



wwPDB X-ray Structure Validation Summary Report i

Oct 23, 2014 – 07:23 PM EDT

PDB ID : 4UQL
Title : High-resolution 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 : 2014-06-24
Resolution : 1.22 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

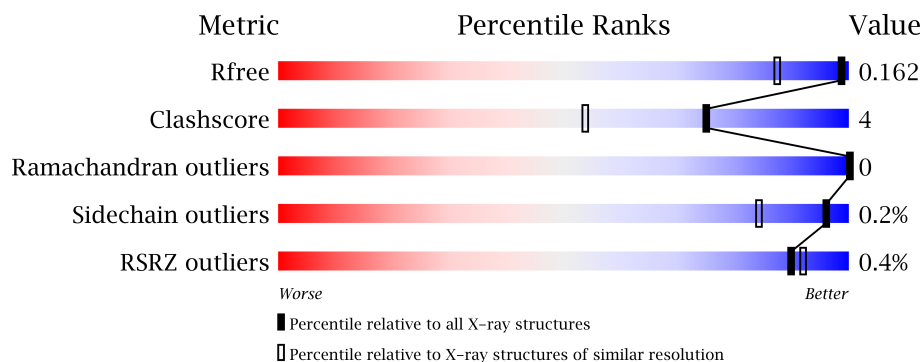
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 1.22 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}	66092	1649 (1.30-1.14)
Clashscore	79885	1059 (1.28-1.16)
Ramachandran outliers	78287	1008 (1.28-1.16)
Sidechain outliers	78261	1006 (1.28-1.16)
RSRZ outliers	66119	1649 (1.30-1.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	
1	B	265	
2	Q	563	
2	R	563	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	A	1268	-	X
5	GOL	A	1269	-	X
5	GOL	B	1269	-	X
5	GOL	B	1270	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	B	1272	-	X
5	GOL	R	1554	-	X
5	GOL	R	1555[A]	-	X
5	GOL	R	1555[B]	-	X
5	GOL	R	1557	-	X
6	GLY	Q	601	-	X
6	GLY	R	601	-	X
7	SOT	B	1268[A]	-	X
7	SOT	B	1268[B]	-	X
8	H2S	B	1271	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14688 atoms, of which 0 are hydrogen and 0 are deuterium.

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	12	0
			2031	1296	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 NICKEL-DEPENDENT HYDROGENASE LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	31	0
			4300	2748	744	783	25			
2	R	545	Total	C	N	O	S	0	35	0
			4328	2765	742	796	25			

There are 32 discrepancies between the modelled and reference sequences:

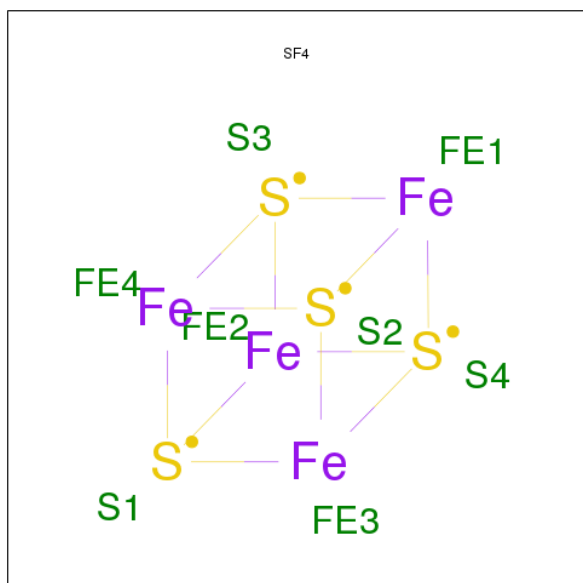
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	EXPRESSION TAG	UNP E1K247
Q	-12	SER	-	EXPRESSION TAG	UNP E1K247
Q	-11	TRP	-	EXPRESSION TAG	UNP E1K247
Q	-10	SER	-	EXPRESSION TAG	UNP E1K247
Q	-9	HIS	-	EXPRESSION TAG	UNP E1K247
Q	-8	PRO	-	EXPRESSION TAG	UNP E1K247
Q	-7	GLN	-	EXPRESSION TAG	UNP 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

