



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2017 – 03:23 PM EDT

PDB ID : 4UDY  
Title : NCO- bound to cluster C of Ni,Fe-CO dehydrogenase at true-atomic resolution  
Authors : Fessler, J.; Jeoung, J.-H.; Dobbek, H.  
Deposited on : 2014-12-12  
Resolution : 1.09 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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029077

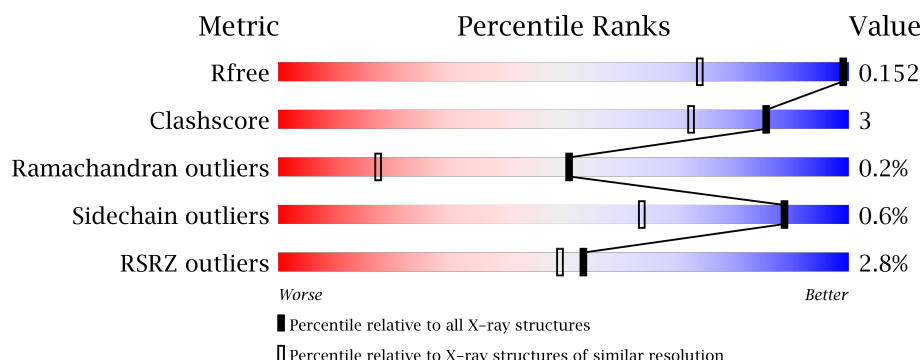
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.09 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))
$R_{free}$	100719	1192 (1.14-1.06)
Clashscore	112137	1244 (1.14-1.06)
Ramachandran outliers	110173	1198 (1.14-1.06)
Sidechain outliers	110143	1196 (1.14-1.06)
RSRZ outliers	101464	1197 (1.14-1.06)

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	X	636	

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
6	0NM	X	1005	-	-	-	X

## 2 Entry composition [i](#)

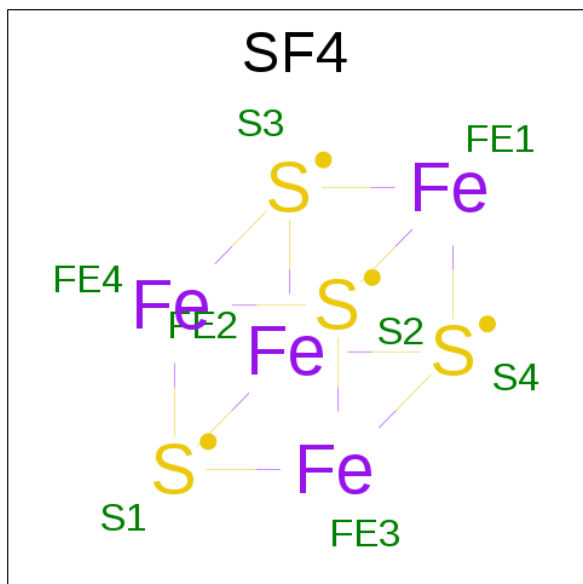
There are 7 unique types of molecules in this entry. The entry contains 10457 atoms, of which 4889 are hydrogens and 0 are deuteriums.

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 CARBON MONOXIDE DEHYDROGENASE 2.

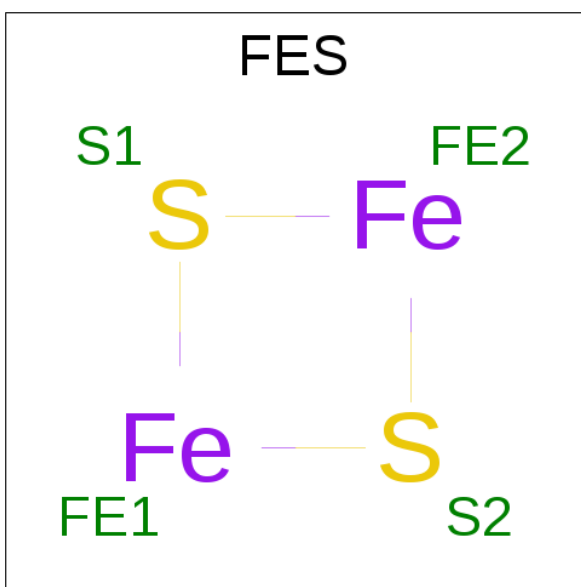
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	X	633	9674	2999	4889	843	903	40	0	26	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



