



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:28 AM GMT

PDB ID : 3CUS
Title : Structure of a double ILE/PHE mutant of NI-FE hydrogenase refined at 2.2 angstrom resolution
Authors : Volbeda, A.
Deposited on : 2008-04-17
Resolution : 2.20 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>

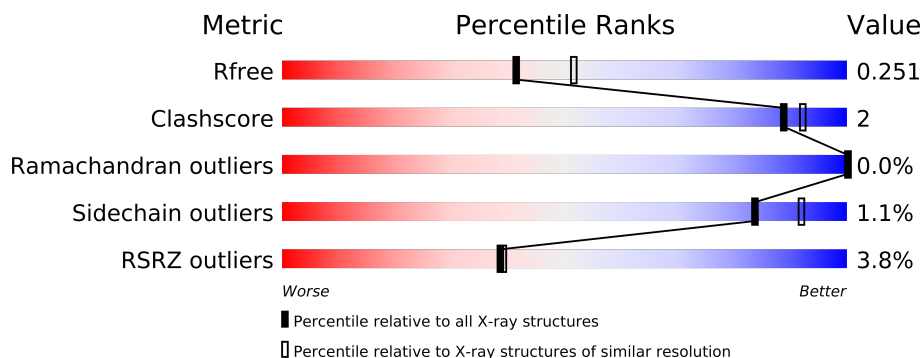
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	264	
1	B	264	
1	C	264	
2	Q	549	
2	R	549	
2	S	549	

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

Mol	Type	Chain	Res	Geometry	Electron density
8	GOL	Q	562	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19590 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 Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1973	1256	330	372	15			
1	B	262	Total	C	N	O	S	0	2	0
			1980	1260	330	375	15			
1	C	260	Total	C	N	O	S	0	1	0
			1965	1251	329	370	15			

- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	4	0
			4185	2668	724	770	23			
2	R	545	Total	C	N	O	S	0	1	0
			4178	2661	725	770	22			
2	S	544	Total	C	N	O	S	0	1	0
			4170	2657	724	767	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	74	ILE	VAL	ENGINEERED MUTATION	UNP P18188
Q	122	PHE	LEU	ENGINEERED MUTATION	UNP P18188
R	74	ILE	VAL	ENGINEERED MUTATION	UNP P18188
R	122	PHE	LEU	ENGINEERED MUTATION	UNP P18188
S	74	ILE	VAL	ENGINEERED MUTATION	UNP P18188
S	122	PHE	LEU	ENGINEERED MUTATION	UNP P18188

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	Ni	0	0
			1	1		

Continued on next page...

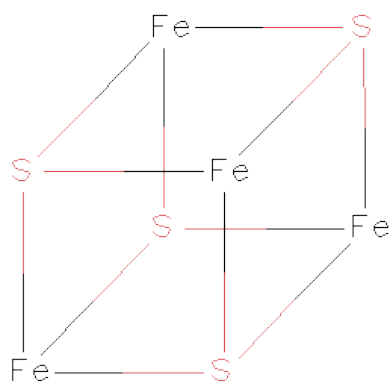
Continued from previous page...

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



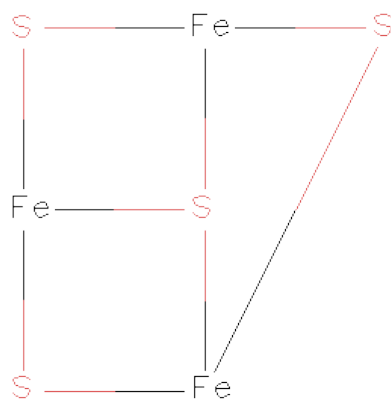
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

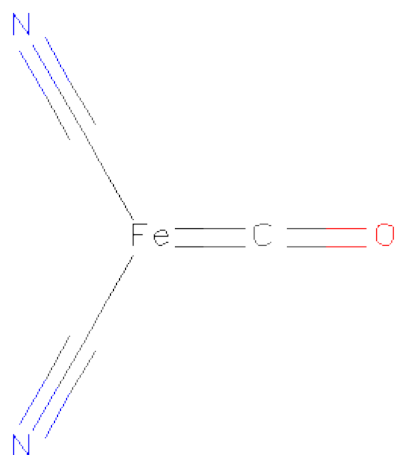
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	Fe	S	0	0
			8	4	4		
5	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



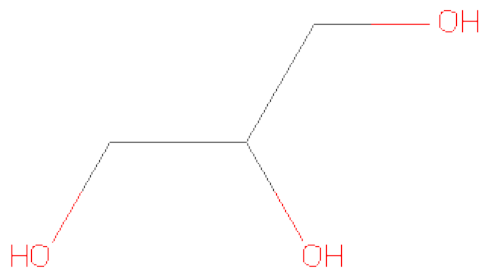
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			7	3	4		
6	B	1	Total	Fe	S	0	0
			7	3	4		
6	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is CARBONMONOXIDE-(DICYANO)IRON (three-letter code: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	134	Total	O	0	0
			134	134		
9	Q	245	Total	O	0	0
			245	245		
9	B	91	Total	O	0	0
			91	91		
9	R	215	Total	O	0	0
			215	215		
9	C	123	Total	O	0	0
			123	123		
9	S	205	Total	O	0	0
			205	205		

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.

