



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:01 PM UTC

PDB ID : 1N5W / pdb_00001n5w
Title : Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Oxidized form
Authors : Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on : 2002-11-07
Resolution : 1.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

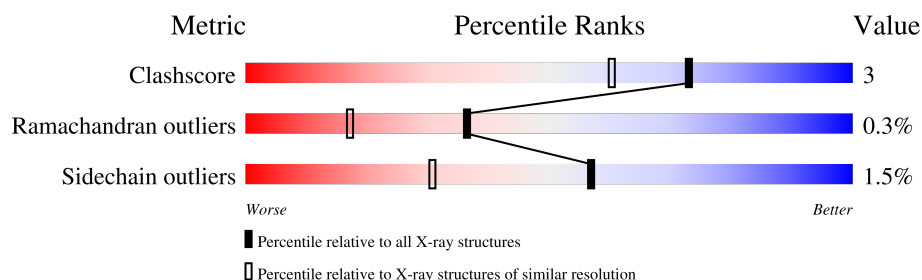
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	166	92% 5% ..
1	D	166	90% .. 5%
2	B	809	89% 8% ..
2	E	809	91% 6% ..
3	C	288	94% 5% .
3	F	288	91% 7% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	3001	-	X	-	-
8	FAD	C	3932	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21572 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	5	0	0
			1204	746	215	228	15			
1	D	158	Total	C	N	O	S	7	0	0
			1175	727	212	221	15			

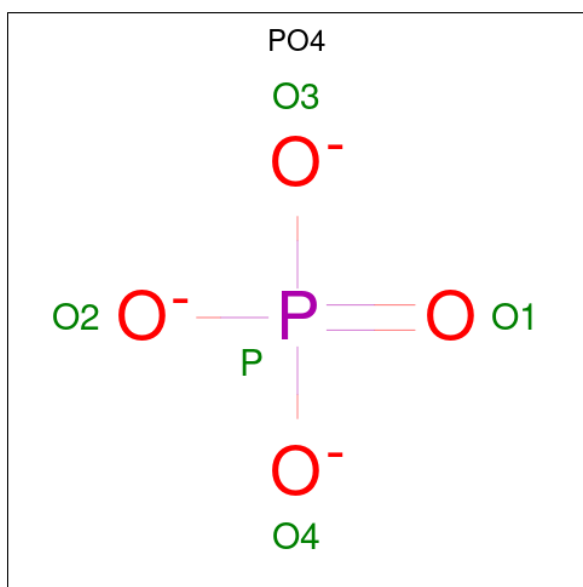
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	804	Total	C	N	O	S	76	1	0
			6206	3942	1062	1161	41			
2	E	795	Total	C	N	O	S	80	1	0
			6138	3902	1050	1145	41			

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

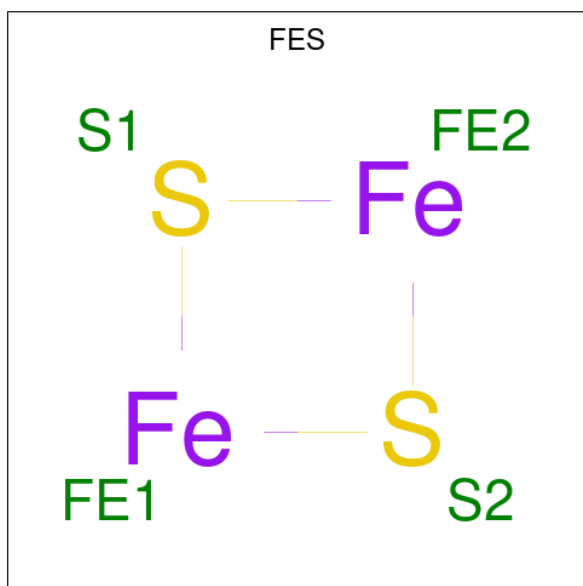
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	27	0	0
			2112	1333	372	396	11			
3	F	286	Total	C	N	O	S	48	0	0
			2103	1327	370	395	11			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



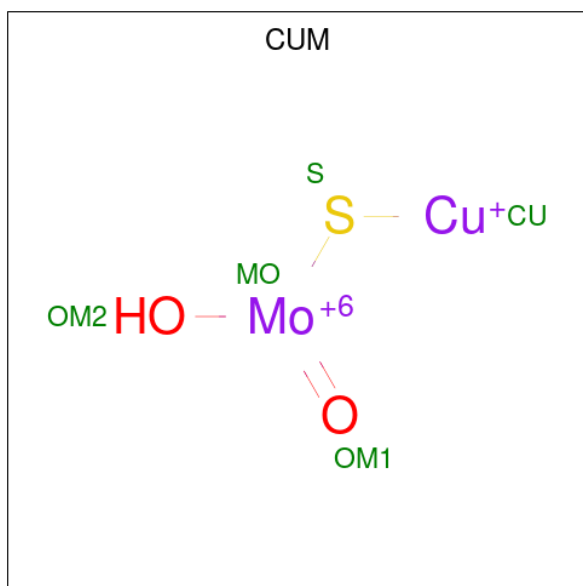
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

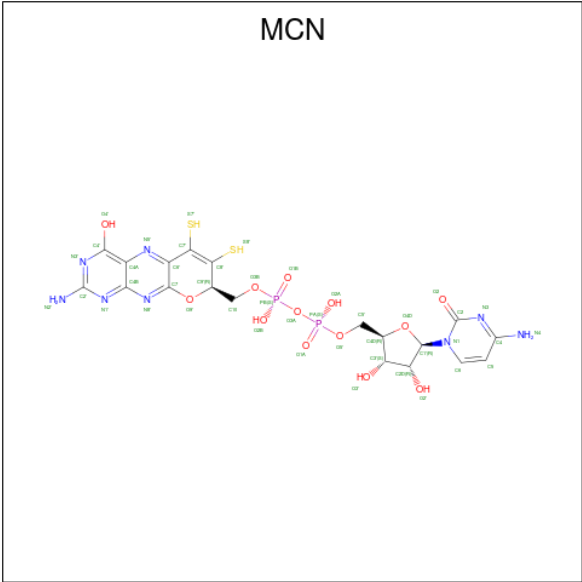
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is CU(I)-S-MO(VI)(=O)OH CLUSTER (CCD ID: CUM) (formula: CuHMoO₂S).



