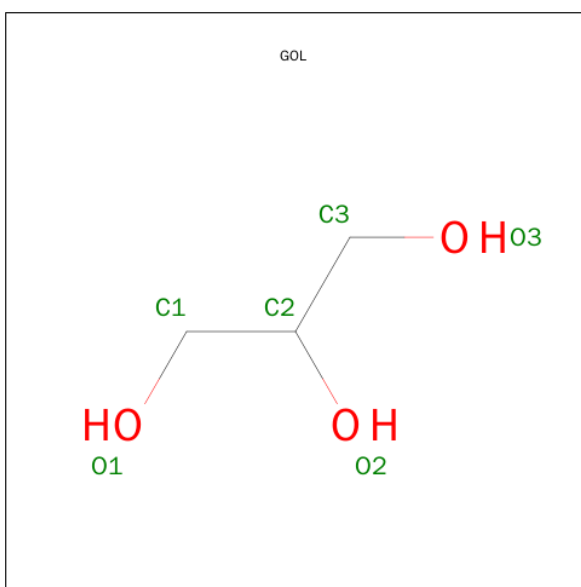
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



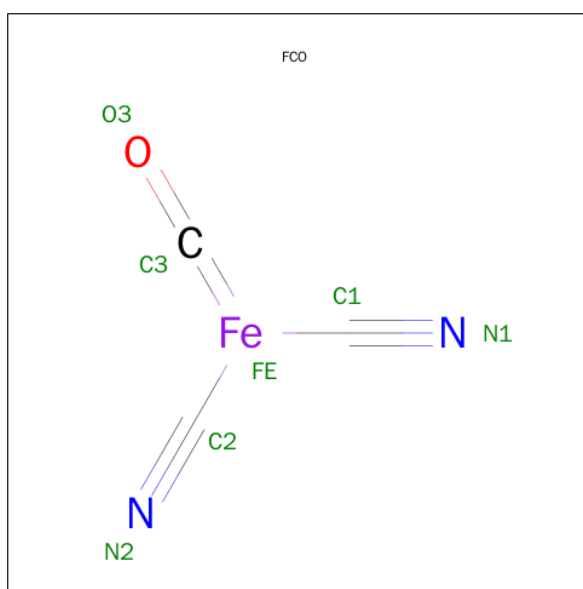
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	S	1	Total	C	O	0	0
			6	3	3		
5	S	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	Q	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
6	R	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
6	S	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	R	1	Total Ni 1 1	0	0
7	Q	1	Total Ni 1 1	0	0
7	S	1	Total Ni 1 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	R	1	Total Mg 1 1	0	0
8	Q	2	Total Mg 2 2	0	0
8	S	1	Total Mg 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	94	Total O 94 94	0	0
9	B	75	Total O 75 75	0	0
9	C	84	Total O 84 84	0	0
9	Q	129	Total O 129 129	0	0
9	R	112	Total O 112 112	0	0
9	S	112	Total O 112 112	0	0

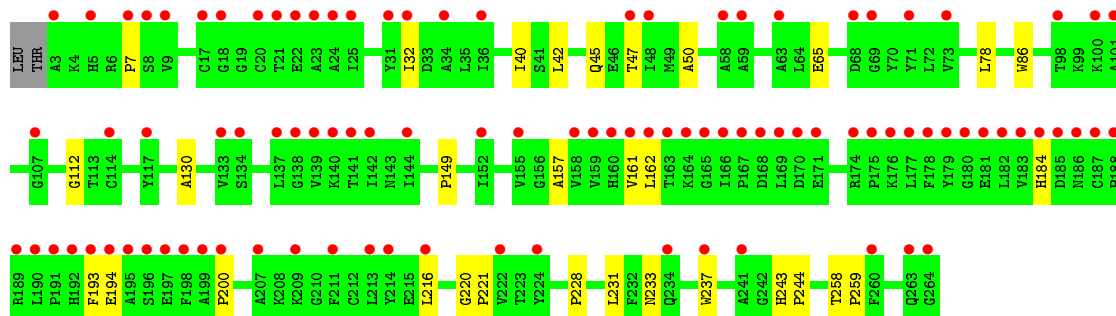
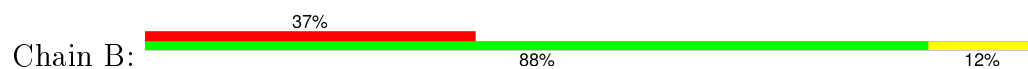
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

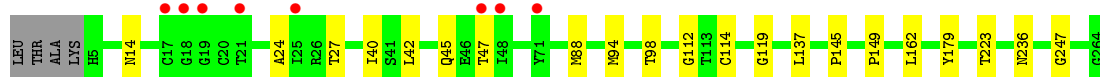
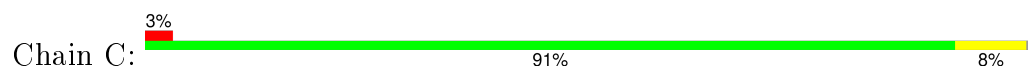
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA