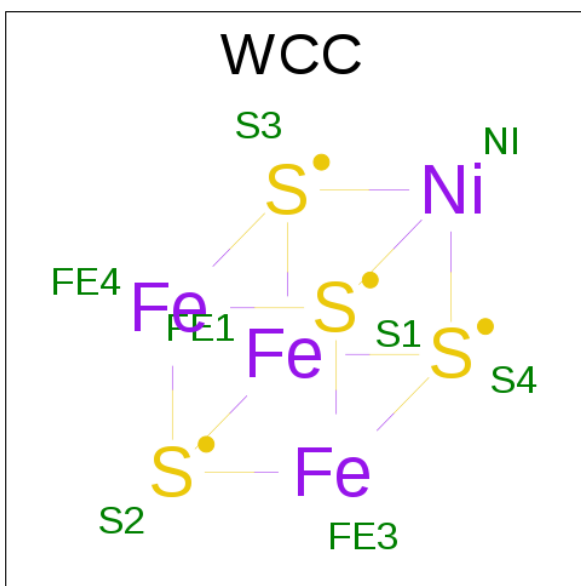
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	X	1	8	4	4	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FE(3)-NI(1)-S(4) CLUSTER (three-letter code: WCC) (formula:  $\text{Fe}_3\text{NiS}_4$ ).

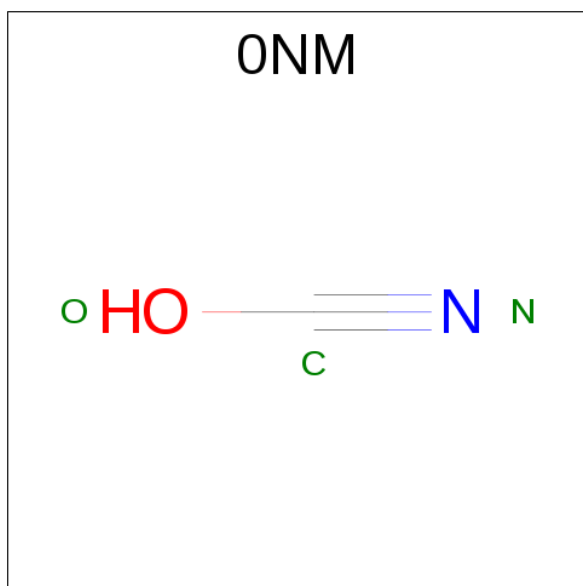


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	X	1	Total	Fe	Ni	S	0	0
			8	3	1	4		

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	1	Total	Fe	0	1
			2	2		

- Molecule 6 is cyanic acid (three-letter code: 0NM) (formula: CHNO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	X	1	Total	C	N	O	0	0
			3	1	1	1		

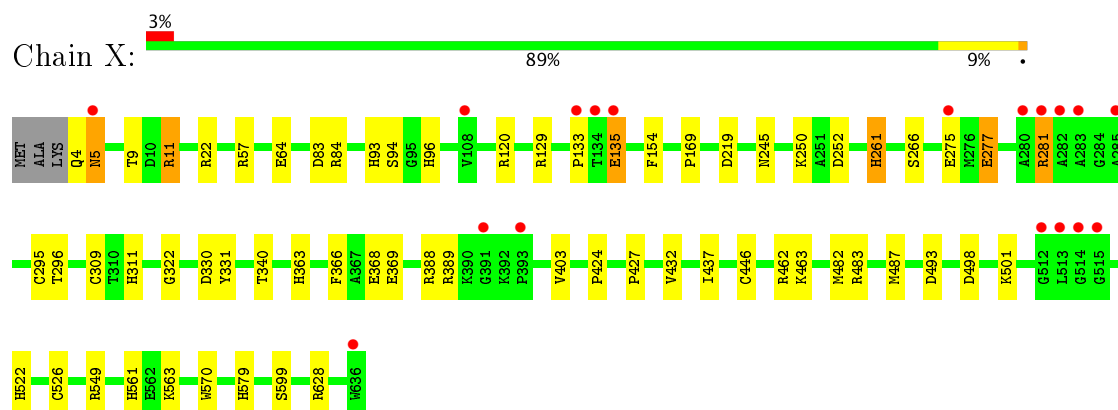
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	X	758	Total	O	0	0
			758	758		