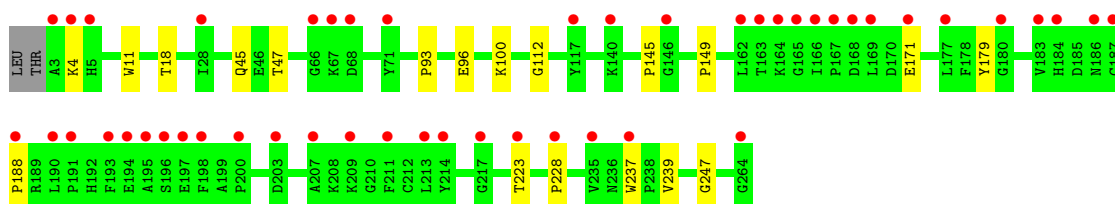
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain A: 



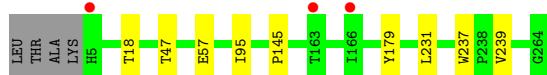
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain B: 



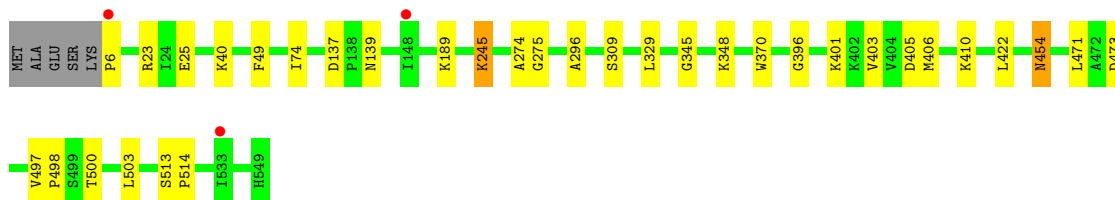
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain C: 



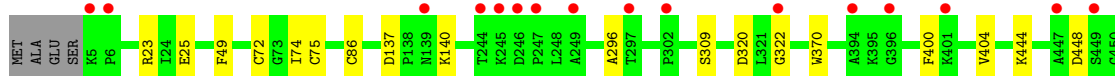
- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

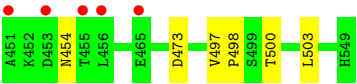
Chain Q: 



- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

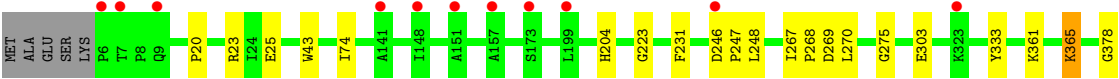
Chain R: 





● Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain S:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.40Å 99.96Å 182.69Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.20) 94.2 (19.99-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.222 0.217 , 0.251	Depositor DCC
R_{free} test set	5400 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.5	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 107158 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19590	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, NI, SF4, MG, F3S, 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	0.62	0/2027	0.60	0/2759
1	B	0.50	0/2043	0.55	0/2781
1	C	0.54	0/2025	0.59	0/2758
2	Q	0.61	0/4302	0.65	0/5835
2	R	0.56	0/4281	0.60	0/5809
2	S	0.55	1/4273 (0.0%)	0.62	0/5798
All	All	0.57	1/18951 (0.0%)	0.61	0/25740

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	303	GLU	CB-CG	-5.21	1.42	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1973	0	1911	11	0
1	B	1980	0	1918	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1965	0	1900	5	0
2	Q	4185	0	4161	23	0
2	R	4178	0	4142	15	0
2	S	4170	0	4138	22	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
5	A	16	0	0	0	0
5	B	16	0	0	0	0
5	C	16	0	0	0	0
6	A	7	0	0	0	0
6	B	7	0	0	0	0
6	C	7	0	0	0	0
7	Q	7	0	0	0	0
7	R	7	0	0	1	0
7	S	7	0	0	1	0
8	A	6	0	8	0	0
8	Q	12	0	16	0	0
8	R	6	0	8	0	0
8	S	6	0	8	0	0
9	A	134	0	0	3	0
9	B	91	0	0	1	0
9	C	123	0	0	5	0
9	Q	245	0	0	4	0
9	R	215	0	0	4	0
9	S	205	0	0	4	0
All	All	19590	0	18210	83	0

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 2.

