



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:14 AM UTC

PDB ID : 4UDX / pdb_00004udx
Title : CO2 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 : 1.03 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

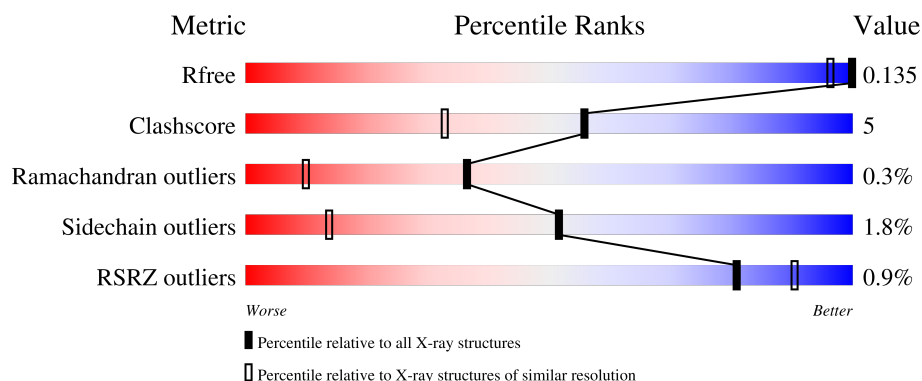
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.03 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	1036 (1.06-1.02)
Clashscore	190562	1063 (1.06-1.02)
Ramachandran outliers	187476	1034 (1.06-1.02)
Sidechain outliers	187428	1035 (1.06-1.02)
RSRZ outliers	180081	1035 (1.06-1.02)

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 $\leq 5\%$. 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	% 87% 10% .

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	CO2	X	1005	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10301 atoms, of which 4742 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	9497	2984	4742	835	894	42	0	22	0

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



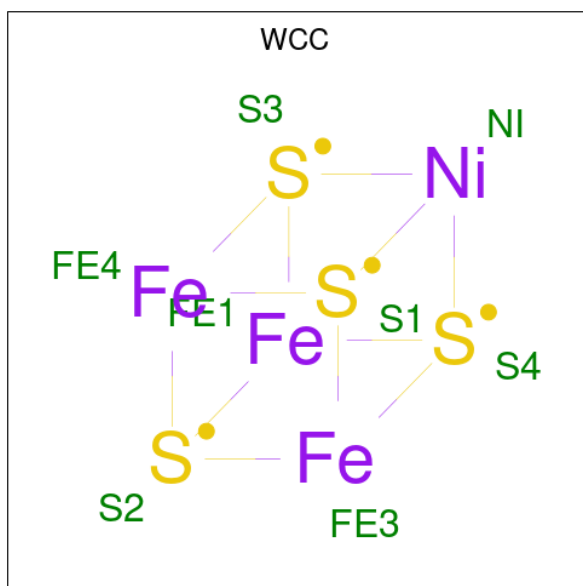
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	X	1	8	4	4	0	0

- 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	0	0
			4	2	2		

- Molecule 4 is FE(3)-NI(1)-S(4) CLUSTER (CCD ID: WCC) (formula: Fe_3NiS_4).

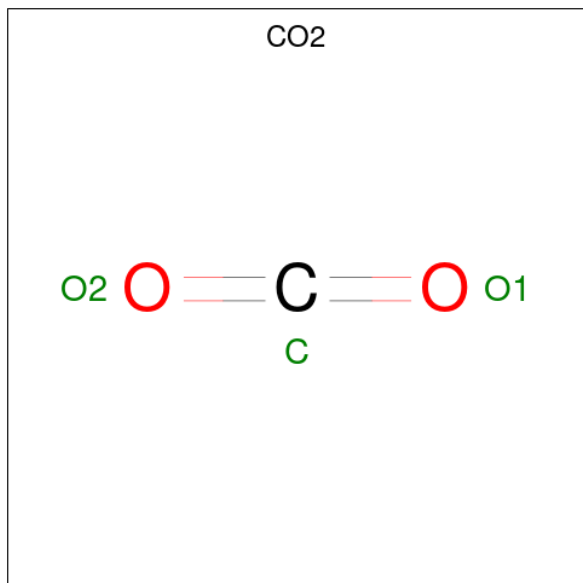


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	X	1	Total	Fe	Ni	S	0	0
			8	3	1	4		

