



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:03 PM GMT

PDB ID : 4UPV  
Title : Low X-ray dose structure of a Ni-A Ni-Sox mixture of the D. fructosovorans NiFe-hydrogenase L122A mutant  
Authors : Volbeda, A.; Martin, L.; Barbier, E.; Gutierrez-Sanz, O.; DeLacey, A.L.; Liebgott, P.P.; Dementin, S.; Rousset, M.; Fontecilla-Camps, J.C.  
Deposited on : 2014-06-18  
Resolution : 1.52 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

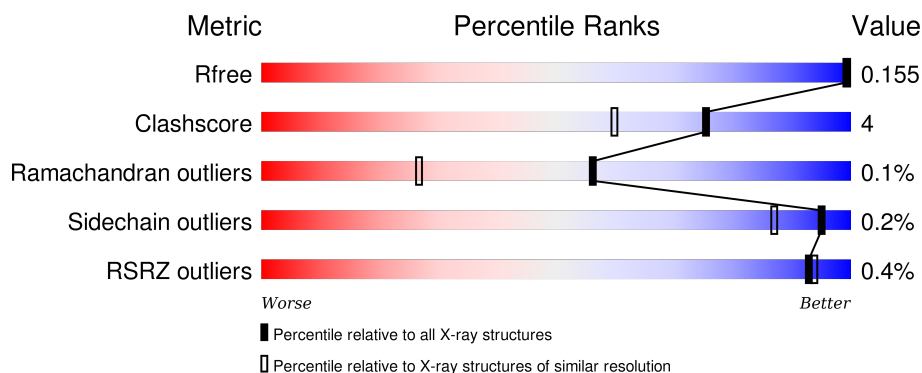
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.52 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	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	265	<div> <div></div> <div>97%</div> <div>..</div> </div>
1	B	265	<div> <div></div> <div>93%</div> <div>6% .</div> </div>
2	Q	564	<div> <div></div> <div>92%</div> <div>. .</div> </div>
2	R	564	<div> <div></div> <div>90%</div> <div>7% .</div> </div>

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
11	MG	R	1552	-	-	-	X
5	GOL	A	1268	-	-	-	X
5	GOL	A	1270	-	-	-	X
5	GOL	B	1269	-	-	X	X
5	GOL	B	1270	-	-	-	X
5	GOL	B	1271	-	-	-	X
5	GOL	B	1273	-	-	-	X
5	GOL	R	1554	-	-	-	X
5	GOL	R	1557	-	-	-	X
5	GOL	R	1558	-	-	-	X
6	GLY	R	601	-	-	-	X
7	SOT	B	1268[A]	-	-	-	X
7	SOT	B	1268[B]	-	-	-	X
8	H2S	B	1272	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 14686 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 NIFE-HYDROGENASE SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	11	0
			2026	1291	336	383	16			
1	B	263	Total	C	N	O	S	0	16	0
			2061	1316	339	390	16			

- Molecule 2 is a protein called NIFE-HYDROGENASE LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	31	0
			4304	2750	745	784	25			
2	R	545	Total	C	N	O	S	0	34	0
			4329	2765	743	796	25			

There are 34 discrepancies between the modelled and reference sequences:

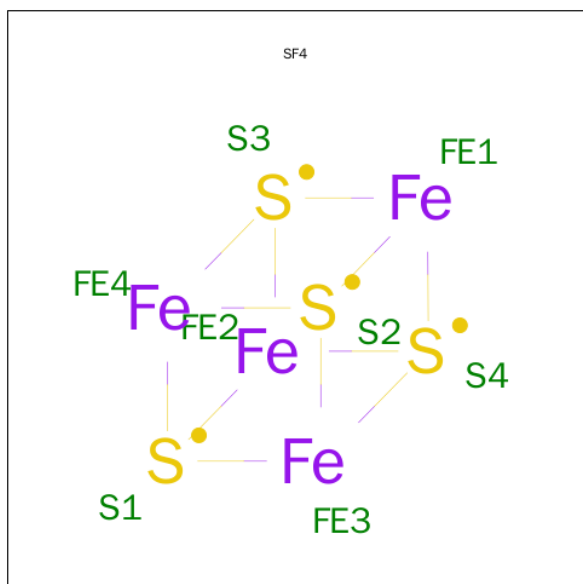
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	EXPRESSION TAG	UNP E1K247
Q	-12	SER	-	EXPRESSION TAG	UNP E1K247
Q	-11	TRP	-	EXPRESSION TAG	UNP E1K247
Q	-10	SER	-	EXPRESSION TAG	UNP E1K247
Q	-9	HIS	-	EXPRESSION TAG	UNP E1K247
Q	-8	PRO	-	EXPRESSION TAG	UNP E1K247
Q	-7	GLN	-	EXPRESSION TAG	UNP E1K247
Q	-6	PHE	-	EXPRESSION TAG	UNP E1K247
Q	-5	GLU	-	EXPRESSION TAG	UNP E1K247
Q	-4	LYS	-	EXPRESSION TAG	UNP E1K247
Q	-3	GLY	-	EXPRESSION TAG	UNP E1K247
Q	-2	ALA	-	EXPRESSION TAG	UNP E1K247
Q	-1	SER	-	EXPRESSION TAG	UNP E1K247
Q	0	GLY	-	EXPRESSION TAG	UNP E1K247
Q	1	ALA	-	EXPRESSION TAG	UNP E1K247
Q	122	ALA	LEU	ENGINEERED MUTATION	UNP E1K247

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	543	CSS	CYS	MICROHETEROGENEITY	UNP E1K247
R	-13	ALA	-	EXPRESSION TAG	UNP E1K247
R	-12	SER	-	EXPRESSION TAG	UNP E1K247
R	-11	TRP	-	EXPRESSION TAG	UNP E1K247
R	-10	SER	-	EXPRESSION TAG	UNP E1K247
R	-9	HIS	-	EXPRESSION TAG	UNP E1K247
R	-8	PRO	-	EXPRESSION TAG	UNP E1K247
R	-7	GLN	-	EXPRESSION TAG	UNP E1K247
R	-6	PHE	-	EXPRESSION TAG	UNP E1K247
R	-5	GLU	-	EXPRESSION TAG	UNP E1K247
R	-4	LYS	-	EXPRESSION TAG	UNP E1K247
R	-3	GLY	-	EXPRESSION TAG	UNP E1K247
R	-2	ALA	-	EXPRESSION TAG	UNP E1K247
R	-1	SER	-	EXPRESSION TAG	UNP E1K247
R	0	GLY	-	EXPRESSION TAG	UNP E1K247
R	1	ALA	-	EXPRESSION TAG	UNP E1K247
R	122	ALA	LEU	ENGINEERED MUTATION	UNP E1K247
R	543	CSS	CYS	MICROHETEROGENEITY	UNP E1K247

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



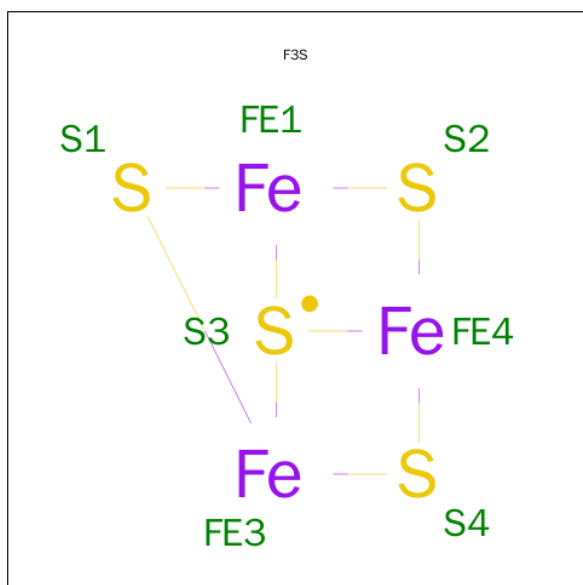
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		