### 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 the various outlier classes 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 ( $\text{RSRZ} > 2$ ). 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: CARBON MONOXIDE DEHYDROGENASE 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.18Å 75.01Å 71.15Å 90.00° 111.22° 90.00°	Depositor
Resolution (Å)	33.16 – 1.09 34.15 – 1.09	Depositor EDS
% Data completeness (in resolution range)	98.0 (33.16-1.09) 98.0 (34.15-1.09)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 1.09Å)	Xtriage
Refinement program	SHELXL	Depositor
R, $R_{free}$	0.136 , 0.165 0.130 , 0.152	Depositor DCC
$R_{free}$ test set	11175 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 72.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.99	EDS
Total number of atoms	10457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0NM, SF4, FE2, WCC, FES

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	X	0.74	4/4919 (0.1%)	1.26	48/6680 (0.7%)

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	X	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	309	CYS	CB-SG	-6.61	1.71	1.82
1	X	599[A]	SER	CB-OG	-6.04	1.34	1.42
1	X	599[B]	SER	CB-OG	-6.04	1.34	1.42
1	X	628	ARG	CZ-NH1	5.74	1.40	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	483	ARG	NE-CZ-NH1	-11.61	114.49	120.30
1	X	11	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	X	628	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	X	120	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	X	483	ARG	CD-NE-CZ	10.10	137.74	123.60
1	X	388	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	X	462	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	X	281	ARG	NE-CZ-NH2	9.30	124.95	120.30
1	X	252	ASP	CB-CG-OD1	8.93	126.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	11	ARG	CD-NE-CZ	8.65	135.71	123.60
1	X	363	HIS	CG-ND1-CE1	8.54	120.15	108.20
1	X	275	GLU	CA-CB-CG	8.41	131.90	113.40
1	X	129	ARG	CD-NE-CZ	8.37	135.32	123.60
1	X	330	ASP	CB-CG-OD1	7.90	125.41	118.30
1	X	366	PHE	CB-CG-CD1	7.82	126.28	120.80
1	X	579	HIS	CG-ND1-CE1	7.74	119.04	108.20
1	X	498	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	X	549	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	X	462	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	X	322	GLY	O-C-N	-7.13	111.29	122.70
1	X	261	HIS	CA-CB-CG	-6.90	101.87	113.60
1	X	570	TRP	CA-CB-CG	6.72	126.47	113.70
1	X	628	ARG	CD-NE-CZ	6.57	132.79	123.60
1	X	389	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	X	154	PHE	CZ-CE2-CD2	6.54	127.95	120.10
1	X	22	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	X	11	ARG	NH1-CZ-NH2	-6.12	112.66	119.40
1	X	561	HIS	CG-ND1-CE1	5.95	116.53	108.20
1	X	322	GLY	C-N-CA	5.91	136.47	121.70
1	X	135	GLU	CB-CG-CD	5.88	130.08	114.20
1	X	84	ARG	CD-NE-CZ	5.84	131.77	123.60
1	X	368[A]	GLU	CA-CB-CG	5.81	126.18	113.40
1	X	368[B]	GLU	CA-CB-CG	5.81	126.18	113.40
1	X	120	ARG	CD-NE-CZ	5.77	131.68	123.60
1	X	57	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	X	493	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	X	369	GLU	OE1-CD-OE2	-5.66	116.50	123.30
1	X	331	TYR	CB-CG-CD1	5.64	124.38	121.00
1	X	389	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	X	311	HIS	CG-ND1-CE1	5.57	116.00	108.20
1	X	366	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	X	5[A]	ASN	CA-CB-CG	5.38	125.23	113.40
1	X	5[B]	ASN	CA-CB-CG	5.38	125.23	113.40
1	X	628	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	X	483	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	X	9	THR	O-C-N	-5.19	114.40	122.70
1	X	363	HIS	ND1-CG-CD2	-5.17	98.77	106.00
1	X	83	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	446	CYS	Peptide