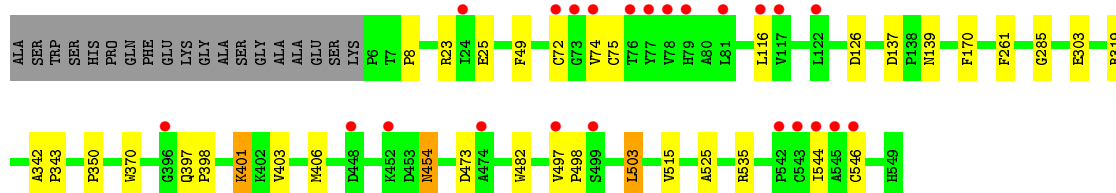
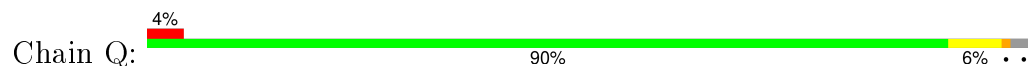
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA



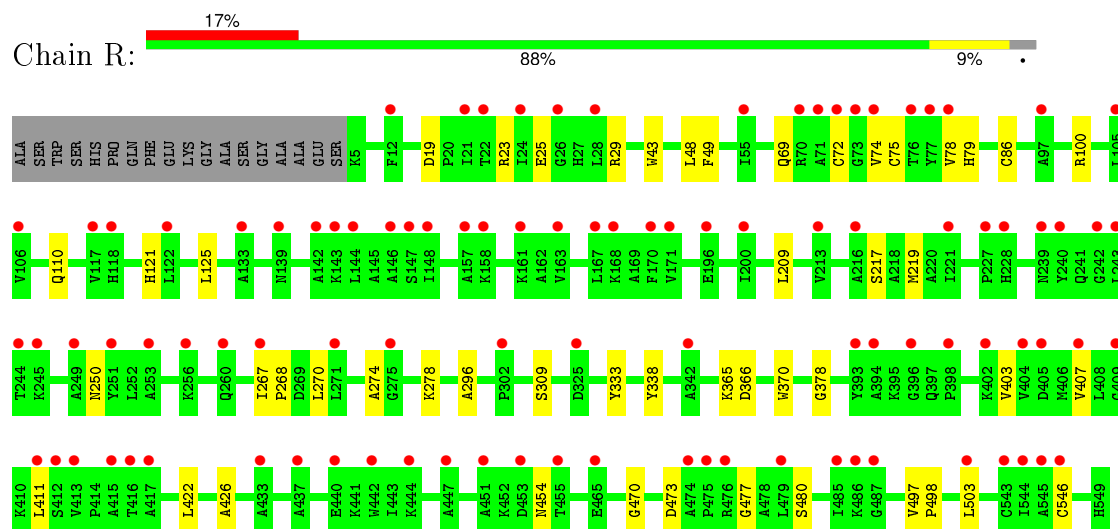
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA



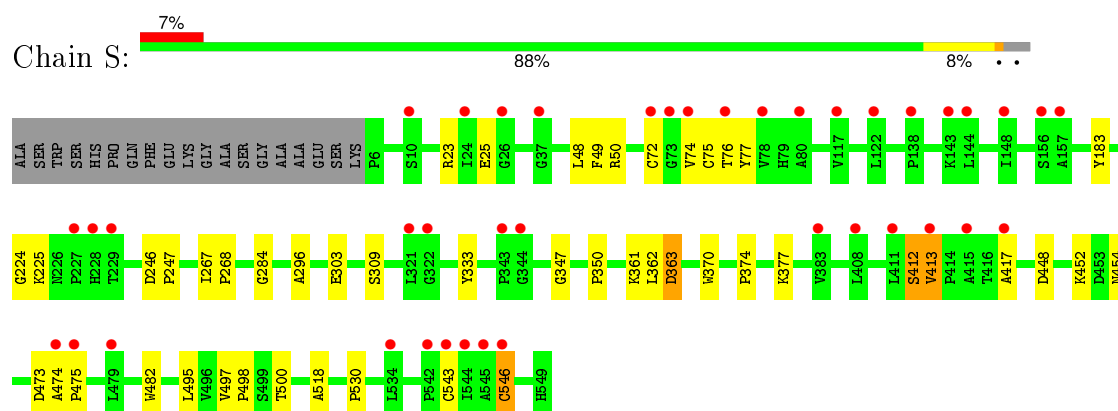
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT



• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT



• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.60Å 99.27Å 182.08Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 46.44 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.00-1.95) 99.2 (46.44-1.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.231 0.218 , 0.250	Depositor DCC
R_{free} test set	8066 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.9	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 160613 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19169	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, NI, SF4, F3S, CSX, FCO

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	0.71	1/2022 (0.0%)	0.71	0/2752
1	B	0.51	0/2031	0.57	0/2767
1	C	0.61	0/2008	0.63	0/2735
2	Q	0.65	0/4313	0.69	0/5854
2	R	0.58	1/4287 (0.0%)	0.63	0/5819
2	S	0.55	1/4264 (0.0%)	0.64	0/5791
All	All	0.60	3/18925 (0.0%)	0.65	0/25718

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	86	CYS	CB-SG	-6.06	1.72	1.82
2	S	303	GLU	CB-CG	-5.73	1.41	1.52
1	A	22	GLU	CD-OE2	-5.01	1.20	1.25

There are no bond angle outliers.