- Molecule 5 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 6 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	X	1	Total	C	O	0	0
			3	1	2		

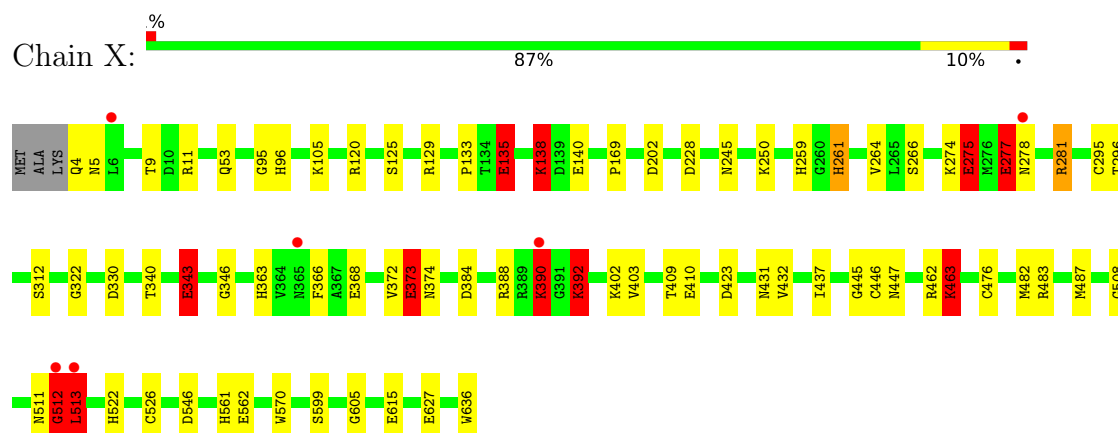
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	X	779	Total	O	0	0
			779	779		

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.52Å 74.87Å 71.08Å 90.00° 111.26° 90.00°	Depositor
Resolution (Å)	50.00 – 1.03 50.00 – 1.03	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-1.03) 98.0 (50.00-1.03)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.03Å)	Xtriage
Refinement program	SHELXL 14	Depositor
R, R_{free}	0.132 , 0.157 0.113 , 0.135	Depositor DCC
R_{free} test set	13236 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	9.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.99	EDS
Total number of atoms	10301	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 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: WCC, FES, SF4, FE2, CO2

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	2.44	21/4891 (0.4%)	1.77	87/6643 (1.3%)

