Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 08:37 am BST

PDB ID	:	4UDY / pdb_00004udy
Title	:	NCO- bound to cluster C of Ni,Fe-CO dehydrogenase at true-atomic resolution
Authors	:	Fesseler, 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

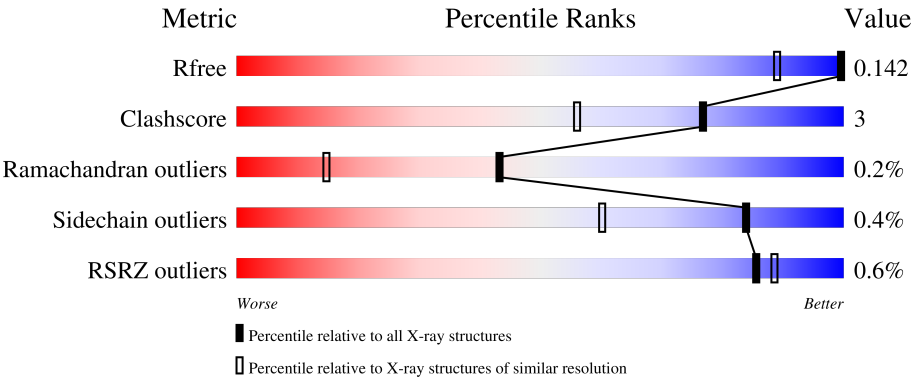
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	% 89% 9% .

2 Entry composition

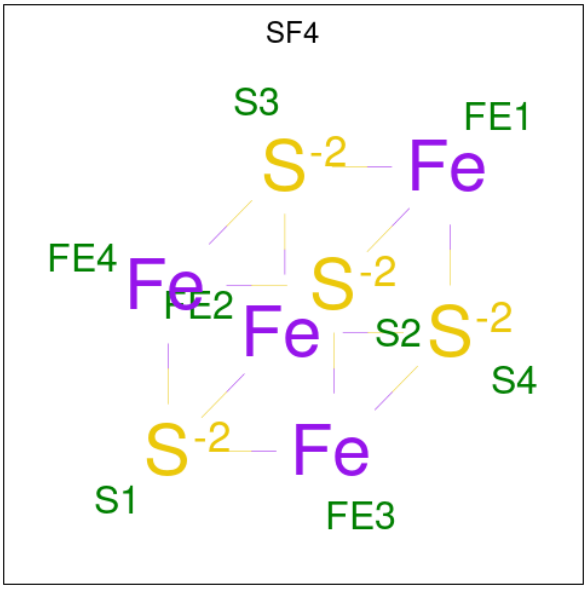
There are 6 unique types of molecules in this entry. The entry contains 10457 atoms, of which 4889 are hydrogens and 0 are deuteriums.

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.

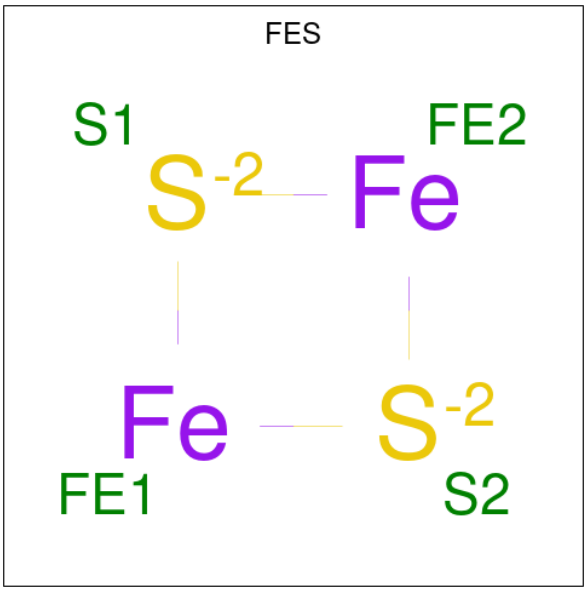
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	X	633	9674	2999	4889	843	903	40	0	26	0