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	A	1968	0	1900	14	0
1	B	1968	0	1881	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1954	0	1884	12	0
2	Q	4185	0	4161	24	0
2	R	4178	0	4152	30	0
2	S	4159	0	4101	33	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	1	0
5	A	18	0	24	6	0
5	Q	18	0	24	2	0
5	R	6	0	8	0	0
5	S	12	0	16	0	0
6	Q	7	0	0	0	0
6	R	7	0	0	0	0
6	S	7	0	0	1	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	Q	2	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0
9	A	94	0	0	1	0
9	B	75	0	0	0	0
9	C	84	0	0	0	0
9	Q	129	0	0	1	0
9	R	112	0	0	1	0
9	S	112	0	0	2	0
All	All	19169	0	18151	125	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (125) 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:A:140:LYS:NZ	5:A:1272:GOL:H11	1.66	1.11
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.02	0.89
1:A:140:LYS:HZ1	5:A:1272:GOL:H11	1.38	0.88
1:A:140:LYS:HZ3	5:A:1272:GOL:H11	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:497:VAL:HG12	2:S:498:PRO:HD2	1.64	0.78
2:S:412:SER:O	2:S:413:VAL:HB	1.88	0.74
2:R:497:VAL:HG12	2:R:498:PRO:HD2	1.73	0.71
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.73	0.70
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.23	0.69
2:R:121:HIS:NE2	2:R:209:LEU:HG	2.12	0.65
2:S:48:LEU:HD21	2:S:50:ARG:HD2	1.80	0.64
1:A:171:GLU:H	1:A:171:GLU:CD	2.01	0.63
1:B:40:ILE:HG22	1:B:162:LEU:HD11	1.82	0.60
2:Q:303:GLU:CG	9:Q:2076:HOH:O	2.51	0.58
1:A:140:LYS:NZ	5:A:1272:GOL:C1	2.57	0.57
2:Q:25:GLU:HB2	2:Q:74:VAL:HG21	1.87	0.57
2:Q:285:GLY:HA3	5:Q:1563:GOL:H2	1.87	0.55
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.42	0.55
1:C:14:ASN:HD22	1:C:94:MET:HG2	1.72	0.55
2:S:374:PRO:CG	2:S:500:THR:HG22	2.37	0.55
1:C:47:THR:O	2:S:23:ARG:HA	2.07	0.55
2:S:448:ASP:O	2:S:452:LYS:HD3	2.08	0.54
1:B:157:ALA:O	1:B:161:VAL:HG23	2.08	0.54
2:Q:116[B]:LEU:HD11	2:Q:261:PHE:HE2	1.72	0.54
1:B:184:HIS:ND1	1:B:221:PRO:HG3	2.22	0.54
1:B:47:THR:O	2:R:23:ARG:HA	2.07	0.54
2:R:43:TRP:CZ2	2:R:365:LYS:HE2	2.44	0.53
1:B:233:ASN:HB3	2:R:217:SER:HA	1.89	0.53
2:R:477:GLY:O	2:R:498:PRO:HG3	2.09	0.53
2:Q:116[B]:LEU:HD11	2:Q:261:PHE:CE2	2.44	0.53
1:B:184:HIS:HB2	1:B:221:PRO:HA	1.91	0.53
2:S:267:ILE:HB	2:S:268:PRO:HD3	1.91	0.53
2:R:296:ALA:HA	2:R:309:SER:HA	1.91	0.53
1:C:42:LEU:HD21	1:C:45:GLN:HG3	1.91	0.52
2:R:267:ILE:HB	2:R:268:PRO:HD3	1.92	0.51
1:B:50:ALA:HB2	2:R:125:LEU:HD13	1.93	0.51
1:A:99:LYS:HE2	9:A:2045:HOH:O	2.11	0.50
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.47	0.50
5:A:1273:GOL:H11	2:Q:170:PHE:HA	1.94	0.50
2:R:110:GLN:HB2	2:R:219:MET:HE3	1.94	0.50
2:R:274:ALA:HA	2:R:422[A]:LEU:HD11	1.94	0.49
2:Q:403:VAL:O	2:Q:406:MET:HB3	2.12	0.49
2:S:497:VAL:HG12	2:S:498:PRO:CD	2.37	0.48
2:R:19:ASP:HB2	2:R:29:ARG:HG3	1.94	0.48
1:B:112:GLY:HA2	1:B:149:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.49	0.48
1:C:14:ASN:ND2	1:C:94:MET:HB3	2.29	0.48
2:R:110:GLN:HB2	2:R:219:MET:CE	2.44	0.48
4:C:1266:F3S:S2	2:S:225:LYS:HE2	2.54	0.48
2:S:75:CSX:OD	2:S:75:CSX:N	2.47	0.48
1:C:40:ILE:HG22	1:C:162:LEU:HD11	1.96	0.48
2:S:25:GLU:HB2	2:S:74:VAL:HG21	1.95	0.47
2:S:543:CYS:SG	2:S:546:CYS:HB2	2.54	0.47
2:Q:137:ASP:OD1	2:Q:139:ASN:HB2	2.13	0.47
2:R:278:LYS:NZ	2:R:411:LEU:O	2.46	0.47
2:S:72:CYS:HB3	2:S:75:CSX:OD	2.14	0.47
2:S:495:LEU:N	2:S:495:LEU:HD12	2.29	0.47
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.96	0.47
2:S:49:PHE:HB2	2:S:370:TRP:CD2	2.50	0.47
1:B:78:LEU:O	1:B:130:ALA:HA	2.15	0.47
1:C:223:THR:OG1	1:C:247:GLY:HA2	2.15	0.47
1:B:193:PHE:HD2	1:B:194:GLU:HG3	1.80	0.46
1:A:47:THR:O	2:Q:23:ARG:HA	2.15	0.46
2:S:284:GLY:HA2	2:S:518:ALA:O	2.16	0.46
2:S:296:ALA:HA	2:S:309:SER:HA	1.96	0.46
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.45	0.46
2:S:361:LYS:HG3	2:S:362:LEU:O	2.16	0.46
2:S:246:ASP:HB2	2:S:247:PRO:HD3	1.98	0.46
2:S:377:LYS:NZ	9:S:2074:HOH:O	2.23	0.46
2:R:333:TYR:OH	2:R:378:GLY:HA2	2.16	0.45
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.98	0.45
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.52	0.45
1:B:184:HIS:CE1	1:B:221:PRO:HG3	2.52	0.45
1:B:32:ILE:HG21	2:R:209:LEU:HD22	1.97	0.45
2:S:350:PRO:HB2	2:S:482:TRP:CG	2.52	0.45
2:R:338:TYR:HA	2:R:366:ASP:O	2.16	0.45
1:B:7:PRO:HG2	1:B:162:LEU:HD13	1.98	0.44
2:S:413:VAL:HG22	2:S:417:ALA:CB	2.47	0.44
1:B:220:GLY:N	1:B:221:PRO:CD	2.80	0.44
1:B:243:HIS:CG	1:B:244:PRO:HD2	2.53	0.44
1:C:112:GLY:HA2	1:C:149:PRO:HD3	2.00	0.44
1:B:42:LEU:HD21	1:B:45:GLN:HG3	2.00	0.44
1:C:236:ASN:HB3	2:S:224:GLY:O	2.17	0.44
1:B:200:PRO:O	1:B:216:LEU:HD21	2.18	0.43
1:B:32:ILE:CG2	2:R:209:LEU:HD22	2.49	0.43
2:R:72:CYS:HB3	2:R:75:CSX:OD	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:75:CSX:O	2:R:78:VAL:HG22	2.18	0.43
2:R:470:GLY:O	2:R:480:SER:HA	2.19	0.43
1:A:137:LEU:HB2	1:A:139:VAL:HG22	2.00	0.43
1:A:24:ALA:O	1:A:27:THR:HG22	2.19	0.42
2:R:69:GLN:HA	2:R:79:HIS:HB2	2.02	0.42
2:Q:319:ARG:HH12	5:Q:1563:GOL:H32	1.84	0.42
1:C:24:ALA:O	1:C:27:THR:HG22	2.20	0.42
2:Q:544:ILE:N	2:Q:544:ILE:HD13	2.34	0.42
2:S:50:ARG:HD3	9:S:2015:HOH:O	2.19	0.42
2:Q:8:PRO:HB2	2:Q:525:ALA:HB2	2.01	0.42
2:Q:126:ASP:HB3	2:Q:535:ARG:HG2	2.01	0.42
2:S:183:TYR:CZ	2:S:530:PRO:HD2	2.55	0.42
1:C:145:PRO:HD2	1:C:179:TYR:CZ	2.55	0.42
1:B:258:THR:HA	1:B:259:PRO:C	2.39	0.41
2:Q:350:PRO:HB2	2:Q:482:TRP:CG	2.55	0.41
1:A:170:ASP:O	5:A:1272:GOL:H32	2.20	0.41
1:A:190:LEU:HB3	1:A:191:PRO:HD3	2.02	0.41
2:Q:401:LYS:HB2	2:Q:401:LYS:HE3	1.39	0.41
2:Q:397:GLN:HA	2:Q:398:PRO:HD3	1.86	0.41
2:Q:454:ASN:H	2:Q:454:ASN:HD22	1.68	0.41
2:S:497:VAL:CG1	2:S:498:PRO:CD	2.87	0.41
2:R:497:VAL:HG11	2:R:546:CYS:HB3	2.03	0.41
2:Q:342:ALA:HB1	2:Q:343:PRO:HD2	2.01	0.41
2:R:100:ARG:HD3	9:R:2038:HOH:O	2.20	0.41
2:S:474:ALA:HB1	2:S:475:PRO:HD2	2.01	0.41
2:Q:503:LEU:HD23	2:Q:515:VAL:HG11	2.02	0.41
2:S:76:THR:O	2:S:77:TYR:HB3	2.21	0.41
2:Q:497:VAL:HG11	2:Q:546:CYS:HB3	2.02	0.41
1:C:114:CYS:HA	1:C:119:GLY:HA3	2.03	0.41
2:R:25:GLU:HB2	2:R:74:VAL:HG21	2.03	0.41
2:S:75:CSX:CB	6:S:1550:FCO:C2	2.98	0.41
1:B:86:TRP:O	2:R:48:LEU:HA	2.22	0.40
2:S:333:TYR:CD2	2:S:347:GLY:HA2	2.55	0.40
2:R:270:LEU:HD21	2:R:426:ALA:HA	2.02	0.40
1:C:98:THR:HG22	1:C:137:LEU:HD11	2.03	0.40
2:Q:72:CYS:HB3	2:Q:75:CSX:OD	2.21	0.40
2:S:362:LEU:O	2:S:363[A]:ASP:HB3	2.22	0.40
2:R:403:VAL:O	2:R:407:VAL:HG23	2.22	0.40
1:A:118:GLY:HA3	1:A:122:LYS:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/264 (98%)	252 (97%)	8 (3%)	0	100	100
1	B	262/264 (99%)	250 (95%)	11 (4%)	1 (0%)	39	27
1	C	258/264 (98%)	248 (96%)	10 (4%)	0	100	100
2	Q	548/563 (97%)	532 (97%)	16 (3%)	0	100	100
2	R	545/563 (97%)	531 (97%)	14 (3%)	0	100	100
2	S	543/563 (96%)	522 (96%)	19 (4%)	2 (0%)	39	27
All	All	2416/2481 (97%)	2335 (97%)	78 (3%)	3 (0%)	56	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	412	SER
2	S	413	VAL
1	B	231	LEU