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	7

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	281	ARG	CZ-NH2	64.52	2.17	1.33
1	X	512	GLY	C-O	55.82	1.99	1.23
1	X	281	ARG	CZ-NH1	52.48	2.06	1.32
1	X	513	LEU	CA-CB	51.18	2.40	1.53
1	X	275	GLU	CD-OE2	40.92	2.03	1.25
1	X	135	GLU	CD-OE1	40.89	2.03	1.25
1	X	275	GLU	CD-OE1	40.80	2.02	1.25
1	X	343	GLU	CD-OE1	40.66	2.02	1.25
1	X	373	GLU	CG-CD	35.01	2.39	1.52
1	X	390	LYS	CD-CE	29.72	2.41	1.52
1	X	392	LYS	CD-CE	29.55	2.41	1.52
1	X	138	LYS	CD-CE	29.44	2.40	1.52
1	X	463	LYS	CE-NZ	25.41	2.25	1.49
1	X	138	LYS	CE-NZ	25.09	2.24	1.49
1	X	281	ARG	NE-CZ	-18.11	1.13	1.33
1	X	512	GLY	C-N	-7.94	1.22	1.33
1	X	561	HIS	ND1-CE1	-6.99	1.25	1.32
1	X	483	ARG	NE-CZ	-5.40	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	259	HIS	C-N	-5.38	1.29	1.33
1	X	363	HIS	ND1-CE1	-5.36	1.27	1.32
1	X	95	GLY	CA-C	5.10	1.57	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	281	ARG	NE-CZ-NH1	55.75	177.25	121.50
1	X	281	ARG	NH1-CZ-NH2	-33.10	76.27	119.30
1	X	275	GLU	OE1-CD-OE2	-22.70	68.42	122.90
1	X	281	ARG	NE-CZ-NH2	-20.23	100.99	119.20
1	X	512	GLY	O-C-N	-18.40	98.78	122.70
1	X	343	GLU	OE1-CD-OE2	-16.12	84.21	122.90
1	X	135	GLU	OE1-CD-OE2	-16.03	84.43	122.90
1	X	392	LYS	CA-CB-CG	14.24	142.57	114.10
1	X	281	ARG	CD-NE-CZ	13.82	143.74	124.40
1	X	374	ASN	OD1-CG-ND2	-12.21	110.39	122.60
1	X	373	GLU	CG-CD-OE1	-11.77	91.32	118.40
1	X	373	GLU	CG-CD-OE2	-11.63	91.65	118.40
1	X	105	LYS	CG-CD-CE	11.08	136.79	111.30
1	X	261	HIS	CA-CB-CG	-10.99	102.81	113.80
1	X	138	LYS	CD-CE-NZ	-10.78	77.41	111.90
1	X	322	GLY	CA-C-N	10.13	138.36	122.26
1	X	322	GLY	C-N-CA	10.13	138.36	122.26
1	X	512	GLY	CA-C-O	-9.92	103.31	120.57
1	X	513	LEU	CA-C-N	9.73	140.47	121.41
1	X	513	LEU	C-N-CA	9.73	140.47	121.41
1	X	513	LEU	N-CA-CB	-9.25	94.86	110.49
1	X	11	ARG	CD-NE-CZ	9.21	137.30	124.40
1	X	129	ARG	CD-NE-CZ	8.99	136.98	124.40
1	X	322	GLY	O-C-N	-8.54	111.59	122.43
1	X	483	ARG	CD-NE-CZ	8.54	136.35	124.40
1	X	512	GLY	CA-C-N	8.42	137.62	121.54
1	X	512	GLY	C-N-CA	8.42	137.62	121.54
1	X	138	LYS	CA-CB-CG	8.26	130.62	114.10
1	X	135	GLU	CG-CD-OE1	-8.14	99.67	118.40
1	X	275	GLU	CG-CD-OE2	-8.11	99.75	118.40
1	X	343	GLU	CG-CD-OE1	-8.02	99.95	118.40
1	X	275	GLU	CG-CD-OE1	-8.01	99.99	118.40
1	X	363	HIS	ND1-CE1-NE2	-7.88	100.52	108.40
1	X	363	HIS	ND1-CG-CD2	-7.48	98.62	106.10
1	X	384	ASP	CA-CB-CG	7.43	120.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	278	ASN	CA-C-O	7.28	128.34	119.31
1	X	343	GLU	CB-CG-CD	7.11	124.68	112.60
1	X	388	ARG	CD-NE-CZ	7.01	134.22	124.40
1	X	605	GLY	CA-C-N	6.93	131.29	121.30
1	X	605	GLY	C-N-CA	6.93	131.29	121.30
1	X	330	ASP	CA-CB-CG	6.67	119.27	112.60
1	X	374	ASN	CA-CB-CG	6.60	119.20	112.60
1	X	462	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	X	627	GLU	CA-CB-CG	6.55	127.19	114.10
1	X	96	HIS	CE1-NE2-CD2	-6.24	102.76	109.00
1	X	447	ASN	CA-CB-CG	6.17	118.78	112.60
1	X	636	TRP	CA-C-O	-6.12	110.39	120.80
1	X	322	GLY	CA-C-O	6.09	125.88	119.06
1	X	363	HIS	CG-ND1-CE1	6.07	119.62	109.30
1	X	570	TRP	CA-CB-CG	5.99	124.98	113.60
1	X	9	THR	CA-C-N	5.96	130.87	121.99
1	X	9	THR	C-N-CA	5.96	130.87	121.99
1	X	390	LYS	CD-CE-NZ	-5.90	93.03	111.90
1	X	546	ASP	CA-CB-CG	5.88	118.48	112.60
1	X	202	ASP	CA-CB-CG	5.88	118.48	112.60
1	X	120	ARG	CG-CD-NE	-5.86	99.10	112.00
1	X	392	LYS	CD-CE-NZ	-5.85	93.19	111.90
1	X	511	ASN	OD1-CG-ND2	5.83	128.43	122.60
1	X	374	ASN	CB-CG-OD1	5.79	132.37	120.80
1	X	277	GLU	N-CA-C	5.77	118.31	111.33
1	X	96	HIS	CG-CD2-NE2	5.72	112.92	107.20
1	X	138	LYS	CB-CG-CD	5.72	124.46	111.30
1	X	343	GLU	CA-C-N	5.71	130.35	120.58
1	X	343	GLU	C-N-CA	5.71	130.35	120.58
1	X	228	ASP	CA-CB-CG	5.71	118.31	112.60
1	X	562	GLU	CA-C-N	5.65	127.85	120.28
1	X	562	GLU	C-N-CA	5.65	127.85	120.28
1	X	5	ASN	CA-CB-CG	5.65	118.25	112.60
1	X	423	ASP	CA-CB-CG	5.63	118.23	112.60
1	X	133	PRO	O-C-N	5.59	129.79	123.03
1	X	53	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	X	274	LYS	CA-C-O	5.44	126.19	120.42
1	X	96	HIS	CA-CB-CG	5.40	119.20	113.80
1	X	277	GLU	CB-CG-CD	-5.31	103.57	112.60
1	X	409	THR	CA-CB-OG1	-5.31	101.64	109.60
1	X	4	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	X	410	GLU	CA-C-N	5.29	127.80	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	410	GLU	C-N-CA	5.29	127.80	120.29
1	X	346	GLY	O-C-N	-5.24	115.56	122.42
1	X	5	ASN	CA-C-O	5.24	125.86	119.05
1	X	259	HIS	CA-C-N	5.24	128.02	122.63
1	X	259	HIS	C-N-CA	5.24	128.02	122.63
1	X	264	VAL	O-C-N	5.19	126.91	121.87
1	X	431	ASN	CA-CB-CG	-5.14	107.45	112.60
1	X	261	HIS	N-CA-C	5.11	119.98	113.18
1	X	366	PHE	CB-CG-CD1	5.09	129.35	120.70
1	X	483	ARG	NE-CZ-NH1	-5.04	116.46	121.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	135	GLU	Sidechain
1	X	275	GLU	Sidechain
1	X	343	GLU	Sidechain
1	X	373	GLU	Sidechain
1	X	446	CYS	Peptide
1	X	512	GLY	Mainchain,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	4755	4742	4894	45	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	779	0	0	10	0
All	All	5559	4742	4894	45	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 5.