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

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



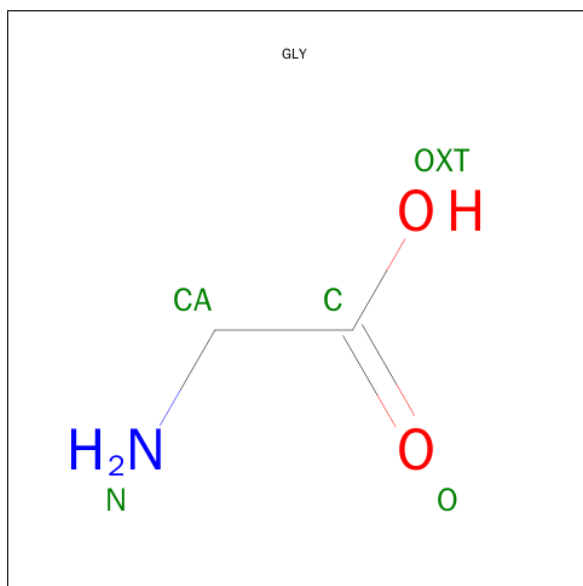
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



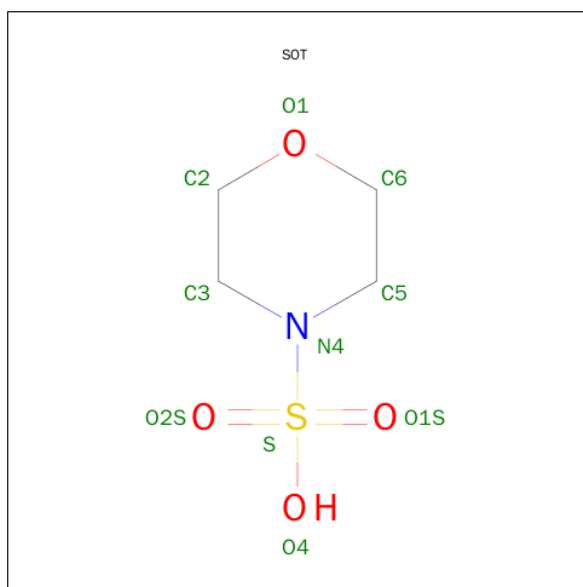
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	1
			7	3	4		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			5	2	1	2		
6	R	1	Total	C	N	O	0	0
			5	2	1	2		

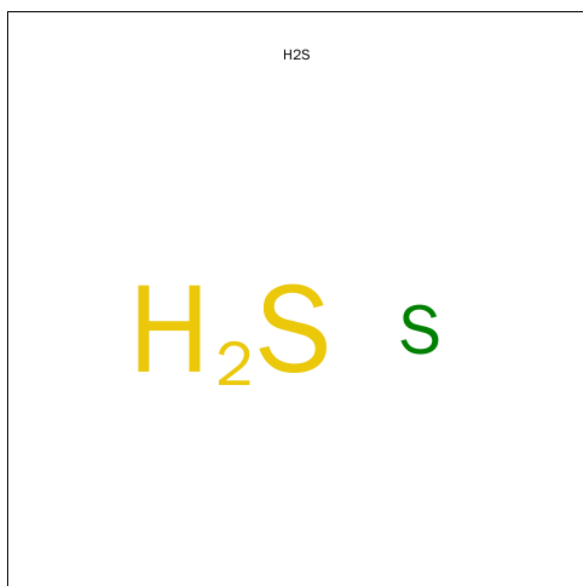
- Molecule 7 is MORPHOLINE-4-SULFONIC ACID (three-letter code: SOT) (formula:  $C_4H_9NO_4S$ ).