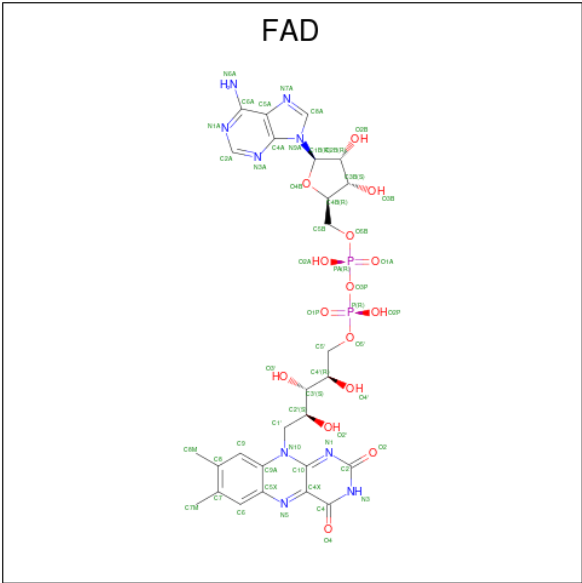
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	Cu	Mo	O	S	0	0
			5	1	1	2	1		
6	E	1	Total	Cu	Mo	O	S	0	0
			5	1	1	2	1		

- Molecule 7 is PTERIN CYTOSINE DINUCLEOTIDE (CCD ID: MCN) (formula: C₁₉H₂₂N₈O₁₃P₂S₂).



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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			18	12	4	2		
8	F	1	Total	C	N	O	0	0
			18	12	4	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	177	Total 177	O 177	0	0
9	B	794	Total 794	O 794	0	0
9	C	308	Total 308	O 308	0	0
9	D	174	Total 174	O 174	0	0
9	E	762	Total 762	O 762	0	0
9	F	264	Total 264	O 264	0	0

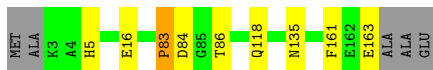
3 Residue-property plots

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. 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. 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:  92% 5% ..



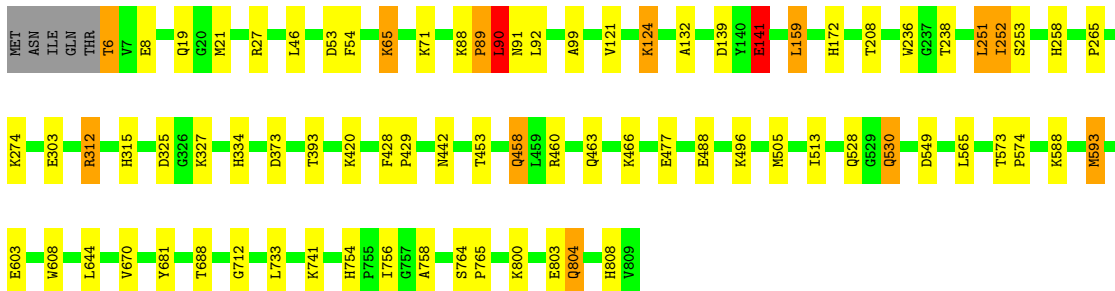
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D:  90% .. 5%



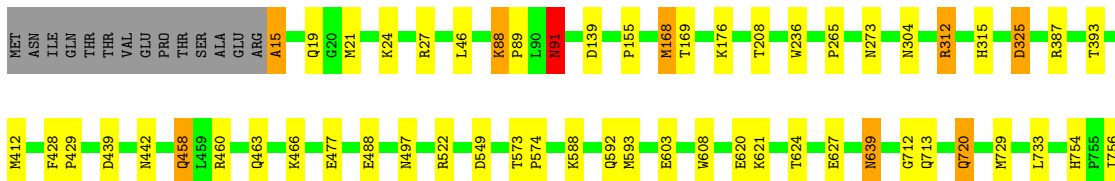
- Molecule 2: Carbon monoxide dehydrogenase large chain

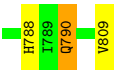
Chain B:  89% 8% ..



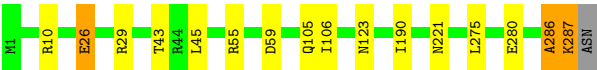
- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain E:  91% 6% ..

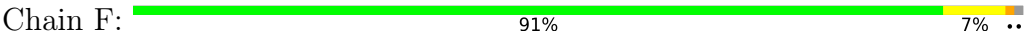




● Molecule 3: Carbon monoxide dehydrogenase medium chain



● Molecule 3: Carbon monoxide dehydrogenase medium chain



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.30Å 132.09Å 159.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 1.50	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.135 , 0.171	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21572	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CUM, PO4, FES, MCN

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	0.91	2/1225 (0.2%)	1.02	0/1656
1	D	1.01	3/1195 (0.3%)	1.01	0/1616
2	B	1.00	13/6365 (0.2%)	1.05	14/8639 (0.2%)
2	E	1.00	14/6296 (0.2%)	1.05	12/8544 (0.1%)
3	C	1.00	4/2149 (0.2%)	1.06	2/2918 (0.1%)
3	F	1.23	3/2140 (0.1%)	1.07	1/2907 (0.0%)
All	All	1.02	39/19370 (0.2%)	1.05	29/26280 (0.1%)

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	1
2	B	1	8
2	E	0	8
3	C	0	5
3	F	0	3
All	All	1	26

