wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:02 PM GMT

PDB ID	:	1N62
Title	:	Crystal Structure of the Mo,Cu-CO Dehydrogenase (CODH), n-butylisocyani de-bound state
Authors	:	Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on	:	2002-11-08
Resolution	:	1.09 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

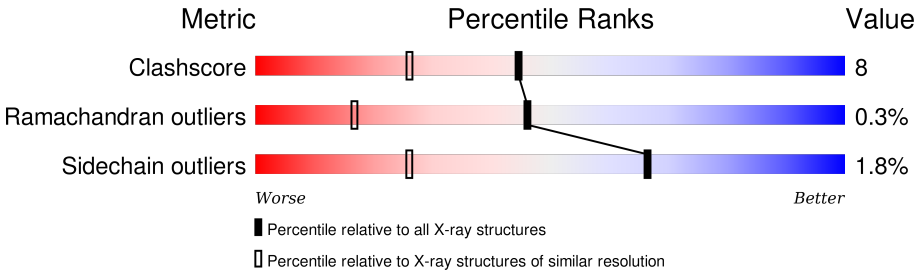
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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))
Clashscore	102246	1055 (1.14-1.06)
Ramachandran outliers	100387	1016 (1.14-1.06)
Sidechain outliers	100360	1014 (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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	166	86% 9%
1	D	166	85% 9%
2	B	809	83% 13%
2	E	809	84% 12%
3	C	288	88% 10%
3	F	288	84% 14%

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	CUB	B	3921	X	-	-	-
6	CUB	E	4921	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22645 atoms, of which 0 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 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	6	6	0
			1225	758	219	231	17			
1	D	159	Total	C	N	O	S	10	8	0
			1218	753	219	228	18			

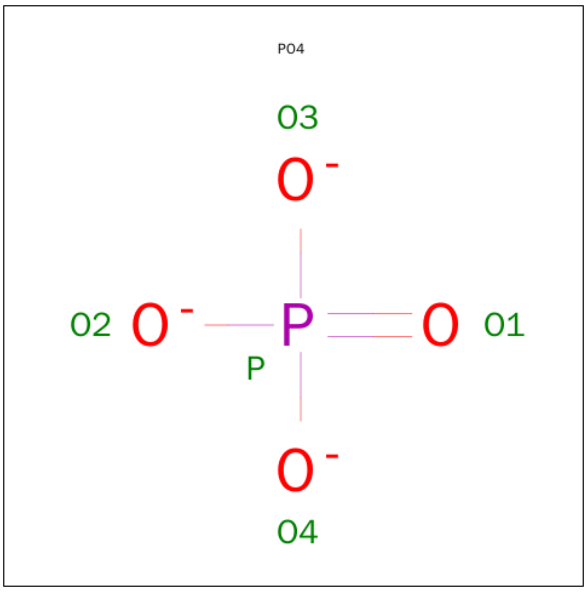
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	804	Total	C	N	O	S	80	15	0
			6256	3977	1067	1164	48			
2	E	796	Total	C	N	O	S	108	20	0
			6221	3959	1061	1154	47			

- Molecule 3 is a protein called Carbon monoxide dehydrogenase medium chain.

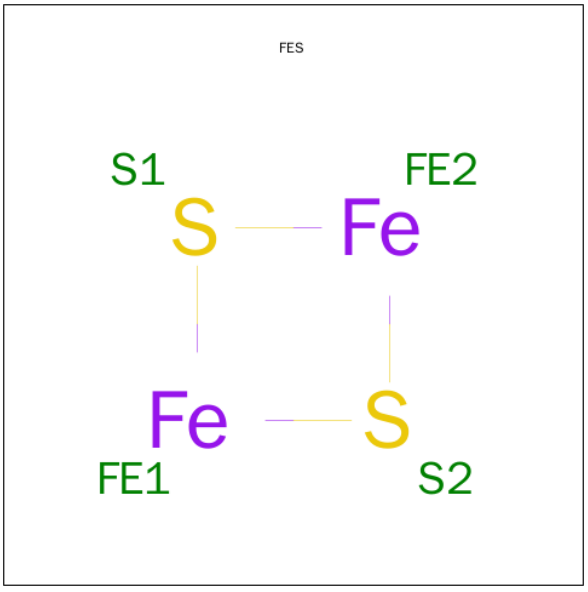
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	33	9	0
			2144	1353	378	401	12			
3	F	286	Total	C	N	O	S	40	6	0
			2125	1341	374	398	12			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