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	206/209 (99%)	205 (100%)	1 (0%)	92	91
1	B	204/209 (98%)	203 (100%)	1 (0%)	92	91
1	C	205/209 (98%)	204 (100%)	1 (0%)	92	91
2	Q	438/447 (98%)	434 (99%)	4 (1%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	435/447 (97%)	431 (99%)	4 (1%)	84	83
2	S	429/447 (96%)	424 (99%)	5 (1%)	78	75
All	All	1917/1968 (97%)	1901 (99%)	16 (1%)	86	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	MET
1	B	65	GLU
1	C	88	MET
2	Q	401	LYS
2	Q	454	ASN
2	Q	473	ASP
2	Q	503	LEU
2	R	250	ASN
2	R	454	ASN
2	R	473	ASP
2	R	503	LEU
2	S	363[A]	ASP
2	S	363[B]	ASP
2	S	454	ASN
2	S	473	ASP
2	S	546	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	C	14	ASN
2	Q	454	ASN
2	Q	509	GLN
2	R	250	ASN
2	R	454	ASN
2	S	454	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	CSX	Q	75	2,7,6	3,6,7	0.68	0	3,6,8	0.90	0
2	CSX	R	75	2,7,6	3,6,7	0.64	0	3,6,8	0.61	0
2	CSX	S	75	2,7,6	3,6,7	0.61	0	3,6,8	0.76	0