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	240	LYS	CB-CG	-26.75	0.72	1.52
3	F	240	LYS	CG-CD	22.13	2.18	1.52
2	B	141	GLU	CG-CD	16.14	1.92	1.52
2	E	639	ASN	CG-OD1	15.28	1.52	1.23
2	B	458	GLN	CD-NE2	-13.01	1.05	1.33
2	B	458	GLN	CD-OE1	11.75	1.45	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	809	VAL	CB-CG2	11.41	1.90	1.52
2	B	124	LYS	CE-NZ	11.24	1.83	1.49
2	E	325	ASP	CG-OD1	10.82	1.46	1.25
2	E	15	ALA	CA-CB	10.76	1.88	1.52
3	C	221	ASN	CG-OD1	10.60	1.43	1.23
1	D	159	VAL	CA-CB	9.14	1.59	1.54
2	B	89	PRO	C-N	-8.96	1.21	1.33
2	E	639	ASN	CG-ND2	-8.78	1.14	1.33
2	B	88	LYS	CD-CE	-8.68	1.26	1.52
2	B	65	LYS	CG-CD	-8.31	1.27	1.52
2	E	458	GLN	CG-CD	-8.24	1.31	1.52
2	E	24	LYS	CE-NZ	7.86	1.73	1.49
3	C	190	ILE	CA-CB	7.78	1.62	1.54
2	E	809	VAL	CB-CG1	-7.45	1.27	1.52
2	B	6	THR	CA-CB	-7.43	1.34	1.54
2	E	91	ASN	CG-OD1	7.01	1.36	1.23
1	D	160	PRO	C-O	-6.99	1.09	1.23
3	C	55	ARG	CD-NE	-6.80	1.36	1.46
2	B	496	LYS	CD-CE	6.55	1.72	1.52
3	C	26	GLU	CB-CG	-6.46	1.33	1.52
2	B	593	MET	SD-CE	-6.29	1.63	1.79
2	E	176	LYS	CA-CB	-6.19	1.43	1.53
2	E	729	MET	SD-CE	-6.06	1.64	1.79
2	E	412	MET	SD-CE	-5.75	1.65	1.79
2	E	497	ASN	CG-ND2	5.74	1.45	1.33
1	A	161	PHE	CA-C	5.64	1.55	1.52
1	D	96	MET	SD-CE	-5.39	1.66	1.79
1	A	83	PRO	CA-CB	-5.35	1.46	1.53
3	F	255	ALA	CA-CB	-5.22	1.46	1.53
2	E	621	LYS	CD-CE	5.17	1.68	1.52
2	B	758	ALA	C-O	-5.13	1.17	1.23
2	B	21	MET	SD-CE	-5.09	1.66	1.79
2	B	91	ASN	CA-CB	5.08	1.61	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	PRO	CA-C-N	12.69	145.77	121.54
2	B	89	PRO	C-N-CA	12.69	145.77	121.54
2	E	720	GLN	OE1-CD-NE2	-12.66	109.94	122.60
3	C	221	ASN	OD1-CG-ND2	12.54	135.15	122.60
2	E	639	ASN	CB-CG-ND2	12.34	134.92	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	240	LYS	CA-CB-CG	-12.09	89.92	114.10
2	B	124	LYS	CD-CE-NZ	-9.79	80.56	111.90
2	B	325	ASP	CA-CB-CG	9.48	122.08	112.60
2	E	458	GLN	CB-CG-CD	9.45	128.67	112.60
2	E	809	VAL	CA-CB-CG1	9.41	126.39	110.40
2	B	458	GLN	CG-CD-OE1	-9.27	102.26	120.80
2	E	639	ASN	CB-CG-OD1	-8.63	103.54	120.80
2	E	639	ASN	OD1-CG-ND2	-8.28	114.32	122.60
2	B	65	LYS	CB-CG-CD	7.87	129.40	111.30
2	B	88	LYS	CG-CD-CE	7.71	129.04	111.30
2	E	15	ALA	CB-CA-C	-7.34	99.49	110.50
2	B	6	THR	N-CA-CB	-7.26	99.16	111.50
2	E	325	ASP	CB-CG-OD1	-6.99	102.32	118.40
2	B	458	GLN	CG-CD-NE2	6.60	126.30	116.40
2	E	325	ASP	OD1-CG-OD2	-6.56	107.16	122.90
2	B	496	LYS	CG-CD-CE	-6.17	97.11	111.30
2	B	90	LEU	N-CA-CB	5.91	120.47	110.49
2	E	439	ASP	N-CA-C	5.70	117.30	111.14
2	B	71	LYS	CG-CD-CE	-5.46	98.74	111.30
3	C	221	ASN	CB-CG-OD1	-5.35	110.10	120.80
2	B	91	ASN	N-CA-CB	-5.33	103.89	111.84
2	E	91	ASN	OD1-CG-ND2	-5.33	117.27	122.60
2	B	741	LYS	CG-CD-CE	-5.22	99.30	111.30
2	E	168	MET	CB-CA-C	-5.08	105.12	111.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	90	LEU	CA

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Mainchain
2	B	141	GLU	Sidechain
2	B	19	GLN	Sidechain
2	B	27	ARG	Sidechain
2	B	312	ARG	Sidechain
2	B	458	GLN	Sidechain
2	B	549	ASP	Sidechain
2	B	89	PRO	Peptide
2	B	90	LEU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	10	ARG	Sidechain
3	C	123	ASN	Sidechain
3	C	286	ALA	Mainchain
3	C	29	ARG	Sidechain
3	C	59	ASP	Sidechain
1	D	138	ARG	Sidechain
2	E	168	MET	Mainchain
2	E	27	ARG	Sidechain
2	E	312	ARG	Sidechain
2	E	325	ASP	Sidechain
2	E	387	ARG	Sidechain
2	E	639	ASN	Sidechain
2	E	720	GLN	Sidechain
2	E	91	ASN	Sidechain
3	F	120	ASP	Sidechain
3	F	158	PHE	Sidechain
3	F	66	GLU	Sidechain

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	A	1204	0	1178	7	1
1	D	1175	0	1157	2	0
2	B	6206	0	6076	58	0
2	E	6138	0	6012	29	0
3	C	2112	0	2168	7	0
3	F	2103	0	2155	17	0
4	A	5	0	0	1	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	5	0	0	1	0
6	E	5	0	0	0	0
7	B	44	0	17	0	0
7	E	44	0	17	0	0
8	C	18	0	9	0	0
8	F	18	0	9	1	0
9	A	177	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	794	0	0	11	1
9	C	308	0	0	2	1
9	D	174	0	0	0	0
9	E	762	0	0	7	2
9	F	264	0	0	6	1
All	All	21572	0	18798	118	3