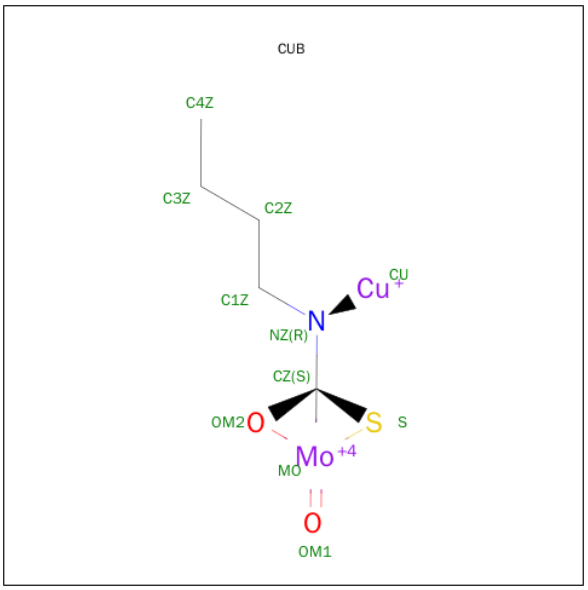
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 4 2 2	0	0
5	A	1	Total Fe S 4 2 2	0	0
5	D	1	Total Fe S 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	D	1	4	2	2	0	0

- Molecule 6 is CU(I)-S-MO(IV)(=O)O-NBIC CLUSTER (three-letter code: CUB) (formula: $C_5H_9CuMoNO_2S$).

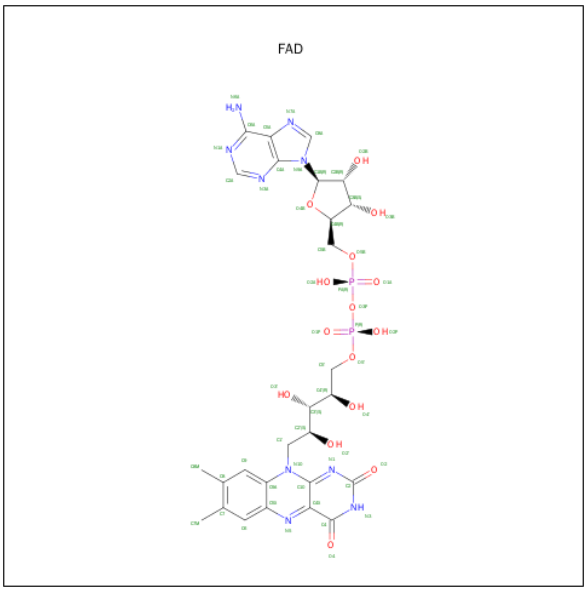


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cu	Mo	N	O	S		
6	B	1	11	5	1	1	1	2	1	0	0
			Total	C	Cu	Mo	N	O	S		
6	E	1	11	5	1	1	1	2	1	0	0

- Molecule 7 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		
7	E	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	217	Total	O	0	0
			217	217		
9	B	1034	Total	O	0	0
			1034	1034		
9	C	427	Total	O	0	0
			427	427		
9	D	222	Total	O	0	0
			222	222		
9	E	962	Total	O	0	0
			962	962		
9	F	357	Total	O	0	0
			357	357		

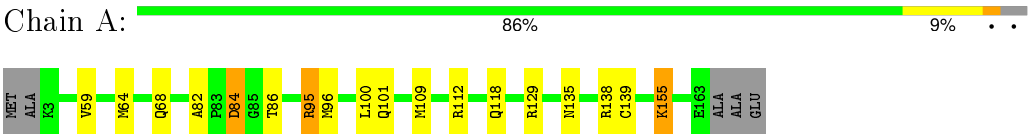
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

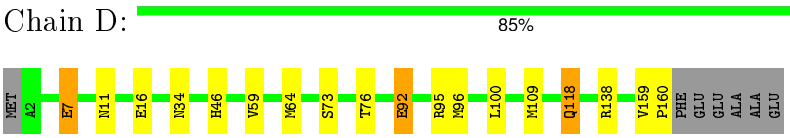
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A:



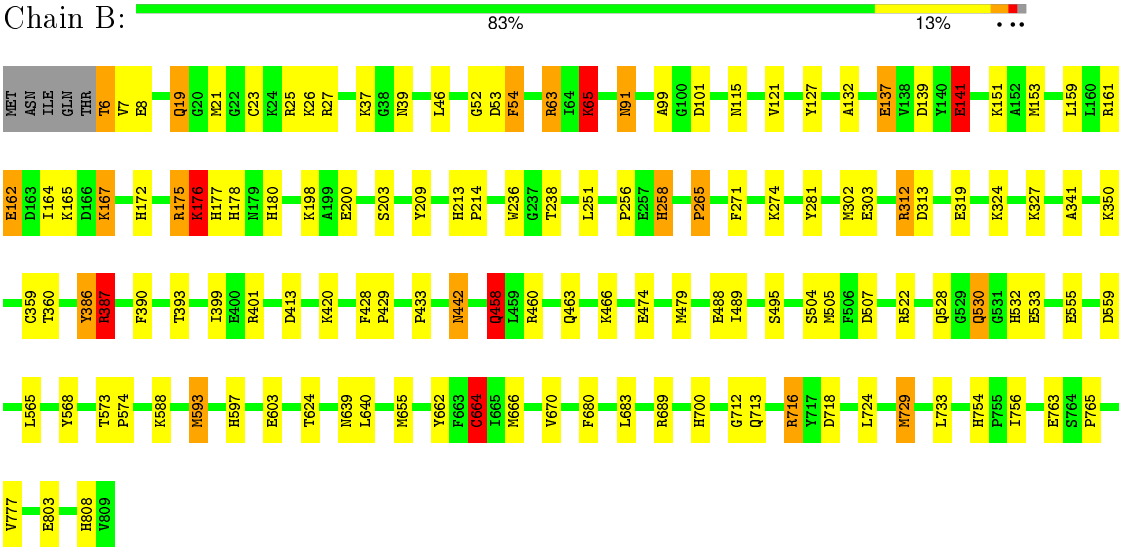
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D:



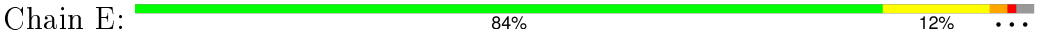
- Molecule 2: Carbon monoxide dehydrogenase large chain

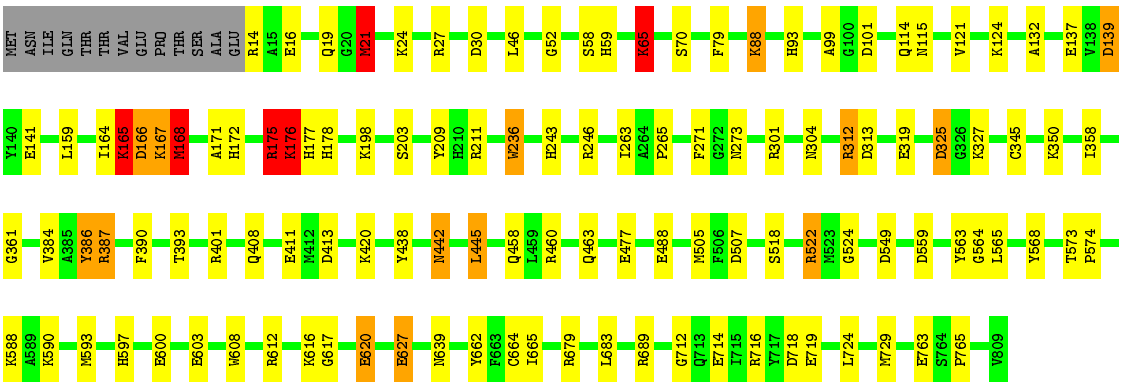
Chain B:



- Molecule 2: Carbon monoxide dehydrogenase large chain

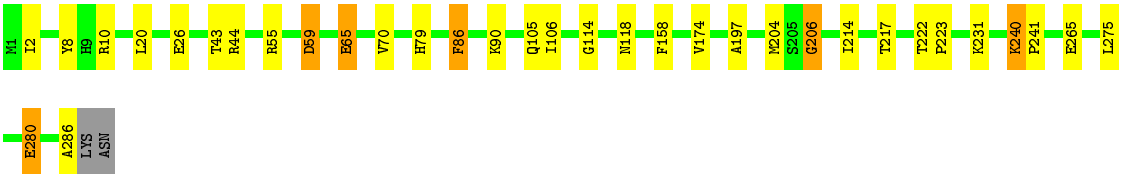
Chain E:





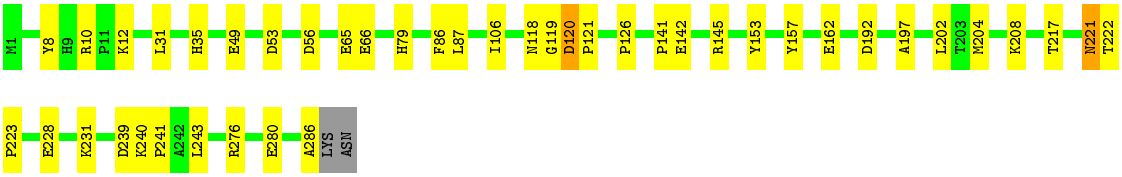
• Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain C:



• Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.86Å 130.02Å 156.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.80 – 1.09	Depositor
% Data completeness (in resolution range)	(Not available) (17.80-1.09)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.172	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22645	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MCN, PO4, CUB, FAD, 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	A	2.66	9/1273 (0.7%)	2.65	10/1719 (0.6%)
1	D	3.27	10/1267 (0.8%)	1.83	10/1710 (0.6%)
2	B	1.15	17/6474 (0.3%)	1.44	28/8780 (0.3%)
2	E	1.35	36/6453 (0.6%)	1.01	45/8747 (0.5%)
3	C	0.94	8/2210 (0.4%)	1.05	10/3000 (0.3%)
3	F	0.83	3/2186 (0.1%)	0.83	2/2969 (0.1%)
All	All	1.53	83/19863 (0.4%)	1.37	105/26925 (0.4%)

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
1	D	0	3
2	B	0	11
2	E	0	14
3	C	0	5
3	F	0	6
All	All	0	40

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92[A]	GLU	CD-OE2	75.22	2.08	1.25
1	D	92[B]	GLU	CD-OE2	75.22	2.08	1.25
1	A	95[A]	ARG	CZ-NH1	52.95	2.01	1.33
1	A	95[B]	ARG	CZ-NH1	52.95	2.01	1.33
2	E	600	GLU	CD-OE1	33.23	1.62	1.25

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	63	ARG	NH1-CZ-NH2	-101.31	7.96	119.40
1	A	95[A]	ARG	NE-CZ-NH2	50.85	145.73	120.30
1	A	95[B]	ARG	NE-CZ-NH2	50.85	145.73	120.30
1	A	95[A]	ARG	NE-CZ-NH1	-49.76	95.42	120.30
1	A	95[B]	ARG	NE-CZ-NH1	-49.76	95.42	120.30

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
2	B	19	GLN	Sidechain
2	B	27	ARG	Sidechain
2	B	54	PHE	Peptide
2	B	6	THR	Mainchain

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	A	1225	0	1203	18	0
1	D	1218	0	1198	30	0
2	B	6256	0	6138	94	3
2	E	6221	0	6103	96	1
3	C	2144	0	2200	28	0
3	F	2125	0	2175	43	0
4	A	5	0	0	0	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	11	0	9	3	0
6	E	11	0	9	4	0
7	B	44	0	17	3	0
7	E	44	0	17	1	0
8	C	53	0	30	0	0
8	F	53	0	31	2	0
9	A	217	0	0	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	1034	0	0	18	7
9	C	427	0	0	7	0
9	D	222	0	0	5	2
9	E	962	0	0	29	2
9	F	357	0	0	13	1
All	All	22645	0	19130	302	9

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 8.

The worst 5 of 302 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)
2:E:21[A]:MET:CG	2:E:21[A]:MET:CB	1.76	1.62
2:E:327[B]:LYS:HD3	9:E:5792:HOH:O	1.23	1.36
3:C:65:GLU:HG2	3:C:86:PHE:CZ	1.65	1.31
2:B:6:THR:CG2	9:B:4489:HOH:O	1.77	1.27
3:C:55[A]:ARG:NH2	9:C:4313:HOH:O	1.66	1.26

The worst 5 of 9 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	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:VAL:CB	9:B:4950:HOH:O[4_477]	1.17	1.03
2:B:7:VAL:CG1	9:B:4950:HOH:O[4_477]	1.51	0.69
2:B:7:VAL:CG2	9:B:4950:HOH:O[4_477]	1.64	0.56
9:B:4928:HOH:O	9:D:5093:HOH:O[4_477]	1.69	0.51
9:E:5511:HOH:O	9:E:5739:HOH:O[2_685]	1.88	0.32