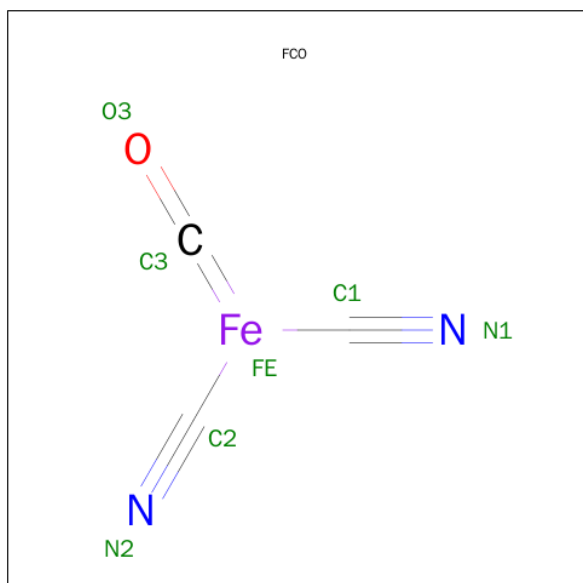
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	1
			18	8	2	6	2		

- Molecule 8 is HYDROSULFURIC ACID (three-letter code: H<sub>2</sub>S) (formula: H<sub>2</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	S	0	0
			1	1		

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C<sub>3</sub>FeN<sub>2</sub>O).



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

- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	R	1	Total	Ni	0	1
			2	2		
10	Q	1	Total	Ni	0	1
			2	2		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	R	1	Total	Mg	0	0
			1	1		
11	Q	1	Total	Mg	0	0
			1	1		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	Q	1	Total	Cl	0	1
			2	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	283	Total	O	0	12
			295	295		
13	B	302	Total	O	0	12
			314	314		
13	Q	541	Total	O	0	12
			553	553		
13	R	606	Total	O	0	16
			622	622		

### 3 Residue-property plots [i](#)

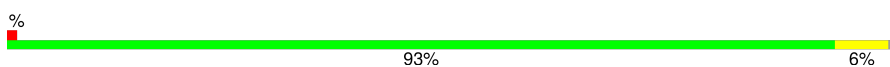
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: NIFE-HYDROGENASE SMALL SUBUNIT

Chain A: 



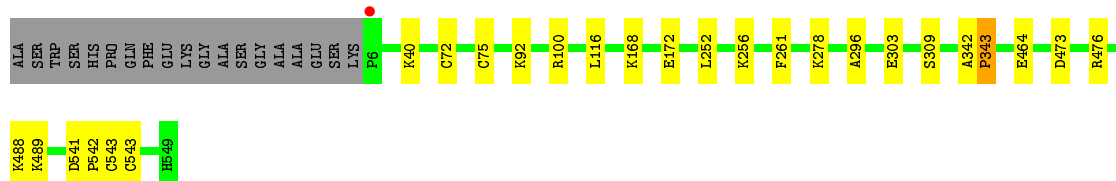
#### • Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT

Chain B: 




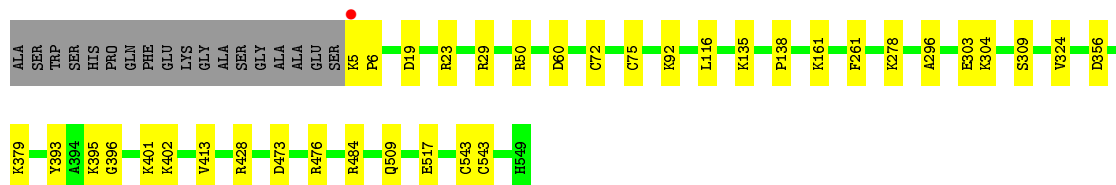
#### • Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT

Chain Q: 



#### • Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT

Chain R: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.69Å 100.85Å 116.70Å 90.00° 105.96° 90.00°	Depositor
Resolution (Å)	30.00 – 1.52 49.03 – 1.52	Depositor EDS
% Data completeness (in resolution range)	90.6 (30.00-1.52) 90.6 (49.03-1.52)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.120 , 0.154 0.121 , 0.155	Depositor DCC
$R_{free}$ test set	10130 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	7.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.0	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 199968 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NI, MG, GOL, CL, SF4, H2S, F3S, CSX, FCO, CSS, SOT