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 (118) 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:593:MET:HG2	2:E:603:GLU:OE1	1.24	1.30
2:B:251:LEU:HD23	2:B:252:ILE:N	1.73	1.03
2:B:124:LYS:CD	2:B:124:LYS:NZ	2.23	1.00
2:B:159:LEU:HB2	9:B:4426:HOH:O	1.61	1.00
2:E:15:ALA:N	9:E:5469:HOH:O	2.02	0.93
2:B:528:GLN:H	2:B:530:GLN:HE22	1.22	0.86
1:D:11:ASN:HD21	1:D:76:THR:H	1.25	0.84
2:E:593:MET:CG	2:E:603:GLU:OE1	2.19	0.82
2:E:208:THR:H	2:E:790:GLN:HE22	1.27	0.81
2:B:460:ARG:HH11	2:B:463:GLN:HE22	1.28	0.79
2:B:303:GLU:OE1	9:B:4483:HOH:O	2.04	0.76
3:F:10:ARG:CZ	9:F:5042:HOH:O	2.34	0.75
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.34	0.74
2:E:458:GLN:HG2	9:E:5504:HOH:O	1.86	0.73
3:F:45:LEU:HG	9:F:5118:HOH:O	1.88	0.72
2:E:477:GLU:OE2	9:E:5278:HOH:O	2.08	0.71
2:B:159:LEU:CA	9:B:4426:HOH:O	2.39	0.69
2:B:303:GLU:OE1	9:B:4213:HOH:O	2.11	0.69
1:A:84:ASP:OD1	1:A:86:THR:HG23	1.92	0.68
2:E:273:ASN:HD21	2:E:304:ASN:HD21	1.42	0.68
2:B:251:LEU:HD23	2:B:251:LEU:C	2.17	0.68
3:F:162:GLU:HB3	3:F:163:PRO:HD2	1.77	0.67
2:B:800:LYS:O	2:B:804:GLN:HG2	1.95	0.67
2:B:528:GLN:H	2:B:530:GLN:NE2	1.92	0.66
1:A:135:ASN:HD21	3:C:105:GLN:HE22	1.43	0.64
2:E:754:HIS:HD2	2:E:756:ILE:H	1.46	0.64
1:A:5:HIS:HD2	4:A:3001:PO4:O2	1.81	0.63
2:B:251:LEU:HD23	2:B:252:ILE:CA	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:592:GLN:NE2	9:E:5296:HOH:O	2.32	0.62
3:F:221:ASN:HD22	3:F:221:ASN:H	1.45	0.62
1:A:5:HIS:HE1	1:A:16:GLU:OE2	1.83	0.62
2:B:670:VAL:O	2:B:808:HIS:HE1	1.84	0.61
6:B:3921:CUM:OM1	6:B:3921:CUM:MO	1.71	0.61
2:B:530:GLN:HE21	2:B:530:GLN:H	1.49	0.60
2:B:803:GLU:OE1	2:B:808:HIS:HD2	1.84	0.60
3:F:221:ASN:ND2	9:F:5073:HOH:O	2.36	0.59
3:C:280:GLU:HG3	9:C:4198:HOH:O	2.02	0.58
2:E:19:GLN:NE2	9:E:5300:HOH:O	2.36	0.58
3:C:286:ALA:O	3:C:287:LYS:HB2	2.04	0.58
2:B:159:LEU:CB	9:B:4426:HOH:O	2.31	0.57
1:A:135:ASN:ND2	3:C:105:GLN:HE22	2.02	0.57
2:E:208:THR:OG1	2:E:315:HIS:HD2	1.87	0.56
2:B:46:LEU:HD11	2:B:236[B]:TRP:CZ3	2.41	0.56
3:C:43:THR:HG22	9:C:4158:HOH:O	2.04	0.56
2:B:124:LYS:NZ	2:B:124:LYS:HD2	2.18	0.56
2:E:46:LEU:HD11	2:E:236[B]:TRP:CZ3	2.40	0.56
2:E:208:THR:H	2:E:790:GLN:NE2	2.02	0.55
2:B:442:ASN:C	2:B:442:ASN:HD22	2.14	0.54
2:B:92:LEU:HD21	2:B:252:ILE:HG23	1.88	0.54
3:F:118:ASN:OD1	3:F:120:ASP:HB2	2.08	0.54
2:B:303:GLU:CD	9:B:4483:HOH:O	2.48	0.53
2:B:334:HIS:HE1	2:B:373:ASP:OD2	1.90	0.53
2:E:754:HIS:CD2	2:E:756:ILE:H	2.26	0.53
3:C:275:LEU:HD23	3:C:275:LEU:C	2.34	0.52
2:B:208:THR:OG1	2:B:315:HIS:HD2	1.93	0.52
2:B:327:LYS:HG2	2:B:420:LYS:HE3	1.91	0.52
2:B:238:THR:HB	2:B:274:LYS:HD3	1.93	0.51
3:F:214:ILE:HD13	3:F:275:LEU:HD11	1.91	0.51
3:F:221:ASN:HD22	3:F:221:ASN:N	2.03	0.50
2:B:466:LYS:HE3	2:B:477:GLU:O	2.11	0.50
1:A:118:GLN:HG2	9:A:4007:HOH:O	2.11	0.50
2:B:513:ILE:HD12	2:B:644:LEU:HD23	1.93	0.50
3:F:276:ARG:O	3:F:280:GLU:HG3	2.12	0.50
3:F:79:HIS:HD2	9:F:5130:HOH:O	1.95	0.49
2:B:754:HIS:HD2	2:B:756:ILE:H	1.58	0.49
3:F:106:ILE:HD13	8:F:4931:FAD:C8	2.43	0.49
2:B:141:GLU:CD	2:B:141:GLU:CB	2.86	0.48
3:F:10:ARG:NH1	9:F:4980:HOH:O	2.43	0.48
2:B:172:HIS:HD2	9:B:4646:HOH:O	1.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:LYS:HB2	2:E:89:PRO:HD3	1.95	0.47
2:B:258:HIS:HE1	2:E:549:ASP:O	1.96	0.47
2:B:530:GLN:NE2	2:B:530:GLN:H	2.11	0.47
3:C:286:ALA:O	3:C:287:LYS:CB	2.62	0.47
2:E:88:LYS:CB	2:E:89:PRO:HD3	2.45	0.47
2:B:573:THR:HB	2:B:574:PRO:HD3	1.98	0.46
2:B:65:LYS:HB2	2:B:139:ASP:OD1	2.15	0.46
2:B:804:GLN:HG3	9:B:4360:HOH:O	2.16	0.46
2:B:252:ILE:HG22	2:B:253:SER:N	2.31	0.46
2:E:428:PHE:HA	2:E:429:PRO:C	2.41	0.46
2:B:428:PHE:HA	2:B:429:PRO:C	2.41	0.45
2:E:442:ASN:HD22	2:E:442:ASN:C	2.24	0.45
2:E:624:THR:OG1	2:E:627:GLU:HG3	2.17	0.45
2:B:99:ALA:O	2:B:172:HIS:HE1	1.99	0.45
2:E:788:HIS:HE2	2:E:790:GLN:NE2	2.14	0.45
2:B:53:ASP:CG	2:B:54:PHE:H	2.25	0.45
3:F:162:GLU:HB3	3:F:163:PRO:CD	2.46	0.45
2:B:159:LEU:HA	9:B:4426:HOH:O	2.13	0.44
2:B:124:LYS:HD2	2:B:124:LYS:HZ2	1.80	0.44
2:B:8:GLU:O	2:B:8:GLU:HG3	2.17	0.44
2:E:155:PRO:HA	2:E:169:THR:HB	1.99	0.44
2:B:460:ARG:NH1	2:B:463:GLN:HE22	2.06	0.43
2:B:688:THR:HG21	2:B:756:ILE:O	2.18	0.43
2:B:593:MET:HG2	2:B:603:GLU:OE2	2.18	0.43
2:E:522:ARG:NH1	9:E:5552:HOH:O	2.48	0.43
2:B:588:LYS:HE3	2:B:608:TRP:CD2	2.53	0.42
2:B:754:HIS:CD2	2:B:756:ILE:H	2.37	0.42
3:F:45:LEU:CG	9:F:5118:HOH:O	2.57	0.42
2:E:713:GLN:NE2	2:E:733:LEU:HD23	2.35	0.42
2:B:92:LEU:CD2	2:B:252:ILE:HG23	2.49	0.42
2:B:251:LEU:C	2:B:251:LEU:CD2	2.84	0.42
3:F:197:ALA:HB3	3:F:217:THR:HB	2.01	0.42
2:B:315:HIS:HE1	9:B:4010:HOH:O	2.02	0.42
2:E:573:THR:HB	2:E:574:PRO:HD3	2.02	0.42
2:E:315:HIS:HE1	9:E:5039:HOH:O	2.03	0.42
1:A:84:ASP:CG	1:A:86:THR:HG23	2.46	0.41
2:B:505:MET:HA	2:B:565:LEU:HG	2.02	0.41
3:F:162:GLU:CB	3:F:163:PRO:HD2	2.50	0.41
3:F:43:THR:OG1	3:F:45:LEU:HG	2.20	0.41
2:B:334:HIS:HD2	9:B:4194:HOH:O	2.04	0.41
2:B:764:SER:N	2:B:765:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:803:GLU:OE1	2:B:808:HIS:CD2	2.69	0.41
2:B:800:LYS:O	2:B:804:GLN:CG	2.67	0.41
2:B:453:THR:HG21	2:B:681:TYR:CE1	2.56	0.41
1:D:159:VAL:HB	1:D:160:PRO:HD3	2.03	0.41
2:E:588:LYS:HE3	2:E:608:TRP:CE2	2.56	0.41
2:B:121:VAL:HG11	2:B:132:ALA:HB3	2.03	0.40
2:B:733:LEU:HD23	2:B:733:LEU:HA	1.84	0.40
2:E:21:MET:HE3	2:E:21:MET:HB3	1.93	0.40