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



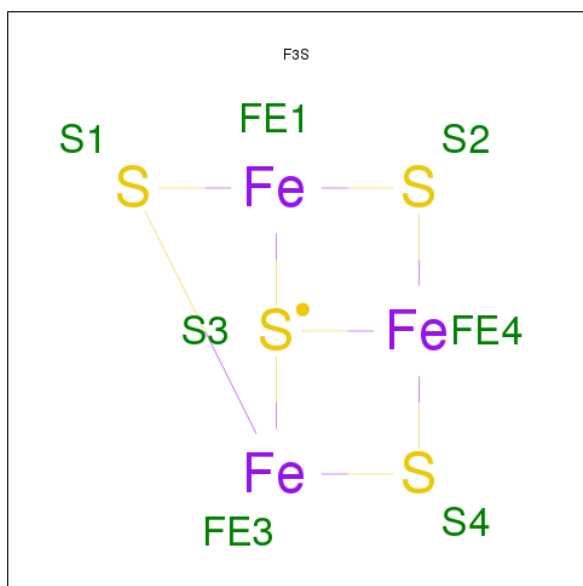
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

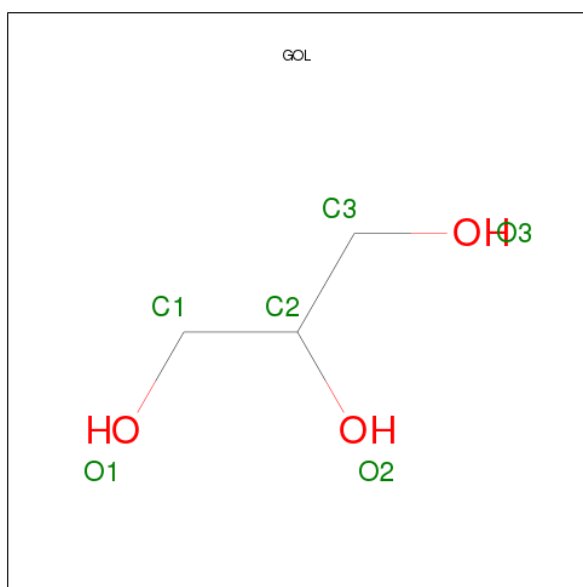
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	Fe	S	0	0
			8	4	4		

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



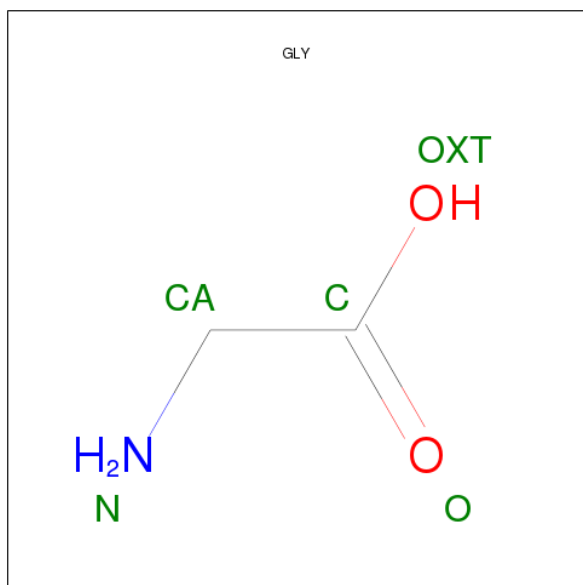
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		

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



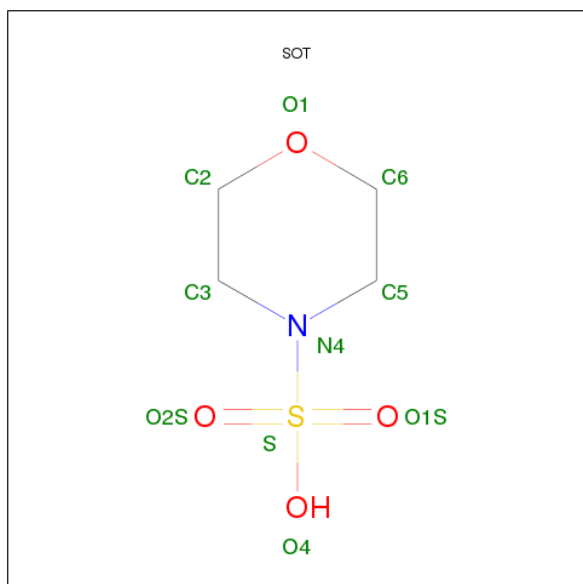
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total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