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
2	CSX	Q	75	2,7,6	-	0/1/5/7	0/0/0/0
2	CSX	R	75	2,7,6	-	0/1/5/7	0/0/0/0
2	CSX	S	75	2,7,6	-	0/1/5/7	0/0/0/0

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	75	CSX	1	0
2	R	75	CSX	2	0
2	S	75	CSX	3	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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	A	1265	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	A	1266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	A	1267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	GOL	A	1271	-	5,5,5	0.27	0	5,5,5	0.99	0
5	GOL	A	1272	-	5,5,5	0.34	0	5,5,5	0.34	0
5	GOL	A	1273	-	5,5,5	0.29	0	5,5,5	0.98	0
3	SF4	B	1265	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	B	1266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	B	1267	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	C	1265	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	C	1266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	C	1267	1	0,12,12	0.00	-	0,24,24	0.00	-
6	FCO	Q	1550	9,2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	Q	1561	-	5,5,5	0.32	0	5,5,5	0.24	0
5	GOL	Q	1562	-	5,5,5	0.54	0	5,5,5	0.54	0
5	GOL	Q	1563	-	5,5,5	0.32	0	5,5,5	0.31	0
6	FCO	R	1550	9,2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	R	1563	-	5,5,5	0.28	0	5,5,5	0.20	0
6	FCO	S	1550	9,2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	S	1561	-	5,5,5	0.38	0	5,5,5	0.20	0
5	GOL	S	1562	-	5,5,5	0.39	0	5,5,5	0.61	0