All (3) 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)
1:A:163:GLU:OE2	9:E:5512:HOH:O[4_477]	1.84	0.36
9:B:4410:HOH:O	9:E:5523:HOH:O[4_477]	1.99	0.21
9:C:4080:HOH:O	9:F:5072:HOH:O[2_684]	2.17	0.03

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	159/166 (96%)	155 (98%)	4 (2%)	0	100	100
1	D	156/166 (94%)	153 (98%)	3 (2%)	0	100	100
2	B	803/809 (99%)	771 (96%)	28 (4%)	4 (0%)	24	8
2	E	794/809 (98%)	766 (96%)	25 (3%)	3 (0%)	30	12
3	C	285/288 (99%)	282 (99%)	3 (1%)	0	100	100
3	F	284/288 (99%)	278 (98%)	6 (2%)	0	100	100
All	All	2481/2526 (98%)	2405 (97%)	69 (3%)	7 (0%)	36	17

All (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
2	B	90	LEU
2	E	265	PRO

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	129/131 (98%)	129 (100%)	0	100	100
1	D	126/131 (96%)	124 (98%)	2 (2%)	55	28
2	B	649/653 (99%)	639 (98%)	10 (2%)	57	31
2	E	641/653 (98%)	633 (99%)	8 (1%)	63	38
3	C	211/212 (100%)	207 (98%)	4 (2%)	50	22
3	F	210/212 (99%)	204 (97%)	6 (3%)	37	10
All	All	1966/1992 (99%)	1936 (98%)	30 (2%)	57	31

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	6	THR
2	B	90	LEU
2	B	141	GLU
2	B	159	LEU
2	B	251	LEU
2	B	252	ILE
2	B	393	THR
2	B	488	GLU
2	B	530	GLN
2	B	804	GLN
3	C	26	GLU
3	C	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	106	ILE
3	C	287	LYS
1	D	3	LYS
1	D	18	LEU
2	E	88	LYS
2	E	91	ASN
2	E	139	ASP
2	E	393	THR
2	E	466	LYS
2	E	488	GLU
2	E	620	GLU
2	E	790	GLN
3	F	20	LEU
3	F	45	LEU
3	F	55	ARG
3	F	126	PRO
3	F	142	GLU
3	F	221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	33	GLN
1	A	34	ASN
1	A	135	ASN
2	B	59	HIS
2	B	115	ASN
2	B	172	HIS
2	B	258	HIS
2	B	273	ASN
2	B	304	ASN
2	B	315	HIS
2	B	334	HIS
2	B	442	ASN
2	B	463	GLN
2	B	530	GLN
2	B	597	HIS
2	B	634	ASN
2	B	639	ASN
2	B	698	GLN
2	B	713	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	720	GLN
2	B	754	HIS
2	B	808	HIS
3	C	118	ASN
3	C	130	GLN
1	D	5	HIS
1	D	11	ASN
2	E	19	GLN
2	E	115	ASN
2	E	273	ASN
2	E	315	HIS
2	E	442	ASN
2	E	457	HIS
2	E	463	GLN
2	E	597	HIS
2	E	698	GLN
2	E	713	GLN
2	E	754	HIS
2	E	790	GLN
3	F	79	HIS
3	F	123	ASN
3	F	221	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](#)

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	D	4907	1	0,4,4	-	-	-		
6	CUM	E	4921	9,2,7	0,4,4	-	-	-		
8	FAD	F	4931	-	20,20,58	3.35	10 (50%)	26,30,89	2.10	9 (34%)
5	FES	A	3907	1	0,4,4	-	-	-		
7	MCN	B	3920	6	42,48,48	2.97	10 (23%)	55,74,74	2.19	16 (29%)
5	FES	D	4908	1	0,4,4	-	-	-		
6	CUM	B	3921	9,2,7	0,4,4	-	-	-		
8	FAD	C	3932	-	20,20,58	3.58	14 (70%)	26,30,89	2.07	8 (30%)
4	PO4	A	3001	-	4,4,4	2.43	2 (50%)	6,6,6	1.78	2 (33%)
5	FES	A	3908	1	0,4,4	-	-	-		
7	MCN	E	4920	6	42,48,48	2.78	14 (33%)	55,74,74	2.34	20 (36%)