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	0.58	0/2129	0.68	2/2893 (0.1%)
1	B	0.57	0/2181	0.71	0/2958
2	Q	0.59	0/4501	0.72	1/6089 (0.0%)
2	R	0.60	0/4555	0.75	3/6166 (0.0%)
All	All	0.59	0/13366	0.72	6/18106 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	428	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	R	50	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	Q	100	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	R	60	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	61[A]	HIS	CB-CA-C	5.08	120.56	110.40

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	2026	0	1960	4	0
1	B	2061	0	1998	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	4304	0	4315	21	0
2	R	4329	0	4314	37	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
5	A	18	0	24	2	0
5	B	24	0	32	9	0
5	Q	6	0	8	0	0
5	R	37	0	46	7	0
6	B	5	0	2	0	0
6	R	5	0	2	1	0
7	B	18	0	16	1	0
8	B	1	0	0	1	0
9	Q	7	0	0	0	0
9	R	7	0	0	0	0
10	Q	2	0	0	0	0
10	R	2	0	0	0	0
11	Q	1	0	0	0	0
11	R	1	0	0	0	0
12	Q	2	0	0	0	0
13	A	295	0	0	2	0
13	B	314	0	0	19	0
13	Q	553	0	0	12	0
13	R	622	0	0	20	0
All	All	14686	0	12717	101	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 4.

The worst 5 of 101 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:Q:92[B]:LYS:HE2	13:Q:2974:HOH:O	1.28	1.29
2:R:278[B]:LYS:HE3	13:R:3163:HOH:O	1.37	1.24
2:Q:489[B]:LYS:HE2	13:Q:3141:HOH:O	1.08	1.20
2:R:92[A]:LYS:HE2	13:R:3254:HOH:O	1.02	1.18
2:R:395[B]:LYS:NZ	5:R:1554:GOL:O1	1.78	1.15

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	272/265 (103%)	265 (97%)	7 (3%)	0	100	100
1	B	277/265 (104%)	270 (98%)	7 (2%)	0	100	100
2	Q	570/564 (101%)	554 (97%)	14 (2%)	2 (0%)	39	14
2	R	575/564 (102%)	565 (98%)	10 (2%)	0	100	100
All	All	1694/1658 (102%)	1654 (98%)	38 (2%)	2 (0%)	56	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	343[A]	PRO
2	Q	343[B]	PRO