All (45) 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:281:ARG:CZ	1:X:281:ARG:NH1	2.06	1.18
1:X:281:ARG:CZ	1:X:281:ARG:NH2	2.17	1.08
1:X:512:GLY:C	1:X:512:GLY:O	1.99	1.06
1:X:275:GLU:OE1	1:X:275:GLU:CD	2.02	1.01
1:X:343:GLU:OE1	1:X:343:GLU:CD	2.02	1.01
1:X:275:GLU:CD	1:X:275:GLU:OE2	2.03	1.01
1:X:135:GLU:CD	1:X:135:GLU:OE1	2.03	1.00
1:X:138:LYS:CE	1:X:138:LYS:NZ	2.24	0.99
1:X:463:LYS:CE	1:X:463:LYS:NZ	2.25	0.99
1:X:392:LYS:CD	1:X:392:LYS:CE	2.41	0.99
1:X:390:LYS:CD	1:X:390:LYS:CE	2.41	0.99
1:X:513:LEU:CA	1:X:513:LEU:CB	2.40	0.99
1:X:138:LYS:CE	1:X:138:LYS:CD	2.40	0.98
1:X:373:GLU:CD	1:X:373:GLU:CG	2.39	0.95
1:X:125:SER:HB3	7:X:2283:HOH:O	1.86	0.76
1:X:312:SER:HB2	1:X:476[B]:CYS:SG	2.27	0.74
1:X:445:GLY:O	1:X:476[B]:CYS:HB2	1.88	0.72
1:X:138:LYS:HE3	1:X:140:GLU:HB2	1.73	0.71
1:X:340[B]:THR:HG23	7:X:2526:HOH:O	1.99	0.62
1:X:169:PRO:HB2	7:X:2369:HOH:O	1.99	0.62
1:X:340[A]:THR:HG22	7:X:2528:HOH:O	2.00	0.61
1:X:526[A]:CYS:CB	6:X:1005:CO2:C	2.78	0.61
1:X:508:GLY:CA	1:X:513:LEU:HD11	2.33	0.59
1:X:403:VAL:HG11	1:X:482[B]:MET:SD	2.43	0.58
1:X:372:VAL:HG12	1:X:373:GLU:OE1	2.07	0.53
1:X:482[B]:MET:HG2	1:X:487[B]:MET:SD	2.48	0.53
1:X:340[A]:THR:CG2	7:X:2528:HOH:O	2.57	0.53
1:X:275:GLU:OE1	1:X:275:GLU:OE2	2.28	0.52
1:X:343:GLU:OE1	1:X:343:GLU:OE2	2.28	0.51
1:X:135:GLU:OE1	1:X:135:GLU:OE2	2.28	0.51
1:X:482[B]:MET:CG	1:X:487[B]:MET:SD	2.99	0.51
1:X:281:ARG:NH1	1:X:281:ARG:NH2	2.61	0.49
1:X:615:GLU:HG3	7:X:2761:HOH:O	2.12	0.48
1:X:512:GLY:HA2	7:X:2693:HOH:O	2.15	0.46
1:X:250:LYS:NZ	7:X:2464:HOH:O	2.49	0.45
1:X:402:LYS:NZ	7:X:2597:HOH:O	2.50	0.45
1:X:261:HIS:N	1:X:296[B]:THR:OG1	2.49	0.45
1:X:261:HIS:CD2	1:X:295[A]:CYS:HB2	2.53	0.44
1:X:277:GLU:O	1:X:281:ARG:HG3	2.18	0.44
1:X:266:SER:HB3	1:X:296[B]:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:512:GLY:O	1:X:513:LEU:N	2.49	0.42
1:X:482[B]:MET:HG3	1:X:487[B]:MET:SD	2.60	0.41
1:X:373:GLU:HG2	7:X:2296:HOH:O	2.21	0.41
1:X:432:VAL:HA	1:X:437:ILE:O	2.21	0.40
1:X:487[B]:MET:SD	1:X:522:HIS:HB2	2.62	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	653/636 (103%)	628 (96%)	23 (4%)	2 (0%)	36 10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	245	ASN
1	X	512	GLY