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	D	4907	1	-	-	0/1/1/1
8	FAD	F	4931	-	-	-	0/3/3/6
5	FES	A	3907	1	-	-	0/1/1/1
7	MCN	B	3920	6	-	1/22/54/54	0/5/5/5
5	FES	D	4908	1	-	-	0/1/1/1
8	FAD	C	3932	-	-	-	0/3/3/6
5	FES	A	3908	1	-	-	0/1/1/1
7	MCN	E	4920	6	-	2/22/54/54	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3920	MCN	C6'-N5'	14.44	1.52	1.32
7	E	4920	MCN	C6'-N5'	8.76	1.44	1.32
7	E	4920	MCN	C7-N8'	8.07	1.48	1.30
8	F	4931	FAD	C9-C8	7.84	1.50	1.39
7	B	3920	MCN	C7-N8'	7.41	1.47	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4920	MCN	C6'-C7	6.51	1.54	1.43
8	C	3932	FAD	C9-C8	6.09	1.47	1.39
8	F	4931	FAD	O4-C4	5.54	1.34	1.23
8	C	3932	FAD	C9-C9A	5.45	1.48	1.39
8	C	3932	FAD	C6-C5X	5.45	1.48	1.40
8	F	4931	FAD	C6-C7	5.24	1.46	1.39
8	C	3932	FAD	O4-C4	4.94	1.32	1.23
8	C	3932	FAD	C9A-C5X	-4.77	1.34	1.41
7	E	4920	MCN	C10-C9'	4.65	1.58	1.51
8	C	3932	FAD	C9A-N10	-4.36	1.32	1.39
8	F	4931	FAD	C9A-C5X	-4.32	1.34	1.41
8	C	3932	FAD	C6-C7	4.22	1.45	1.39
8	F	4931	FAD	C4X-N5	4.14	1.39	1.30
7	E	4920	MCN	PB-O3A	4.04	1.63	1.59
8	C	3932	FAD	C8-C7	4.04	1.50	1.40
8	F	4931	FAD	C6-C5X	3.95	1.46	1.40
4	A	3001	PO4	P-O1	3.94	1.59	1.50
7	E	4920	MCN	C4A-N5'	3.83	1.45	1.37
8	C	3932	FAD	C7M-C7	3.75	1.58	1.51
8	F	4931	FAD	C8-C7	3.61	1.49	1.40
7	B	3920	MCN	C4A-N5'	3.51	1.44	1.37
8	F	4931	FAD	C9-C9A	3.50	1.45	1.39
7	E	4920	MCN	C2'-N3'	3.43	1.41	1.35
7	B	3920	MCN	C6'-C7	3.37	1.49	1.43
7	B	3920	MCN	PA-O3A	3.36	1.63	1.59
7	E	4920	MCN	O3'-C3'	3.29	1.51	1.43
8	F	4931	FAD	O2-C2	3.26	1.30	1.24
8	C	3932	FAD	C10-N10	-3.19	1.32	1.36
8	C	3932	FAD	C10-N1	3.14	1.38	1.32
8	F	4931	FAD	C7M-C7	3.03	1.56	1.51
7	B	3920	MCN	O3'-C3'	2.73	1.49	1.43
7	E	4920	MCN	PB-O2B	-2.73	1.42	1.55
7	E	4920	MCN	C1'-N1	-2.71	1.39	1.47
4	A	3001	PO4	P-O3	2.62	1.62	1.54
7	E	4920	MCN	C2-N3	2.62	1.41	1.36
8	C	3932	FAD	C4X-C10	-2.57	1.36	1.43
7	B	3920	MCN	C4'-N3'	2.46	1.42	1.36
8	C	3932	FAD	C5X-N5	-2.36	1.35	1.39
8	C	3932	FAD	C2-N1	-2.33	1.31	1.36
7	E	4920	MCN	O4D-C1'	2.26	1.47	1.42
7	E	4920	MCN	C5-C4	2.23	1.48	1.42
7	B	3920	MCN	C4B-N1'	2.19	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3920	MCN	C1'-N1	2.16	1.53	1.47
7	E	4920	MCN	C2D-C1'	2.15	1.60	1.53
7	B	3920	MCN	C5'-C4D	2.03	1.57	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	4920	MCN	O9'-C7-C6'	-7.44	109.34	120.97
7	E	4920	MCN	O9'-C7-N8'	-5.71	107.59	115.12
7	E	4920	MCN	N1'-C2'-N3'	-5.64	120.04	127.21
7	B	3920	MCN	O9'-C7-N8'	-5.51	107.84	115.12
7	B	3920	MCN	O9'-C7-C6'	-5.40	112.53	120.97
7	E	4920	MCN	C4A-C4B-N1'	5.13	129.69	121.74
7	B	3920	MCN	C6'-N5'-C4A	-4.93	106.76	117.06
8	F	4931	FAD	C6-C5X-C9A	4.93	123.43	118.69
7	B	3920	MCN	C4B-C4A-N5'	4.62	127.50	122.35
8	C	3932	FAD	C6-C5X-N5	-4.60	110.80	118.44
7	B	3920	MCN	C2'-N3'-C4'	4.23	125.43	116.31
7	B	3920	MCN	O4'-C4'-C4A	4.19	127.29	119.53
8	C	3932	FAD	C5X-N5-C4X	-3.82	111.91	118.09
8	F	4931	FAD	O2-C2-N3	-3.76	111.37	118.58
7	E	4920	MCN	O2-C2-N1	3.71	126.17	118.90
8	C	3932	FAD	C9A-C5X-N5	3.68	126.77	121.25
7	B	3920	MCN	C4-N3-C2	3.65	126.01	120.26
8	F	4931	FAD	C9-C9A-C5X	3.51	124.56	119.37
8	F	4931	FAD	C4-N3-C2	-3.49	119.44	125.64
7	E	4920	MCN	O4D-C1'-C2D	-3.47	99.18	106.62
7	E	4920	MCN	C4D-O4D-C1'	3.47	117.13	109.47
8	F	4931	FAD	N3-C2-N1	3.32	126.56	119.50
7	B	3920	MCN	N1-C2-N3	-3.30	113.08	118.80
8	C	3932	FAD	C6-C5X-C9A	3.26	121.83	118.69
4	A	3001	PO4	O3-P-O2	3.16	117.74	107.91
7	B	3920	MCN	C4A-C4B-N1'	3.11	126.56	121.74
7	E	4920	MCN	C3'-C2D-C1'	3.07	107.28	101.46
7	E	4920	MCN	C4B-C4A-N5'	3.04	125.74	122.35
7	B	3920	MCN	C6-N1-C2	3.00	125.52	120.46
7	B	3920	MCN	N1'-C2'-N3'	-2.95	123.46	127.21
8	C	3932	FAD	C4-N3-C2	-2.94	120.41	125.64
8	C	3932	FAD	C9-C9A-C5X	2.85	123.58	119.37
8	F	4931	FAD	C7M-C7-C8	-2.77	115.11	120.76
7	B	3920	MCN	O2-C2-N3	2.75	126.66	122.33
7	E	4920	MCN	C6'-N5'-C4A	-2.64	111.54	117.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	4920	MCN	N4-C4-N3	2.62	122.59	117.91
8	F	4931	FAD	C9A-C9-C8	-2.55	114.49	119.92
8	F	4931	FAD	C6-C5X-N5	-2.53	114.25	118.44
8	C	3932	FAD	C4X-C4-N3	2.53	119.68	113.25
7	E	4920	MCN	O4'-C4'-C4A	2.47	124.11	119.53
8	F	4931	FAD	C5X-C6-C7	-2.47	116.25	120.83
7	E	4920	MCN	C2'-N3'-C4'	2.46	121.61	116.31
7	B	3920	MCN	C5-C6-N1	-2.45	117.86	121.84
7	E	4920	MCN	O2-C2-N3	-2.42	118.52	122.33
7	E	4920	MCN	C6-N1-C2	2.40	124.52	120.46
4	A	3001	PO4	O2-P-O1	-2.35	102.65	110.95
7	E	4920	MCN	C7-N8'-C4B	2.32	120.08	117.01
7	B	3920	MCN	C5-C4-N3	-2.27	117.50	121.32
7	E	4920	MCN	C4A-C4B-N8'	-2.24	118.27	121.74
7	B	3920	MCN	N4-C4-N3	2.16	121.76	117.91
7	E	4920	MCN	N1-C2-N3	-2.13	115.11	118.80
7	E	4920	MCN	N2'-C2'-N1'	2.11	121.08	117.79
7	B	3920	MCN	O3'-C3'-C2D	-2.04	105.27	111.82
7	E	4920	MCN	C1'-N1-C2	-2.04	113.93	118.44
8	C	3932	FAD	C5X-C6-C7	-2.02	117.08	120.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	3920	MCN	C10-O3B-PB-O1B
7	E	4920	MCN	C10-O3B-PB-O1B
7	E	4920	MCN	C10-O3B-PB-O3A