The worst 5 of 83 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:322:GLY:HA3	9:R:721:HOH:O	1.71	0.89
9:C:341:HOH:O	2:S:361:LYS:HE3	1.81	0.81
1:C:57:GLU:HB2	9:C:390:HOH:O	1.84	0.78
2:S:385:PRO:HB2	9:S:614:HOH:O	1.86	0.75
1:A:215:GLU:HG3	9:A:373:HOH:O	1.88	0.72

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%)	254 (98%)	6 (2%)	0	100	100
1	B	262/264 (99%)	252 (96%)	10 (4%)	0	100	100
1	C	259/264 (98%)	252 (97%)	6 (2%)	1 (0%)	43	45
2	Q	545/549 (99%)	532 (98%)	13 (2%)	0	100	100
2	R	543/549 (99%)	529 (97%)	14 (3%)	0	100	100
2	S	542/549 (99%)	527 (97%)	15 (3%)	0	100	100
All	All	2411/2439 (99%)	2346 (97%)	64 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	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	208/210 (99%)	207 (100%)	1 (0%)	94	98
1	B	210/210 (100%)	207 (99%)	3 (1%)	78	88
1	C	208/210 (99%)	207 (100%)	1 (0%)	94	98
2	Q	438/438 (100%)	432 (99%)	6 (1%)	78	88
2	R	435/438 (99%)	430 (99%)	5 (1%)	84	92
2	S	434/438 (99%)	429 (99%)	5 (1%)	82	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1933/1944 (99%)	1912 (99%)	21 (1%)	84	92

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	171	GLU
2	R	454	ASN
2	S	452	LYS
1	B	100	LYS
2	S	454	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	14	ASN
2	S	454	ASN
2	R	454	ASN
1	A	61	HIS
1	C	14	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	CSO	Q	543	3,2	6,6,7	7.90	4 (66%)	3,6,8	4.01	1 (33%)
2	CSO	R	543	3,2	6,6,7	7.61	3 (50%)	3,6,8	4.30	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CSO	S	543	3,2	6,6,7	7.50	3 (50%)	3,6,8	5.25	1 (33%)

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	CSO	Q	543	3,2	-	0/2/5/7	0/0/0/0
2	CSO	R	543	3,2	-	0/2/5/7	0/0/0/0
2	CSO	S	543	3,2	-	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	Q	543	CSO	O-C	18.42	1.24	1.11
2	S	543	CSO	O-C	17.64	1.23	1.11
2	R	543	CSO	O-C	17.55	1.23	1.11
2	R	543	CSO	OD-SG	4.54	1.81	1.62
2	R	543	CSO	CA-C	3.80	1.55	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	543	CSO	C-CA-N	-8.97	104.87	113.83
2	R	543	CSO	C-CA-N	-7.37	106.47	113.83
2	Q	543	CSO	C-CA-N	-6.67	107.17	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 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\# Z > 2$
5	SF4	A	265	1	12,12,12	5.74	9 (75%)	0,24,24	0.00	-
6	F3S	A	266	1	3,9,9	14.44	3 (100%)	0,15,15	0.00	-
5	SF4	A	267	1	12,12,12	5.23	7 (58%)	0,24,24	0.00	-
8	GOL	A	271	-	5,5,5	0.31	0	5,5,5	0.21	0
5	SF4	B	265	1	12,12,12	3.82	8 (66%)	0,24,24	0.00	-
6	F3S	B	266	1	3,9,9	17.16	3 (100%)	0,15,15	0.00	-
5	SF4	B	267	1	12,12,12	4.18	8 (66%)	0,24,24	0.00	-
5	SF4	C	265	1	12,12,12	6.06	11 (91%)	0,24,24	0.00	-
6	F3S	C	266	1	3,9,9	15.27	3 (100%)	0,15,15	0.00	-
5	SF4	C	267	1	12,12,12	5.07	8 (66%)	0,24,24	0.00	-
7	FCO	Q	550	2	2,6,6	0.19	0	0,6,6	0.00	-
8	GOL	Q	561	-	5,5,5	0.46	0	5,5,5	0.20	0
8	GOL	Q	562	-	5,5,5	0.42	0	5,5,5	0.55	0
7	FCO	R	550	2	2,6,6	0.20	0	0,6,6	0.00	-
8	GOL	R	563	-	5,5,5	0.36	0	5,5,5	0.36	0
7	FCO	S	550	2	2,6,6	0.02	0	0,6,6	0.00	-
8	GOL	S	561	-	5,5,5	0.29	0	5,5,5	0.51	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
5	SF4	A	265	1	-	0/0/48/48	0/0/5/5
6	F3S	A	266	1	-	0/0/24/24	0/0/3/3
5	SF4	A	267	1	-	0/0/48/48	0/0/5/5
8	GOL	A	271	-	-	0/4/4/4	0/0/0/0
5	SF4	B	265	1	-	0/0/48/48	0/0/5/5
6	F3S	B	266	1	-	0/0/24/24	0/0/3/3
5	SF4	B	267	1	-	0/0/48/48	0/0/5/5
5	SF4	C	265	1	-	0/0/48/48	0/0/5/5
6	F3S	C	266	1	-	0/0/24/24	0/0/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	C	267	1	-	0/0/48/48	0/0/5/5
7	FCO	Q	550	2	-	0/0/6/6	0/0/0/0
8	GOL	Q	561	-	-	0/4/4/4	0/0/0/0
8	GOL	Q	562	-	-	0/4/4/4	0/0/0/0
7	FCO	R	550	2	-	0/0/6/6	0/0/0/0
8	GOL	R	563	-	-	0/4/4/4	0/0/0/0
7	FCO	S	550	2	-	0/0/6/6	0/0/0/0
8	GOL	S	561	-	-	0/4/4/4	0/0/0/0