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	518/498 (104%)	508 (98%)	10 (2%)	50 11

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	138	LYS
1	X	277	GLU
1	X	368[A]	GLU
1	X	368[B]	GLU
1	X	373	GLU
1	X	390	LYS
1	X	392	LYS
1	X	463	LYS
1	X	513	LEU
1	X	599	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	431	ASN
1	X	436	ASN
1	X	455	GLN

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](#)

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	$\# Z > 2$
3	FES	X	1002	1	0,4,4	-	-	-		
6	CO2	X	1005	5,4	2,2,2	2.81	2 (100%)	1,1,1	6.71	1 (100%)
4	WCC	X	1003	6,5,1	0,12,12	-	-	-		
2	SF4	X	1001	1	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
3	FES	X	1002	1	-	-	0/1/1/1
4	WCC	X	1003	6,5,1	-	-	0/6/5/5
2	SF4	X	1001	1	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	1005	CO2	O1-C	2.83	1.32	1.16
6	X	1005	CO2	O2-C	2.79	1.32	1.16

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	1005	CO2	O2-C-O1	-6.71	114.65	175.36

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	CO2	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.56	6 (0%) 81 90	4, 13, 35, 103	22 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	513	LEU	5.7
1	X	512	GLY	2.6
1	X	6	LEU	2.3
1	X	278	ASN	2.2
1	X	390	LYS	2.1
1	X	365[A]	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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
5	FE2	X	1004[A]	1/1	0.97	0.07	18,18,18,18	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FE2	X	1004[B]	1/1	0.97	0.07	8,8,8,8	1
6	CO2	X	1005	3/3	0.98	0.05	8,8,8,9	3
2	SF4	X	1001	8/8	1.00	0.01	5,6,6,6	0
3	FES	X	1002	4/4	1.00	0.01	6,6,7,7	0
4	WCC	X	1003	8/8	1.00	0.01	6,7,8,9	8

6.5 Other polymers [i](#)

There are no such residues in this entry.