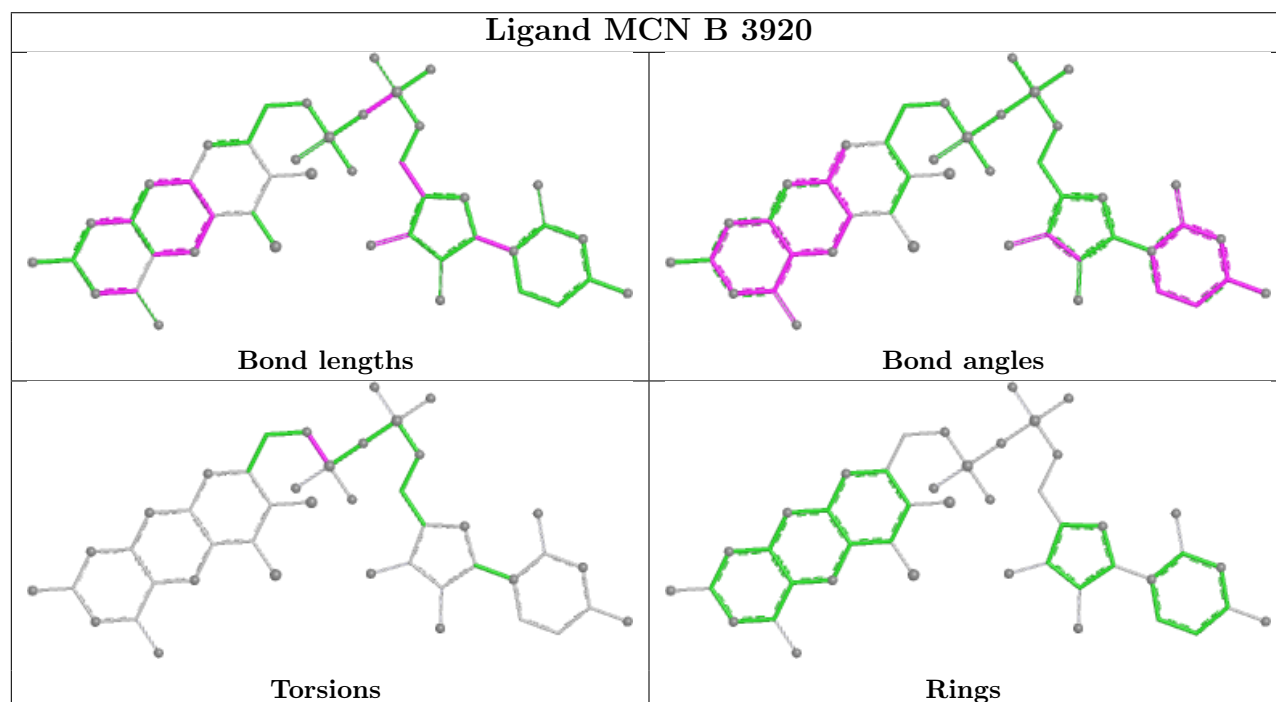
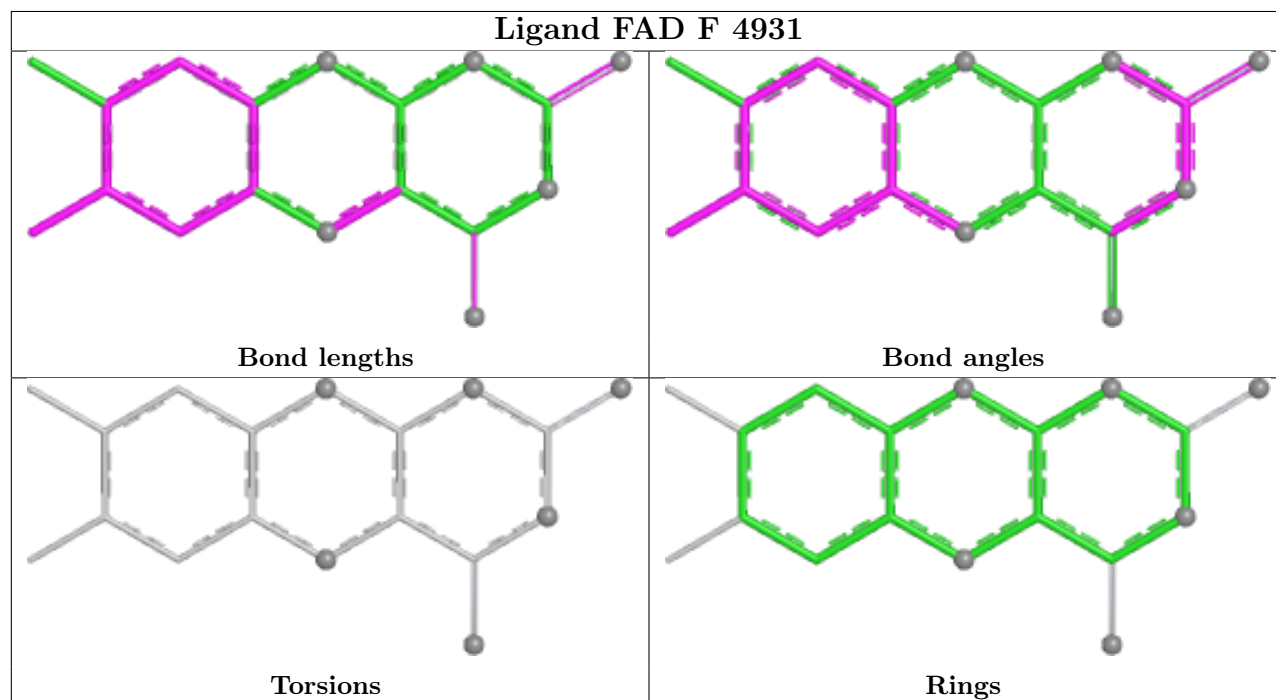
There are no ring outliers.