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	A	1265	1	-	0/0/48/48	0/6/5/5
4	F3S	A	1266	1	-	0/0/24/24	0/0/3/3
3	SF4	A	1267	1	-	0/0/48/48	0/6/5/5
5	GOL	A	1271	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1272	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1273	-	-	0/4/4/4	0/0/0/0
3	SF4	B	1265	1	-	0/0/48/48	0/6/5/5
4	F3S	B	1266	1	-	0/0/24/24	0/0/3/3
3	SF4	B	1267	1	-	0/0/48/48	0/6/5/5
3	SF4	C	1265	1	-	0/0/48/48	0/6/5/5
4	F3S	C	1266	1	-	0/0/24/24	0/0/3/3
3	SF4	C	1267	1	-	0/0/48/48	0/6/5/5
6	FCO	Q	1550	9,2	-	0/0/6/6	0/0/0/0
5	GOL	Q	1561	-	-	0/4/4/4	0/0/0/0
5	GOL	Q	1562	-	-	0/4/4/4	0/0/0/0
5	GOL	Q	1563	-	-	0/4/4/4	0/0/0/0
6	FCO	R	1550	9,2	-	0/0/6/6	0/0/0/0
5	GOL	R	1563	-	-	0/4/4/4	0/0/0/0
6	FCO	S	1550	9,2	-	0/0/6/6	0/0/0/0
5	GOL	S	1561	-	-	0/4/4/4	0/0/0/0
5	GOL	S	1562	-	-	0/4/4/4	0/0/0/0

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 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1272	GOL	5	0
5	A	1273	GOL	1	0
4	C	1266	F3S	1	0
5	Q	1563	GOL	2	0
6	S	1550	FCO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	A	262/264 (99%)	0.26	8 (3%) 52 62	18, 28, 43, 58	9 (3%)
1	B	262/264 (99%)	1.95	98 (37%) 0 0	35, 65, 104, 122	4 (1%)
1	C	260/264 (98%)	0.31	8 (3%) 52 62	24, 35, 52, 61	5 (1%)
2	Q	543/563 (96%)	0.30	23 (4%) 40 51	19, 30, 42, 54	9 (1%)
2	R	544/563 (96%)	1.04	98 (18%) 2 2	26, 44, 76, 97	11 (2%)
2	S	543/563 (96%)	0.60	40 (7%) 17 27	22, 41, 67, 83	9 (1%)
All	All	2414/2481 (97%)	0.71	275 (11%) 7 11	18, 37, 75, 122	47 (1%)