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	A	165/166 (99%)	162 (98%)	3 (2%)	0	100	100
1	D	165/166 (99%)	162 (98%)	3 (2%)	0	100	100
2	B	817/809 (101%)	785 (96%)	28 (3%)	4 (0%)	34	8
2	E	813/809 (100%)	788 (97%)	22 (3%)	3 (0%)	39	12
3	C	293/288 (102%)	287 (98%)	6 (2%)	0	100	100
3	F	290/288 (101%)	285 (98%)	5 (2%)	0	100	100
All	All	2543/2526 (101%)	2469 (97%)	67 (3%)	7 (0%)	46	17

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	265	PRO
2	B	312	ARG
2	B	712	GLY
2	E	312	ARG
2	E	712	GLY

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	135/131 (103%)	134 (99%)	1 (1%)	88	63
1	D	134/131 (102%)	133 (99%)	1 (1%)	88	63
2	B	663/653 (102%)	645 (97%)	18 (3%)	52	12
2	E	661/653 (101%)	647 (98%)	14 (2%)	61	19
3	C	219/212 (103%)	218 (100%)	1 (0%)	92	72
3	F	216/212 (102%)	213 (99%)	3 (1%)	74	37
All	All	2028/1992 (102%)	1990 (98%)	38 (2%)	66	24

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	664[A]	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	21[A]	MET
3	F	87	LEU
3	C	59	ASP
2	E	21[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	754	HIS
1	D	11	ASN
3	F	79	HIS
3	C	79	HIS
2	E	59	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\|>2$
5	FES	A	3907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	A	3908	1	0,4,4	0.00	-	0,4,4	0.00	-
4	PO4	A	4001	-	4,4,4	0.76	0	6,6,6	0.31	0
7	MCN	B	3920	6	32,48,48	1.70	6 (18%)	39,74,74	1.64	7 (17%)
6	CUB	B	3921	2,7	3,12,12	2.03	2 (66%)	3,20,20	1.82	1 (33%)
8	FAD	C	3932	-	48,58,58	1.36	6 (12%)	54,89,89	2.32	6 (11%)
5	FES	D	4907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	D	4908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	MCN	E	4920	6	32,48,48	1.95	9 (28%)	39,74,74	1.90	7 (17%)
6	CUB	E	4921	2,7	3,12,12	1.98	1 (33%)	3,20,20	1.35	1 (33%)
8	FAD	F	4931	-	48,58,58	1.29	5 (10%)	54,89,89	1.82	10 (18%)

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	FES	A	3907	1	-	0/0/4/4	0/1/1/1
5	FES	A	3908	1	-	0/0/4/4	0/1/1/1
4	PO4	A	4001	-	-	0/0/0/0	0/0/0/0
7	MCN	B	3920	6	-	0/18/54/54	0/5/5/5
6	CUB	B	3921	2,7	1/1/3/3	0/2/25/25	0/0/2/2
8	FAD	C	3932	-	-	0/30/50/50	0/6/6/6
5	FES	D	4907	1	-	0/0/4/4	0/1/1/1
5	FES	D	4908	1	-	0/0/4/4	0/1/1/1
7	MCN	E	4920	6	-	0/18/54/54	0/5/5/5
6	CUB	E	4921	2,7	1/1/3/3	0/2/25/25	0/0/2/2
8	FAD	F	4931	-	-	0/30/50/50	0/6/6/6

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4931	FAD	C10-N10	-3.94	1.34	1.39
8	C	3932	FAD	C10-N10	-3.75	1.34	1.39
7	B	3920	MCN	C6-C5	-3.71	1.30	1.38
7	B	3920	MCN	O4D-C1'	-3.37	1.36	1.41
8	F	4931	FAD	O4B-C4B	-2.94	1.38	1.45

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	3932	FAD	N3A-C2A-N1A	-8.47	122.41	128.89
8	C	3932	FAD	C4X-C4-N3	-5.34	116.28	123.59
7	E	4920	MCN	N1'-C2'-N3'	-4.96	119.89	127.44
7	E	4920	MCN	C5-C4-N4	-4.86	113.85	121.31
7	B	3920	MCN	N1'-C2'-N3'	-4.79	120.15	127.44

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	3921	CUB	CZ
6	E	4921	CUB	CZ

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3920	MCN	3	0
6	B	3921	CUB	3	0
7	E	4920	MCN	1	0
6	E	4921	CUB	4	0
8	F	4931	FAD	2	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.