### 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	220/210 (105%)	220 (100%)	0	100	100
1	B	225/210 (107%)	223 (99%)	2 (1%)	84	65
2	Q	460/446 (103%)	459 (100%)	1 (0%)	95	87
2	R	467/446 (105%)	466 (100%)	1 (0%)	95	87
All	All	1372/1312 (105%)	1368 (100%)	4 (0%)	95	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88[A]	MET
1	B	88[B]	MET
2	Q	473	ASP
2	R	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	B	5	HIS
1	B	14	ASN
2	Q	250	ASN
2	Q	509	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CSS	Q	543[A]	10,2	4,6,7	0.85	0	3,6,8	1.02	0
2	CSX	Q	75	9,10,2	3,6,7	0.66	0	3,6,8	0.89	0
2	CSS	R	543[A]	10,2	4,6,7	0.66	0	3,6,8	1.05	0
2	CSX	R	75	9,10,2	3,6,7	0.53	0	3,6,8	0.88	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	CSS	Q	543[A]	10,2	-	0/1/5/7	0/0/0/0
2	CSX	Q	75	9,10,2	-	0/1/5/7	0/0/0/0
2	CSS	R	543[A]	10,2	-	0/1/5/7	0/0/0/0
2	CSX	R	75	9,10,2	-	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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	543[A]	CSS	1	0
2	Q	75	CSX	1	0
2	R	543[A]	CSS	1	0
2	R	75	CSX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 1 is modelled with single atom and 8 are monoatomic - leaving 27 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	1268	-	5,5,5	0.23	0	5,5,5	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	1269	-	5,5,5	0.51	0	5,5,5	0.80	0
5	GOL	A	1270	-	5,5,5	0.26	0	5,5,5	0.38	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	-
7	SOT	B	1268[A]	1	6,9,10	0.64	0	5,11,14	8.26	5 (100%)
7	SOT	B	1268[B]	-	6,9,10	0.35	0	5,11,14	3.41	2 (40%)
5	GOL	B	1269	-	5,5,5	0.22	0	5,5,5	0.71	0
5	GOL	B	1270	-	5,5,5	0.17	0	5,5,5	0.51	0
5	GOL	B	1271	-	5,5,5	0.22	0	5,5,5	0.46	0
5	GOL	B	1273	-	5,5,5	0.32	0	5,5,5	0.63	0
6	GLY	B	301	-	1,4,4	0.83	0	0,4,4	0.00	-
9	FCO	Q	1550	13,2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	Q	1553	-	5,5,5	0.59	0	5,5,5	0.37	0
9	FCO	R	1550	13,2	0,6,6	0.00	-	0,6,6	0.00	-
5	GOL	R	1553	-	5,5,5	0.59	0	5,5,5	0.19	0
5	GOL	R	1554	-	5,5,5	0.47	0	5,5,5	0.42	0
5	GOL	R	1555[A]	-	5,5,5	0.44	0	5,5,5	0.50	0
5	GOL	R	1555[B]	-	5,5,5	0.45	0	5,5,5	0.60	0
5	GOL	R	1556	-	5,5,5	0.33	0	5,5,5	0.79	0
5	GOL	R	1557	-	5,5,5	0.20	0	5,5,5	0.55	0
5	GOL	R	1558	-	5,5,5	0.18	0	5,5,5	0.52	0
6	GLY	R	601	-	1,4,4	0.83	0	0,4,4	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1268	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1269	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1270	-	-	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
7	SOT	B	1268[A]	1	-	0/0/12/14	0/1/1/1
7	SOT	B	1268[B]	-	-	0/0/12/14	0/1/1/1
5	GOL	B	1269	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1270	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1271	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1273	-	-	0/4/4/4	0/0/0/0
6	GLY	B	301	-	-	0/0/2/2	0/0/0/0
9	FCO	Q	1550	13,2	-	0/0/6/6	0/0/0/0
5	GOL	Q	1553	-	-	0/4/4/4	0/0/0/0
9	FCO	R	1550	13,2	-	0/0/6/6	0/0/0/0
5	GOL	R	1553	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1554	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1555[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1555[B]	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1556	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1557	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1558	-	-	0/4/4/4	0/0/0/0
6	GLY	R	601	-	-	0/0/2/2	0/0/0/0

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1268[A]	SOT	O1-C6-C5	2.48	117.53	111.84
7	B	1268[A]	SOT	O1-C2-C3	3.20	119.18	111.84
7	B	1268[A]	SOT	C6-O1-C2	3.60	122.02	109.89
7	B	1268[B]	SOT	C2-C3-N4	5.11	111.70	108.19
7	B	1268[B]	SOT	C6-C5-N4	5.49	111.96	108.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1269	GOL	2	0
7	B	1268[B]	SOT	1	0
5	B	1269	GOL	8	0
5	B	1270	GOL	3	0
5	B	1271	GOL	1	0
5	R	1554	GOL	2	0
5	R	1555[A]	GOL	1	0
5	R	1556	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1558	GOL	3	0
6	R	601	GLY	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/265 (98%)	-0.51	3 (1%) 82 85	5, 10, 20, 48	4 (1%)
1	B	263/265 (99%)	-0.59	2 (0%) 87 89	6, 9, 18, 34	3 (1%)
2	Q	542/564 (96%)	-0.52	1 (0%) 95 95	5, 10, 20, 36	6 (1%)
2	R	543/564 (96%)	-0.63	1 (0%) 95 95	5, 9, 17, 39	4 (0%)
All	All	1610/1658 (97%)	-0.57	7 (0%) 93 94	5, 9, 19, 48	17 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	8.3
1	A	4	LYS	4.3
2	Q	6	PRO	2.8
1	B	2	THR	2.4
1	B	264[A]	GLY	2.3