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	9.2
1	B	264	GLY	8.2
1	B	169	LEU	7.9
1	B	71	TYR	7.8
1	B	191	PRO	7.6
1	B	163	THR	7.4
1	B	142	ILE	7.3
1	B	180	GLY	7.3
1	B	179	TYR	6.5
1	B	198	PHE	6.5
1	B	162	LEU	6.3
1	B	177	LEU	6.2
2	R	74	VAL	5.9
2	R	148	ILE	5.8
2	R	163	VAL	5.8
1	B	166	ILE	5.8
2	R	437	ALA	5.7
1	B	211	PHE	5.6
1	B	140	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
2	S	413	VAL	5.5
1	B	167	PRO	5.5
1	B	165	GLY	5.5
1	B	159	VAL	5.4
1	B	7	PRO	5.4
1	B	168	ASP	5.3
1	B	195	ALA	5.2
1	B	171	GLU	5.0
1	B	188	PRO	4.9
2	S	24	ILE	4.9
1	B	197	GLU	4.8
2	R	243	LEU	4.8
1	B	190	LEU	4.7
1	B	107	GLY	4.7
2	S	148	ILE	4.6
1	B	181	GLU	4.5
2	R	393	TYR	4.4
2	R	394	ALA	4.3
1	B	183	VAL	4.3
2	S	74	VAL	4.2
1	B	224	TYR	4.2
2	R	404	VAL	4.1
1	B	214	TYR	4.1
1	B	139	VAL	4.1
1	B	209	LYS	4.1
2	R	440	GLU	4.1
2	Q	24	ILE	4.0
1	B	187	CYS	4.0
2	R	73	GLY	4.0
2	S	78	VAL	4.0
2	R	143	LYS	4.0
2	R	451	ALA	4.0
1	B	178	PHE	3.9
1	B	160	HIS	3.9
2	R	260	GLN	3.8
1	B	193	PHE	3.8
1	C	17	CYS	3.8
2	R	24	ILE	3.8
2	R	249	ALA	3.8
2	R	415	ALA	3.8
2	S	122	LEU	3.7
2	S	143	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	211	PHE	3.7
2	R	409	GLY	3.7
1	B	192	HIS	3.7
2	Q	78	VAL	3.6
2	R	161	LYS	3.6
2	R	72	CYS	3.6
2	R	543	CYS	3.6
1	C	48	ILE	3.6
2	R	442	TRP	3.6
2	R	455	THR	3.6
2	R	545	ALA	3.6
2	R	245	LYS	3.6
1	A	18	GLY	3.5
2	S	72	CYS	3.5
2	S	73	GLY	3.5
1	B	68	ASP	3.5
2	R	170	PHE	3.5
2	R	267	ILE	3.5
1	B	176	LYS	3.5
2	R	97	ALA	3.5
1	B	184	HIS	3.5
2	R	167	LEU	3.5
2	Q	74	VAL	3.5
2	Q	72	CYS	3.5
2	R	200	ILE	3.5
1	B	158	VAL	3.4
2	R	76	THR	3.4
2	R	485	ILE	3.4
2	Q	546	CYS	3.4
1	B	25	ILE	3.4
2	R	544	ILE	3.4
1	B	182	LEU	3.4
2	S	344	GLY	3.4
1	B	194	GLU	3.4
2	R	412	SER	3.4
1	B	20	CYS	3.3
2	R	71	ALA	3.3
2	R	227	PRO	3.3
1	B	47	THR	3.3
1	B	137	LEU	3.3
1	B	161	VAL	3.3
2	R	405	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	R	444	LYS	3.3
2	R	407	VAL	3.3
2	S	544	ILE	3.3
1	B	18	GLY	3.2
1	B	175	PRO	3.2
2	S	157	ALA	3.2
2	Q	76	THR	3.2
2	S	117	VAL	3.2
1	B	48	ILE	3.2
2	R	417	ALA	3.2
2	R	487	GLY	3.2
2	S	343	PRO	3.2
2	R	157	ALA	3.2
2	R	244	THR	3.2
2	R	117	VAL	3.1
1	A	17	CYS	3.1
2	S	37	GLY	3.1
2	S	417	ALA	3.1
2	Q	542	PRO	3.1
1	A	48	ILE	3.1
2	R	78	VAL	3.1
2	R	139	ASN	3.1
2	S	411	LEU	3.0
1	B	170	ASP	3.0
2	Q	122	LEU	3.0
1	B	133	VAL	3.0
1	B	164	LYS	3.0
1	B	222	VAL	3.0
1	B	196	SER	3.0
2	S	543	CYS	3.0
2	S	10	SER	3.0
2	R	302	PRO	3.0
2	R	146	ALA	3.0
1	C	25	ILE	2.9
1	B	5	HIS	2.9
1	B	185	ASP	2.9
2	R	158	LYS	2.9
2	R	474	ALA	2.9
2	R	486	LYS	2.9
1	A	19	GLY	2.9
1	B	134[A]	SER	2.8
2	R	105	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	R	453	ASP	2.8
2	R	228	HIS	2.8
2	R	396	GLY	2.8
2	R	546	CYS	2.8
2	Q	73	GLY	2.8
2	R	144	LEU	2.8
2	R	411	LEU	2.8
1	B	189	ARG	2.8
2	R	465	GLU	2.8
1	B	69	GLY	2.8
1	B	22	GLU	2.8
1	B	100	LYS	2.8
1	B	8	SER	2.7
2	R	240	TYR	2.7
2	R	133	ALA	2.7
1	B	36	ILE	2.7
1	B	23	ALA	2.7
2	R	256	LYS	2.7
2	S	542	PRO	2.7
2	R	55	ILE	2.7
1	C	19	GLY	2.7
1	C	21	THR	2.6
1	B	144	ILE	2.6
2	R	106	VAL	2.6
2	R	171	VAL	2.6
1	B	101	ALA	2.6
2	Q	545	ALA	2.6
2	R	213	VAL	2.6
1	B	152	ILE	2.6
2	R	77	TYR	2.6
2	R	196	GLU	2.6
1	B	21	THR	2.6
2	R	503	LEU	2.6
1	B	73	VAL	2.6
2	S	156	SER	2.6
1	A	20	CYS	2.5
1	B	138	GLY	2.5
2	R	271	LEU	2.5
2	Q	543	CYS	2.5
1	B	199	ALA	2.5
2	R	122	LEU	2.5
2	R	28	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	S	546	CYS	2.5
2	Q	452	LYS	2.5
2	R	21	ILE	2.5
1	B	17	CYS	2.5
2	Q	117	VAL	2.5
2	S	321	LEU	2.5
2	Q	79	HIS	2.4
1	B	234	GLN	2.4
2	S	383	VAL	2.4
2	R	398	PRO	2.4
1	B	34	ALA	2.4
2	R	142	ALA	2.4
2	R	251	TYR	2.4
2	R	402	LYS	2.4
2	S	80	ALA	2.4
1	B	174	ARG	2.4
1	C	47	THR	2.4
2	R	275	GLY	2.4
1	B	213	LEU	2.4
2	S	415	ALA	2.4
1	B	32	ILE	2.3
2	R	216	ALA	2.3
2	S	474	ALA	2.3
1	B	9	VAL	2.3
1	B	59	ALA	2.3
2	S	545	ALA	2.3
1	A	4	LYS	2.3
2	Q	544	ILE	2.3
2	Q	499	SER	2.3
2	S	76	THR	2.3
2	S	138	PRO	2.3
2	S	229	THR	2.3
1	B	114	CYS	2.3
1	B	186	ASN	2.3
1	B	207	ALA	2.3
1	B	200	PRO	2.2
2	R	253	ALA	2.2
2	R	242	GLY	2.2
1	B	263	GLN	2.2
1	B	31	TYR	2.2
1	B	216	LEU	2.2
2	R	221	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	S	534	LEU	2.2
2	R	413	VAL	2.2
2	R	325	ASP	2.1
2	S	26	GLY	2.1
2	R	70	ARG	2.1
2	R	476	ARG	2.1
1	B	141	THR	2.1
2	Q	77	TYR	2.1
2	S	479	LEU	2.1
2	R	12	PHE	2.1
1	A	147	CYS	2.1
2	R	22	THR	2.1
1	C	18	GLY	2.1
2	S	322	GLY	2.1
1	B	241	ALA	2.1
2	R	433	ALA	2.1
1	B	155	VAL	2.1
2	Q	448	ASP	2.1
1	B	260	PHE	2.1
2	Q	116[A]	LEU	2.1
2	S	144	LEU	2.1
1	B	63	ALA	2.1
2	R	447	ALA	2.1
2	Q	497	VAL	2.1
2	R	118	HIS	2.1
2	S	227	PRO	2.1
1	B	58	ALA	2.1
1	C	71	TYR	2.1
2	Q	81	LEU	2.1
2	Q	396	GLY	2.1
2	R	479	LEU	2.0
1	B	98	THR	2.0
2	R	416	THR	2.0
2	R	239	ASN	2.0
1	B	117	TYR	2.0
2	R	26	GLY	2.0
2	R	168	LYS	2.0
2	S	228	HIS	2.0
2	S	408	LEU	2.0
1	B	237	TRP	2.0
2	R	475	PRO	2.0
2	S	475	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	R	147	SER	2.0
1	B	24	ALA	2.0
2	Q	474	ALA	2.0
2	R	342	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	CSX	S	75	7/8	0.97	0.21	-	22,24,27,28	1
2	CSX	Q	75	7/8	0.96	0.18	-	21,22,25,25	1
2	CSX	R	75	7/8	0.98	0.21	-	31,32,35,36	1