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



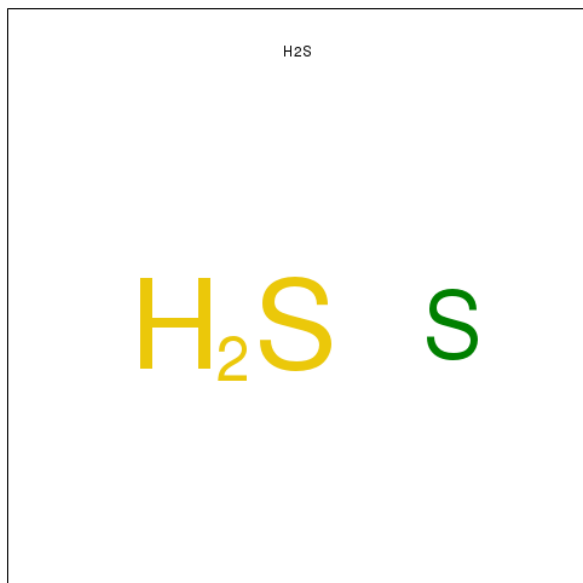
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			5	2	1	2		
6	Q	1	Total	C	N	O	0	0
			5	2	1	2		
6	R	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 7 is MORPHOLINE-4-SULFONICACID (three-letter code: SOT) (formula: C₄H₉NO₄S).



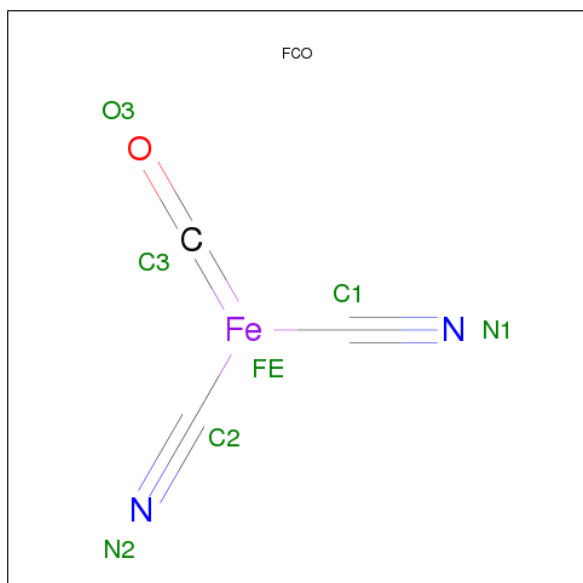
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	1
			18	8	2	6	2		

- Molecule 8 is HYDROSULFURIC ACID (three-letter code: H₂S) (formula: H₂S).



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: C₃FeN₂O).



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	0
			1	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	283	Total	O	0	12
			295	295		
13	B	307	Total	O	0	9
			316	316		
13	Q	544	Total	O	0	13
			557	557		
13	R	618	Total	O	0	14
			632	632		

3 Residue-property plots

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

Chain A: 



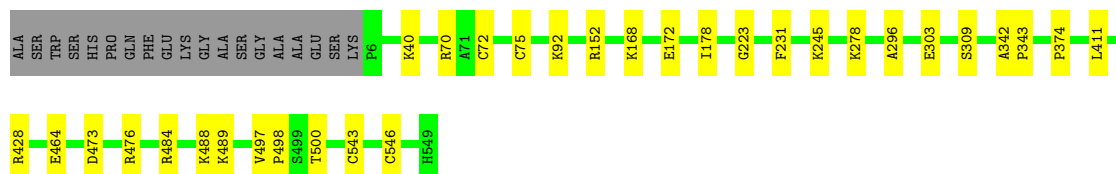
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain B: 



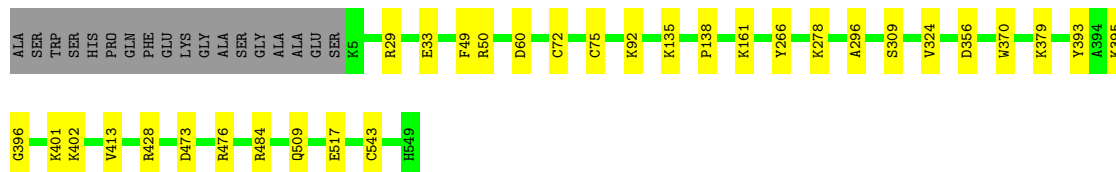
- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain Q: 