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



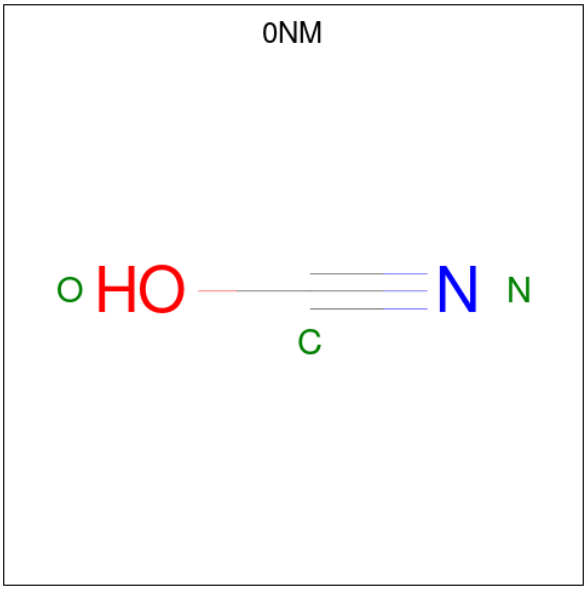
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	X	1	8	4	4	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



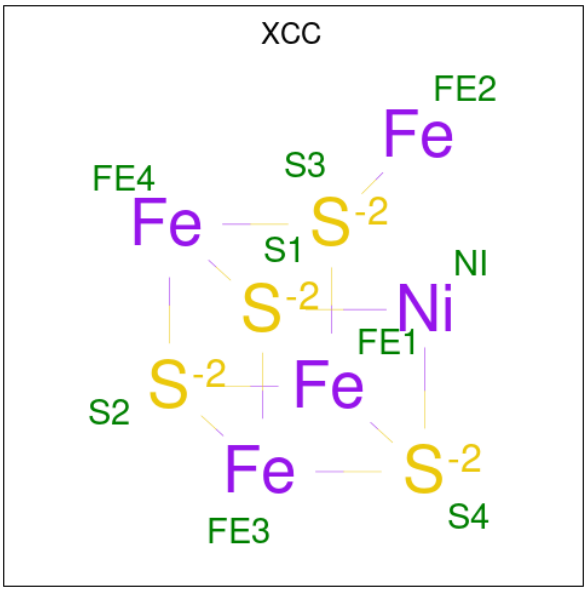
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	1	Total Fe S 4 2 2	0	0

- Molecule 4 is cyanic acid (CCD ID: 0NM) (formula: CHNO).



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

- Molecule 5 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe_4NiS_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	X	1	Total	Fe	Ni	S	0	1
			10	5	1	4		

- Molecule 6 is water.

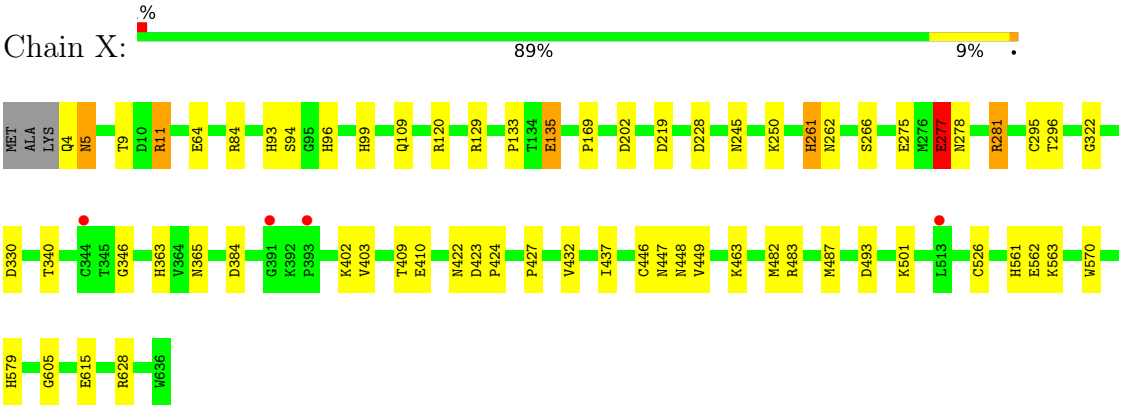
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	X	758	Total	O	0	0
			758	758		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (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