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	266	F3S	S3-FE4	-19.69	2.20	2.33
6	B	266	F3S	S3-FE1	-17.82	2.21	2.33
6	C	266	F3S	S3-FE4	-16.98	2.21	2.33
6	A	266	F3S	S3-FE4	-16.85	2.21	2.33
6	A	266	F3S	S3-FE1	-14.98	2.23	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	262/264 (99%)	0.15	6 (2%) 57 58	13, 15, 17, 26	8 (3%)
1	B	262/264 (99%)	0.95	48 (18%) 2 2	13, 15, 17, 23	9 (3%)
1	C	260/264 (98%)	0.03	3 (1%) 75 76	13, 15, 17, 21	5 (1%)
2	Q	544/549 (99%)	0.06	3 (0%) 86 88	12, 14, 17, 23	12 (2%)
2	R	545/549 (99%)	0.33	21 (3%) 37 38	12, 15, 18, 22	13 (2%)
2	S	544/549 (99%)	0.17	12 (2%) 59 59	12, 15, 17, 22	15 (2%)
All	All	2417/2439 (99%)	0.25	93 (3%) 38 39	12, 15, 17, 26	62 (2%)

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	PHE	4.6
1	B	228	PRO	4.6
1	C	5	HIS	4.4
1	B	183	VAL	4.3
1	B	3	ALA	4.3

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, 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	CSO	S	543	7/8	0.11	-0.91	14,14,15,16	0
2	CSO	R	543	7/8	0.11	-1.14	14,14,14,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CSO	Q	543	7/8	0.12	-1.40	14,14,16,16	0

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
8	GOL	Q	562	6/6	0.18	2.93	13,16,16,16	0
8	GOL	A	271	6/6	0.17	1.38	18,20,20,21	0
8	GOL	S	561	6/6	0.14	0.43	13,14,14,15	0
8	GOL	R	563	6/6	0.18	-0.01	16,18,19,19	0
7	FCO	S	550	7/7	0.12	-0.48	14,14,14,15	0
8	GOL	Q	561	6/6	0.11	-0.53	10,11,12,12	0
5	SF4	A	265	8/8	0.13	-0.62	12,13,13,14	0
5	SF4	A	267	8/8	0.14	-0.63	12,13,14,15	0
4	MG	Q	553	1/1	0.13	-0.72	13,13,13,13	0
5	SF4	C	265	8/8	0.11	-0.79	12,13,14,14	0
7	FCO	Q	550	7/7	0.13	-0.97	13,14,15,15	0
3	NI	S	551	1/1	0.10	-1.18	14,14,14,14	0
7	FCO	R	550	7/7	0.10	-1.30	13,13,14,14	0
6	F3S	A	266	7/7	0.13	-1.34	13,14,14,14	0
6	F3S	C	266	7/7	0.11	-1.36	13,14,14,15	0
5	SF4	C	267	8/8	0.11	-1.36	13,14,14,15	0
6	F3S	B	266	7/7	0.10	-1.49	13,14,15,15	0
4	MG	S	553	1/1	0.12	-1.69	13,13,13,13	0
4	MG	R	553	1/1	0.08	-1.87	13,13,13,13	0
5	SF4	B	265	8/8	0.11	-1.91	14,14,15,16	0
5	SF4	B	267	8/8	0.07	-2.26	13,14,15,15	0
3	NI	Q	551	1/1	0.10	-3.72	15,15,15,15	0
3	NI	R	551	1/1	0.04	-5.16	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.