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CSS	R	543[A]	7/8	0.99	0.05	-	5,6,10,10	7
2	CSX	R	75	7/8	0.99	0.05	-	5,6,7,7	1
2	CSS	Q	543[A]	7/8	0.99	0.06	-	6,7,11,11	7
2	CSX	Q	75	7/8	1.00	0.05	-	6,6,8,8	1

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	GLY	R	601	5/5	0.94	0.22	15.97	10,12,12,16	5
5	GOL	B	1269	6/6	0.95	0.26	11.83	15,18,19,20	6
5	GOL	B	1273	6/6	0.93	0.17	9.01	19,23,27,33	0
5	GOL	B	1270	6/6	0.83	0.44	8.30	24,25,27,32	6
5	GOL	A	1268	6/6	0.90	0.13	4.79	27,29,32,34	0
5	GOL	R	1554	6/6	0.94	0.14	4.43	16,17,19,23	1
8	H2S	B	1272	1/1	0.97	0.28	4.40	31,31,31,31	1
5	GOL	R	1558	6/6	0.70	0.20	3.48	22,27,29,34	6
5	GOL	A	1270	6/6	0.72	0.17	2.79	24,28,29,30	6
7	SOT	B	1268[A]	9/10	0.97	0.11	2.79	9,13,15,19	9
7	SOT	B	1268[B]	9/10	0.97	0.11	2.63	17,17,20,20	9
5	GOL	B	1271	6/6	0.79	0.17	2.13	21,25,26,32	6
5	GOL	R	1557	6/6	0.90	0.12	2.09	16,24,26,26	6
11	MG	R	1552	1/1	1.00	0.06	2.05	6,6,6,6	0
6	GLY	B	301	5/5	0.87	0.15	1.54	16,16,18,21	5
5	GOL	A	1269	6/6	0.93	0.16	1.43	22,29,30,35	0
5	GOL	R	1553	6/6	0.97	0.06	0.89	8,8,10,10	0
5	GOL	R	1556	6/6	0.94	0.12	0.69	12,14,16,17	6
3	SF4	B	1267	8/8	1.00	0.05	-0.41	6,6,6,6	0
5	GOL	Q	1553	6/6	0.98	0.06	-0.54	8,9,9,10	0
3	SF4	A	1265	8/8	1.00	0.04	-1.04	7,7,8,8	0
11	MG	Q	1552	1/1	1.00	0.05	-1.24	6,6,6,6	0
9	FCO	R	1550	7/7	1.00	0.05	-1.26	6,7,7,7	0
3	SF4	B	1265	8/8	1.00	0.04	-1.41	7,7,8,8	0
3	SF4	A	1267	8/8	1.00	0.05	-1.41	6,6,6,6	0
9	FCO	Q	1550	7/7	1.00	0.05	-1.54	6,7,8,9	0
10	NI	R	1551[B]	1/1	1.00	0.04	-1.94	8,8,8,8	1
4	F3S	A	1266	7/7	1.00	0.05	-2.04	6,6,7,7	0
4	F3S	B	1266	7/7	1.00	0.04	-2.06	6,7,7,7	0
10	NI	Q	1551[B]	1/1	1.00	0.03	-7.21	8,8,8,8	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	NI	Q	1551[A]	1/1	1.00	0.03	-	9,9,9,9	1
10	NI	R	1551[A]	1/1	1.00	0.04	-	9,9,9,9	1
5	GOL	R	1555[B]	6/6	0.97	0.09	-	12,21,24,25	1
12	CL	Q	1554[B]	1/1	0.98	0.04	-	37,37,37,37	1
5	GOL	R	1555[A]	6/6	0.97	0.09	-	12,21,24,30	1
12	CL	Q	1554[A]	1/1	0.98	0.04	-	30,30,30,30	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.