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.18Å 75.01Å 71.15Å 90.00° 111.22° 90.00°	Depositor
Resolution (Å)	33.16 – 1.09 33.16 – 1.09	Depositor EDS
% Data completeness (in resolution range)	98.0 (33.16-1.09) 98.0 (33.16-1.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 1.09Å)	Xtriage
Refinement program	SHELXL 14	Depositor
R, R_{free}	0.136 , 0.165 0.116 , 0.142	Depositor DCC
R_{free} test set	11175 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	9.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, XCC, FES, SF4

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	0.92	5/4919 (0.1%)	1.41	63/6680 (0.9%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	363	HIS	ND1-CE1	-7.49	1.25	1.32
1	X	579	HIS	CG-ND1	-7.23	1.30	1.38
1	X	561	HIS	ND1-CE1	-5.95	1.26	1.32
1	X	628	ARG	CZ-NH1	5.55	1.40	1.32
1	X	449	VAL	N-CA	-5.17	1.39	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	261	HIS	CA-CB-CG	-11.93	101.87	113.80
1	X	135	GLU	CB-CG-CD	10.28	130.08	112.60
1	X	483	ARG	CD-NE-CZ	9.53	137.74	124.40
1	X	322	GLY	CA-C-N	9.02	136.47	122.49
1	X	322	GLY	C-N-CA	9.02	136.47	122.49
1	X	275	GLU	CA-CB-CG	8.90	131.90	114.10
1	X	322	GLY	O-C-N	-8.77	111.29	122.43
1	X	363	HIS	ND1-CE1-NE2	-8.50	99.90	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	384	ASP	CA-CB-CG	8.35	120.95	112.60
1	X	11	ARG	CD-NE-CZ	8.08	135.71	124.40
1	X	9	THR	CA-C-N	8.04	133.97	121.99
1	X	9	THR	C-N-CA	8.04	133.97	121.99
1	X	129	ARG	CD-NE-CZ	7.80	135.32	124.40
1	X	363	HIS	ND1-CG-CD2	-7.33	98.77	106.10
1	X	483	ARG	NE-CZ-NH1	-7.01	114.49	121.50
1	X	570	TRP	CA-CB-CG	6.77	126.47	113.60
1	X	605	GLY	CA-C-N	6.69	130.93	121.30
1	X	605	GLY	C-N-CA	6.69	130.93	121.30
1	X	410	GLU	CA-C-N	6.44	129.43	120.29
1	X	410	GLU	C-N-CA	6.44	129.43	120.29
1	X	562	GLU	CA-C-N	6.40	128.85	120.28
1	X	562	GLU	C-N-CA	6.40	128.85	120.28
1	X	281	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	X	363	HIS	CG-ND1-CE1	6.38	120.15	109.30
1	X	5[A]	ASN	CA-CB-CG	-6.34	106.26	112.60
1	X	5[B]	ASN	CA-CB-CG	-6.34	106.26	112.60
1	X	330	ASP	CA-CB-CG	6.26	118.86	112.60
1	X	99[A]	HIS	CA-CB-CG	-6.17	107.62	113.80
1	X	99[B]	HIS	CA-CB-CG	-6.17	107.62	113.80
1	X	448	ASN	CA-C-N	6.04	130.94	120.86
1	X	448	ASN	C-N-CA	6.04	130.94	120.86
1	X	628	ARG	CD-NE-CZ	5.99	132.79	124.40
1	X	278	ASN	CA-C-O	5.83	126.67	119.79
1	X	409	THR	CA-CB-OG1	-5.79	100.92	109.60
1	X	9	THR	O-C-N	-5.78	114.40	122.37
1	X	579	HIS	CG-ND1-CE1	5.73	119.04	109.30
1	X	277	GLU	CB-CG-CD	-5.61	103.06	112.60
1	X	262[A]	ASN	N-CA-C	5.60	116.72	109.72
1	X	262[B]	ASN	N-CA-C	5.60	116.72	109.72
1	X	322	GLY	CA-C-O	5.57	125.29	119.06
1	X	561	HIS	ND1-CG-CD2	-5.50	100.59	106.10
1	X	365[A]	ASN	CA-CB-CG	-5.48	107.12	112.60
1	X	365[B]	ASN	CA-CB-CG	-5.48	107.12	112.60
1	X	423	ASP	CA-CB-CG	5.46	118.06	112.60
1	X	579	HIS	ND1-CE1-NE2	-5.46	102.94	108.40
1	X	363	HIS	CE1-NE2-CD2	5.44	114.44	109.00
1	X	228	ASP	CA-CB-CG	5.35	117.95	112.60
1	X	410	GLU	O-C-N	-5.33	116.47	122.12
1	X	363	HIS	CB-CG-ND1	5.29	130.63	122.70
1	X	493	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	605	GLY	O-C-N	-5.27	115.98	122.46
1	X	84	ARG	CD-NE-CZ	5.26	131.77	124.40
1	X	129	ARG	O-C-N	5.24	128.35	122.22
1	X	615	GLU	CB-CG-CD	5.24	121.50	112.60
1	X	346	GLY	CA-C-N	5.22	128.29	120.87
1	X	346	GLY	C-N-CA	5.22	128.29	120.87
1	X	120	ARG	CD-NE-CZ	5.20	131.68	124.40
1	X	11	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
1	X	109	GLN	OE1-CD-NE2	5.09	127.69	122.60
1	X	447	ASN	CA-CB-CG	5.09	117.69	112.60
1	X	562	GLU	O-C-N	-5.04	116.46	122.20
1	X	202	ASP	CA-CB-CG	5.03	117.63	112.60
1	X	422	ASN	CA-CB-CG	-5.02	107.58	112.60