## 5.2 Too-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 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	X	4785	4889	4914	25	0
2	X	8	0	0	0	0
3	X	4	0	0	0	0
4	X	8	0	0	0	0
5	X	2	0	0	0	0
6	X	3	0	0	1	0
7	X	758	0	0	10	0
All	All	5568	4889	4914	25	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 (25) 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:X:463:LYS:HD3	7:X:2736:HOH:O	1.98	0.64
1:X:94[B]:SER:HB3	7:X:2240:HOH:O	1.98	0.62
1:X:277:GLU:O	1:X:281:ARG:HG3	2.00	0.62
1:X:169:PRO:HB2	7:X:2377:HOH:O	2.01	0.59
1:X:403:VAL:HG11	1:X:482[B]:MET:SD	2.44	0.57
1:X:526:CYS:CB	6:X:1005:0NM:C	2.85	0.54
1:X:501:LYS:HE2	7:X:2664:HOH:O	2.11	0.51
1:X:340[B]:THR:HG23	7:X:2515:HOH:O	2.13	0.49
1:X:482[B]:MET:CG	1:X:487[B]:MET:SD	3.01	0.48
1:X:4:GLN:N	7:X:2001:HOH:O	2.46	0.48
1:X:93[B]:HIS:CE1	1:X:563:LYS:HB3	2.50	0.47
1:X:250:LYS:HE3	7:X:2461:HOH:O	2.13	0.47
1:X:133:PRO:HB3	1:X:135:GLU:OE2	2.14	0.47
1:X:482[B]:MET:HG2	1:X:487[B]:MET:SD	2.55	0.46
1:X:261:HIS:N	1:X:296[B]:THR:OG1	2.48	0.46
1:X:261:HIS:CD2	1:X:295[A]:CYS:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:432:VAL:HA	1:X:437:ILE:O	2.17	0.44
1:X:482[B]:MET:HG3	1:X:487[B]:MET:SD	2.57	0.44
1:X:266:SER:HB3	1:X:296[B]:THR:HG23	2.00	0.44
1:X:93[B]:HIS:ND1	1:X:219:ASP:OD1	2.51	0.43
1:X:64[A]:GLU:HG3	7:X:2205:HOH:O	2.20	0.42
1:X:93[B]:HIS:O	1:X:96:HIS:HB3	2.19	0.41
1:X:11:ARG:NH2	7:X:2034:HOH:O	2.49	0.41
1:X:424:PRO:O	1:X:427:PRO:HD2	2.21	0.41
1:X:94[B]:SER:CB	7:X:2240:HOH:O	2.65	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	X	657/636 (103%)	634 (96%)	22 (3%)	1 (0%)	51 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	245	ASN

### 5.3.2 Protein sidechains [i](#)

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	X	520/498 (104%)	516 (99%)	4 (1%)	85 54

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

Mol	Chain	Res	Type
1	X	5[A]	ASN
1	X	5[B]	ASN
1	X	277	GLU
1	X	522	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
2	SF4	X	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FES	X	1002	1	0,4,4	0.00	-	0,4,4	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	WCC	X	1003	1,5,6	0,12,12	0.00	-	0,24,24	0.00	-
6	0NM	X	1005	5,4	1,2,2	3.33	1 (100%)	0,1,1	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
2	SF4	X	1001	1	-	0/0/48/48	0/6/5/5
3	FES	X	1002	1	-	0/0/4/4	0/1/1/1
4	WCC	X	1003	1,5,6	-	0/0/48/48	0/6/5/5
6	0NM	X	1005	5,4	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	1005	0NM	C-N	3.33	1.40	1.16

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	1005	0NM	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	X	633/636 (99%)	-0.27	18 (2%) 53 49	6, 11, 30, 57	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	513	LEU	7.0
1	X	514	GLY	3.7
1	X	515	GLY	3.5
1	X	283	ALA	3.0
1	X	280	ALA	2.8
1	X	5[A]	ASN	2.8
1	X	281	ARG	2.7
1	X	285	ALA	2.6
1	X	135	GLU	2.5
1	X	512	GLY	2.4
1	X	275	GLU	2.4
1	X	391	GLY	2.3
1	X	393	PRO	2.3
1	X	133	PRO	2.1
1	X	282	ALA	2.1
1	X	636	TRP	2.0
1	X	134	THR	2.0
1	X	108	VAL	2.0

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

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

### 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, 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( $\text{\AA}^2$ )	Q<0.9
6	0NM	X	1005	3/3	0.99	0.16	7.89	7,7,7,8	3
4	WCC	X	1003	8/8	1.00	0.07	0.73	6,7,8,9	8
2	SF4	X	1001	8/8	1.00	0.05	0.27	5,6,6,6	0
3	FES	X	1002	4/4	1.00	0.05	-0.08	6,6,7,7	0
5	FE2	X	1004[B]	1/1	1.00	0.06	-1.17	8,8,8,8	1
5	FE2	X	1004[A]	1/1	1.00	0.06	-1.53	21,21,21,21	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.