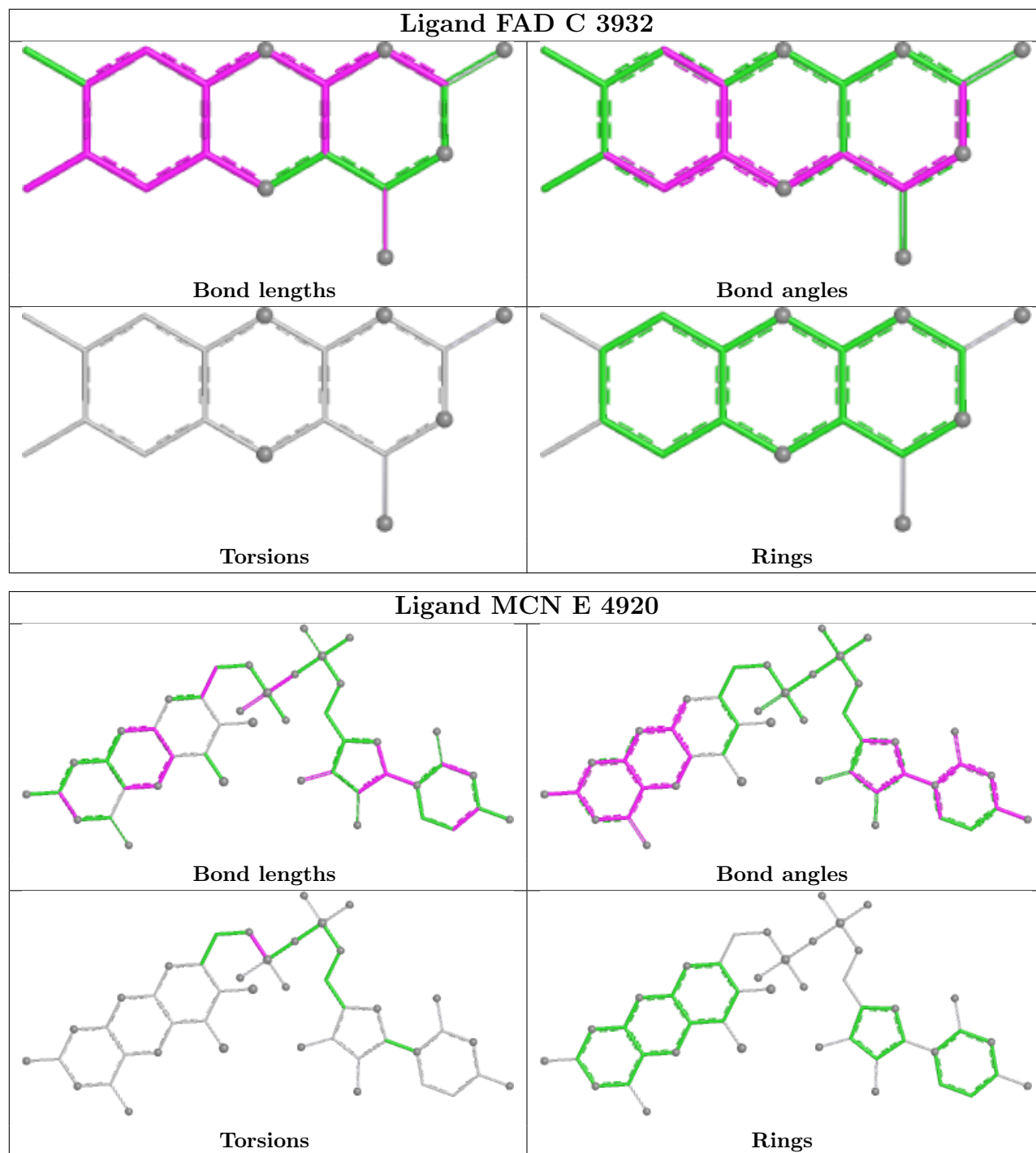
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	4931	FAD	1	0
6	B	3921	CUM	1	0
4	A	3001	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.