- Molecule 2: NICKEL-DEPENDENT 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, α , β , γ	64.69Å 100.85Å 116.70Å 90.00° 105.96° 90.00°	Depositor
Resolution (Å)	30.00 – 1.22 45.99 – 1.15	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-1.22) 95.9 (45.99-1.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.15Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.120 , 0.152 0.132 , 0.162	Depositor DCC
R_{free} test set	20888 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	6.4	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.6	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 487248 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14688	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.63	0/2137	0.75	1/2904 (0.0%)
1	B	0.63	0/2181	0.79	2/2958 (0.1%)
2	Q	0.63	0/4495	0.80	3/6081 (0.0%)
2	R	0.63	0/4555	0.84	5/6166 (0.1%)
All	All	0.63	0/13368	0.81	11/18109 (0.1%)

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
1	A	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	428	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	R	50	ARG	NE-CZ-NH2	-6.95	116.82	120.30
2	Q	152	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	Q	428	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	R	266	TYR	CB-CG-CD1	5.75	124.45	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ARG	Sidechain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2031	0	1971	10	1
1	B	2061	0	1998	21	0
2	Q	4300	0	4316	31	0
2	R	4328	0	4320	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	12	0	16	0	0
5	B	18	0	24	2	0
5	Q	6	0	8	0	0
5	R	31	0	38	5	0
6	B	5	0	2	0	0
6	Q	5	0	2	1	0
6	R	5	0	2	1	0
7	B	18	0	16	0	0
8	B	1	0	0	0	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	1	0	0	0	0
13	A	295	0	0	4	1
13	B	316	0	0	18	0
13	Q	557	0	0	17	1
13	R	632	0	0	27	1
All	All	14688	0	12713	103	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 103 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Q:245[B]:LYS:HE2	13:Q:2510:HOH:O	1.16	1.25
2:R:92[B]:LYS:HE3	13:R:2558:HOH:O	1.11	1.25
5:B:1269:GOL:O3	13:B:2305:HOH:O	1.52	1.25
2:Q:489[B]:LYS:HE2	13:Q:2441:HOH:O	1.13	1.24
2:Q:92[B]:LYS:HE2	13:Q:2272:HOH:O	1.41	1.18

All (2) 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	Distance(Å)	Clash(Å)
1:A:168[B]:ASP:OD1	13:Q:2496:HOH:O[2_556]	1.66	0.54
13:A:2200[B]:HOH:O	13:R:2587:HOH:O[2_555]	1.80	0.40

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	273/265 (103%)	266 (97%)	7 (3%)	0	100	100
1	B	277/265 (104%)	271 (98%)	6 (2%)	0	100	100
2	Q	570/563 (101%)	554 (97%)	16 (3%)	0	100	100
2	R	576/563 (102%)	566 (98%)	10 (2%)	0	100	100
All	All	1696/1656 (102%)	1657 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	221/210 (105%)	221 (100%)	0	100	100
1	B	225/210 (107%)	223 (99%)	2 (1%)	87	63
2	Q	459/445 (103%)	458 (100%)	1 (0%)	96	84
2	R	467/445 (105%)	466 (100%)	1 (0%)	96	84
All	All	1372/1310 (105%)	1368 (100%)	4 (0%)	96	83

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 (4) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 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	5,5,7	7.54	3 (60%)	2,5,8	5.41	2 (100%)
2	CSS	Q	543[B]	10	5,6,7	7.29	1 (20%)	4,6,8	3.97	2 (50%)
2	CSX	Q	75	9,10,2	4,6,7	8.53	1 (25%)	3,6,8	3.97	2 (66%)
2	CSS	R	543[A]	10	5,5,7	9.26	3 (60%)	2,5,8	4.89	1 (50%)
2	CSS	R	543[B]	10	5,6,7	9.09	1 (20%)	4,6,8	3.77	2 (50%)
2	CSX	R	75	9,10,2	4,6,7	8.32	1 (25%)	3,6,8	4.01	2 (66%)

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	-	0/2/4/7	0/0/0/0
2	CSS	Q	543[B]	10	-	0/2/5/7	0/0/0/0
2	CSX	Q	75	9,10,2	-	0/2/5/7	0/0/0/0
2	CSS	R	543[A]	10	-	0/2/4/7	0/0/0/0
2	CSS	R	543[B]	10	-	0/2/5/7	0/0/0/0
2	CSX	R	75	9,10,2	-	0/2/5/7	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	543[B]	CSS	O-C	20.22	1.25	1.11
2	R	543[A]	CSS	O-C	20.22	1.25	1.11
2	Q	75	CSX	O-C	17.01	1.23	1.11
2	R	75	CSX	O-C	16.55	1.22	1.11
2	Q	543[B]	CSS	O-C	16.19	1.22	1.11