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	A	1271	6/6	0.85	0.29	5.93	45,50,52,53	0
5	GOL	Q	1563	6/6	0.77	0.26	5.28	43,47,51,55	0
5	GOL	A	1272	6/6	0.83	0.21	5.22	45,47,49,50	0
5	GOL	Q	1562	6/6	0.90	0.19	5.08	33,38,40,41	0
5	GOL	S	1562	6/6	0.70	0.30	1.55	48,52,56,57	6
5	GOL	Q	1561	6/6	0.95	0.14	1.31	37,40,41,41	0
5	GOL	A	1273	6/6	0.83	0.20	0.71	40,49,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	R	1563	6/6	0.90	0.16	-0.12	44,49,50,51	0
8	MG	Q	1553	1/1	0.97	0.10	-0.65	26,26,26,26	0
6	FCO	S	1550	7/7	0.99	0.17	-0.98	23,25,28,28	0
4	F3S	C	1266	7/7	0.99	0.09	-1.14	20,25,27,29	0
5	GOL	S	1561	6/6	0.95	0.09	-1.27	33,38,41,42	0
4	F3S	A	1266	7/7	0.99	0.09	-1.37	22,25,26,26	0
3	SF4	A	1267	8/8	0.99	0.12	-1.49	20,21,24,25	0
3	SF4	C	1267	8/8	0.99	0.12	-1.51	24,27,28,29	0
3	SF4	B	1267	8/8	0.95	0.11	-1.80	44,48,52,52	0
4	F3S	B	1266	7/7	0.87	0.08	-1.81	66,71,73,75	0
6	FCO	Q	1550	7/7	0.99	0.15	-1.86	14,22,24,25	0
6	FCO	R	1550	7/7	0.99	0.14	-1.98	26,30,30,37	0
8	MG	S	1553	1/1	0.96	0.09	-2.05	24,24,24,24	0
8	MG	Q	1559	1/1	0.96	0.06	-2.08	47,47,47,47	0
3	SF4	B	1265	8/8	0.96	0.07	-2.26	83,93,97,98	0
7	NI	R	1551	1/1	1.00	0.14	-2.36	34,34,34,34	0
3	SF4	C	1265	8/8	0.99	0.07	-2.66	27,29,31,31	0
3	SF4	A	1265	8/8	0.98	0.06	-2.67	29,32,33,33	0
8	MG	R	1553	1/1	0.95	0.05	-2.98	28,28,28,28	0
7	NI	S	1551	1/1	0.99	0.12	-3.49	28,28,28,28	0
7	NI	Q	1551	1/1	0.96	0.12	-5.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.