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 (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	X	4785	4889	4914	28	0
2	X	8	0	0	0	0
3	X	4	0	0	0	0
4	X	3	0	0	1	0
5	X	10	0	0	0	0
6	X	758	0	0	12	0
All	All	5568	4889	4914	28	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 (28) 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	6:X:2736:HOH:O	1.98	0.64
1:X:94[B]:SER:HB3	6: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	6: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	4:X:1005:0NM:C	2.85	0.54
1:X:501:LYS:HE2	6:X:2664:HOH:O	2.11	0.51
1:X:340[B]:THR:HG23	6: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	6: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	6: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:482[B]:MET:HE1	6:X:2497:HOH:O	2.17	0.45
1:X:261:HIS:CD2	1:X:295[A]:CYS:HB2	2.52	0.44
1:X:402:LYS:NZ	6:X:2585:HOH:O	2.50	0.44
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:135:GLU:CD	1:X:135:GLU:H	2.27	0.43
1:X:64[A]:GLU:HG3	6: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	6: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	6: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%)	43 15

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%)	517 (99%)	3 (1%)	78 49

All (3) 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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	431	ASN
1	X	436	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands 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	$\#\|Z\| > 2$
3	FES	X	1002	1	0,4,4	-	-	-		
5	XCC	X	1006[A]	1,4	0,12,12	-	-	-		
2	SF4	X	1001	1	0,12,12	-	-	-		
4	0NM	X	1005	5	1,2,2	3.72	1 (100%)	0,1,1	-	-
5	XCC	X	1006[B]	1,4	0,12,12	-	-	-		

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	-	-	0/6/5/5
3	FES	X	1002	1	-	-	0/1/1/1
5	XCC	X	1006[B]	1,4	-	-	0/4/4/4
5	XCC	X	1006[A]	1,4	-	-	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	1005	0NM	C-N	3.72	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
4	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, 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	X	633/636 (99%)	-0.55	4 (0%)	85	88	4, 13, 35, 64	26 (4%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	513	LEU	3.0
1	X	393	PRO	2.3
1	X	391	GLY	2.1
1	X	344	CYS	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

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	0NM	X	1005	3/3	0.99	0.04	7,7,7,8	3
3	FES	X	1002	4/4	1.00	0.01	6,6,7,7	0
2	SF4	X	1001	8/8	1.00	0.01	5,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	XCC	X	1006[A]	9/9	1.00	0.02	6,7,9,21	9
5	XCC	X	1006[B]	9/9	1.00	0.02	6,7,8,9	9

6.5 Other polymers (i)

There are no such residues in this entry.