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	543[B]	CSS	C-CA-N	-7.34	106.50	113.83
2	Q	543[A]	CSS	C-CA-N	-7.34	106.50	113.83
2	R	543[B]	CSS	C-CA-N	-6.91	106.92	113.83
2	R	543[A]	CSS	C-CA-N	-6.91	106.92	113.83
2	Q	75	CSX	C-CA-N	-6.05	107.78	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 1 is modelled with single atom and 7 are monoatomic - leaving 25 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	12,12,12	5.42	8 (66%)	0,24,24	0.00	-
4	F3S	A	1266	1	3,9,9	4.38	3 (100%)	0,15,15	0.00	-
3	SF4	A	1267	1	12,12,12	6.60	8 (66%)	0,24,24	0.00	-
5	GOL	A	1268	-	5,5,5	0.20	0	5,5,5	0.92	0
5	GOL	A	1269	-	5,5,5	0.48	0	5,5,5	0.74	0
3	SF4	B	1265	1	12,12,12	5.13	9 (75%)	0,24,24	0.00	-
4	F3S	B	1266	1	3,9,9	5.06	3 (100%)	0,15,15	0.00	-
3	SF4	B	1267	1	12,12,12	6.32	6 (50%)	0,24,24	0.00	-
7	SOT	B	1268[A]	1	9,9,10	1.68	1 (11%)	9,11,14	5.22	7 (77%)
7	SOT	B	1268[B]	-	9,9,10	2.55	2 (22%)	9,11,14	2.00	1 (11%)
5	GOL	B	1269	-	5,5,5	0.50	0	5,5,5	0.72	0
5	GOL	B	1270	-	5,5,5	0.25	0	5,5,5	0.40	0
5	GOL	B	1272	-	5,5,5	0.40	0	5,5,5	0.78	0
6	GLY	B	301	-	4,4,4	1.13	1 (25%)	4,4,4	1.39	1 (25%)
9	FCO	Q	1550	13,2	2,6,6	0.41	0	0,6,6	0.00	-
5	GOL	Q	1553	-	5,5,5	0.32	0	5,5,5	0.33	0
6	GLY	Q	601	-	4,4,4	0.97	0	4,4,4	0.78	0
9	FCO	R	1550	13,2	2,6,6	0.23	0	0,6,6	0.00	-
5	GOL	R	1553	-	5,5,5	0.37	0	5,5,5	0.34	0
5	GOL	R	1554	-	5,5,5	0.67	0	5,5,5	0.26	0
5	GOL	R	1555[A]	-	5,5,5	0.38	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	R	1555[B]	-	5,5,5	0.47	0	5,5,5	1.34	1 (20%)
5	GOL	R	1556	-	5,5,5	0.30	0	5,5,5	0.91	0
5	GOL	R	1557	-	5,5,5	0.25	0	5,5,5	0.73	0
6	GLY	R	601	-	4,4,4	0.91	0	4,4,4	0.81	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	1268	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1269	-	-	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	-	1/4/12/14	0/1/1/1
7	SOT	B	1268[B]	-	-	1/4/12/14	0/1/1/1
5	GOL	B	1269	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1270	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1272	-	-	0/4/4/4	0/0/0/0
6	GLY	B	301	-	-	0/2/2/2	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
6	GLY	Q	601	-	-	0/2/2/2	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
6	GLY	R	601	-	-	0/2/2/2	0/0/0/0

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1267	SF4	S4-FE2	-13.10	2.24	2.33
3	A	1267	SF4	S2-FE4	-12.92	2.24	2.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1267	SF4	S4-FE2	-12.23	2.25	2.33
3	B	1267	SF4	S3-FE1	-11.60	2.25	2.33
3	A	1267	SF4	S3-FE1	-9.72	2.26	2.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1268[A]	SOT	O2S-S-O1S	9.65	121.48	113.03
7	B	1268[A]	SOT	C6-C5-N4	7.72	117.76	108.44
7	B	1268[A]	SOT	C2-C3-N4	6.33	116.08	108.44
7	B	1268[B]	SOT	C5-N4-C3	5.06	127.17	112.48
7	B	1268[A]	SOT	O1-C2-C3	3.96	121.10	111.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1268[A]	SOT	O2S-S-N4-C5
7	B	1268[B]	SOT	O1S-S-N4-C5

There are no ring outliers.

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	262/265 (98%)	-0.41	4 (1%) 70 76	4, 8, 20, 48	4 (1%)
1	B	263/265 (99%)	-0.48	3 (1%) 77 82	4, 7, 17, 32	3 (1%)
2	Q	544/563 (96%)	-0.44	0 100 100	4, 9, 19, 37	7 (1%)
2	R	545/563 (96%)	-0.47	0 100 100	4, 7, 15, 40	5 (0%)
All	All	1614/1656 (97%)	-0.45	7 (0%) 90 92	4, 8, 18, 48	19 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	8.1
1	A	163	THR	3.6
1	A	164[A]	LYS	3.0
1	B	264[A]	GLY	2.5
1	A	4	LYS	2.5

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CSS	R	543[A]	6/8	0.08	1.18	3,4,5,7	2
2	CSS	Q	543[B]	7/8	0.07	0.61	5,5,8,9	3
2	CSS	Q	543[A]	6/8	0.07	0.61	5,5,6,8	2
2	CSS	R	543[B]	7/8	0.08	0.57	3,4,7,8	3
2	CSX	Q	75	7/8	0.06	-0.99	4,4,5,6	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CSX	R	75	7/8	0.06	-1.59	3,4,5,5	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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GLY	Q	601	5/5	0.30	20.12	12,12,14,16	5
6	GLY	R	601	5/5	0.33	17.77	9,10,12,14	5
5	GOL	A	1268	6/6	0.14	14.15	26,27,30,33	0
5	GOL	R	1557	6/6	0.24	8.25	14,23,25,26	6
8	H2S	B	1271	1/1	0.25	6.97	18,18,18,18	1
5	GOL	R	1555[B]	6/6	0.09	6.83	11,18,22,24	1
5	GOL	B	1269	6/6	0.14	6.45	20,22,27,28	1
7	SOT	B	1268[B]	9/10	0.10	6.01	15,17,22,22	9
5	GOL	B	1272	6/6	0.14	5.78	17,20,25,37	0
5	GOL	R	1555[A]	6/6	0.09	5.61	11,18,22,24	1
7	SOT	B	1268[A]	9/10	0.10	4.96	11,12,14,16	9
5	GOL	B	1270	6/6	0.15	2.37	20,22,27,33	6
5	GOL	R	1554	6/6	0.10	2.18	14,15,17,20	1
5	GOL	A	1269	6/6	0.14	2.06	18,27,30,32	0
6	GLY	B	301	5/5	0.15	1.76	14,16,16,18	5
5	GOL	R	1556	6/6	0.12	1.46	11,14,15,17	6
12	CL	Q	1554	1/1	0.08	0.09	32,32,32,32	1
11	MG	R	1552	1/1	0.05	0.02	4,4,4,4	0
5	GOL	R	1553	6/6	0.05	-0.01	6,6,7,8	0
9	FCO	Q	1550	7/7	0.05	-1.36	5,5,6,7	0
5	GOL	Q	1553	6/6	0.03	-1.59	6,7,8,8	0
4	F3S	A	1266	7/7	0.03	-2.26	4,4,5,5	0
3	SF4	B	1265	8/8	0.03	-2.28	5,5,5,5	0
3	SF4	A	1265	8/8	0.02	-2.33	5,5,5,6	0
3	SF4	A	1267	8/8	0.03	-2.34	4,4,4,4	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SF4	B	1267	8/8	0.03	-2.38	4,4,4,4	0
4	F3S	B	1266	7/7	0.03	-2.62	4,4,5,5	0
9	FCO	R	1550	7/7	0.04	-2.89	5,5,5,6	0
10	NI	Q	1551[B]	1/1	0.02	-3.30	7,7,7,7	1
10	NI	Q	1551[A]	1/1	0.02	-3.44	8,8,8,8	1
10	NI	R	1551[A]	1/1	0.02	-4.00	7,7,7,7	1
10	NI	R	1551[B]	1/1	0.02	-4.09	8,8,8,8	1
11	MG	Q	1552	1/1	0.02	-4.22	4,4,4,4	0

6.5 Other polymers ⓘ

There are no such residues in this entry.