



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:10 PM EDT

PDB ID : 1N61 / pdb_00001n61
Title : Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Dithionite reduced state
Authors : Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on : 2002-11-08
Resolution : 1.30 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)	:	2.50

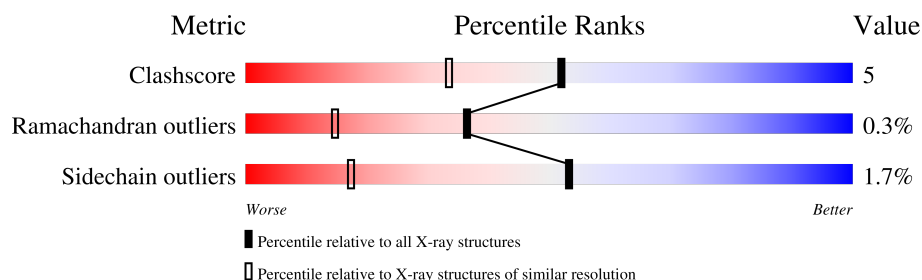
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)

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	87% 9% ..
1	D	166	84% 8% • 5%
2	B	809	86% 11% ..
2	E	809	88% 8% ..
3	C	288	91% 7% •
3	F	288	91% 6% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22269 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	4	0
			1216	754	215	231	16			
1	D	158	Total	C	N	O	S	5	3	0
			1186	734	213	223	16			

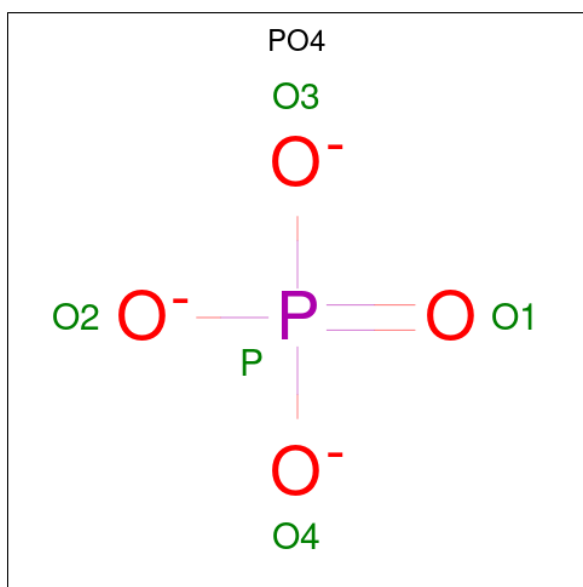
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	804	Total	C	N	O	S	76	8	0
			6232	3959	1067	1163	43			
2	E	795	Total	C	N	O	S	65	11	0
			6171	3926	1052	1147	46			

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

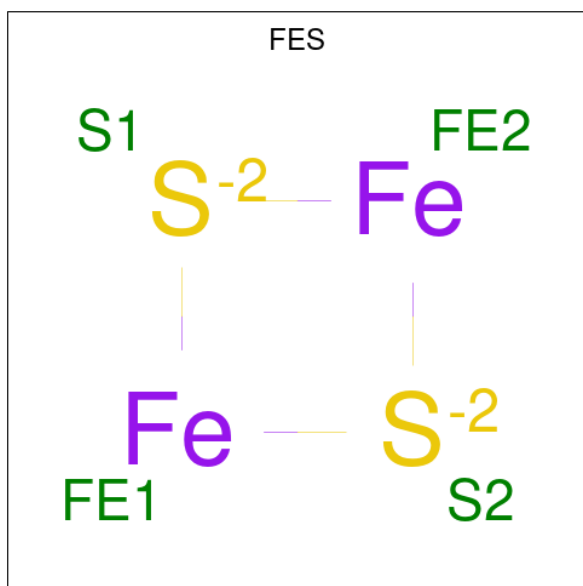
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	26	6	0
			2130	1345	373	400	12			
3	F	286	Total	C	N	O	S	34	4	0
			2114	1336	370	397	11			

- 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).



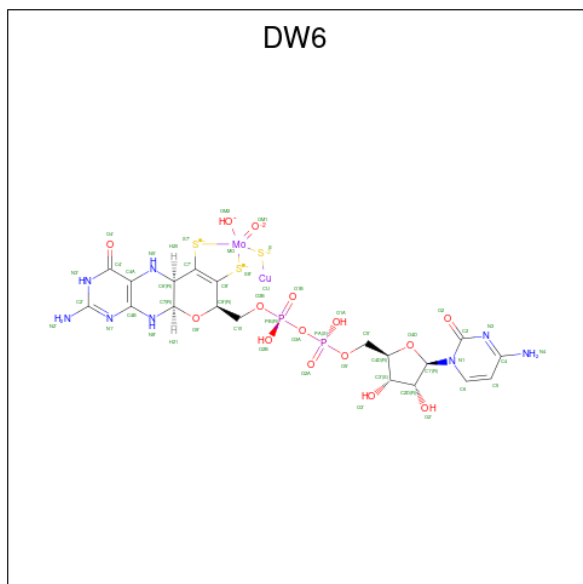
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

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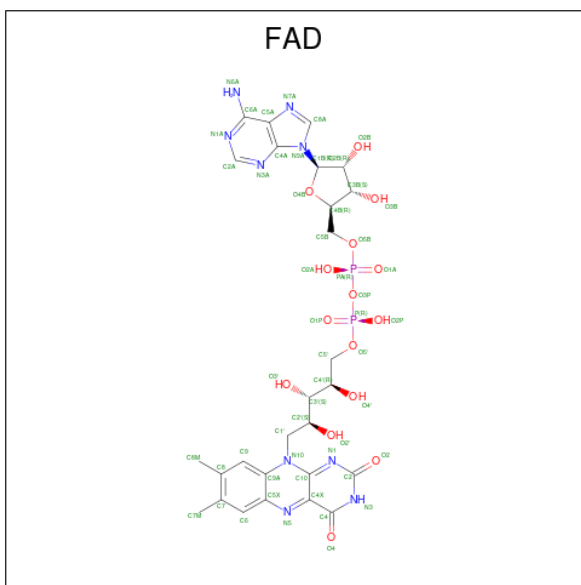
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is CuSMo(=O)OH pterin (CCD ID: DW6) (formula: $C_{19}H_{25}CuMoN_8O_{15}P_2S_3$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
6	B	1	Total	C	Cu	Mo	N	O	P	S	0	0
			49	19	1	1	8	15	2	3		
6	E	1	Total	C	Cu	Mo	N	O	P	S	0	0
			49	19	1	1	8	15	2	3		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	207	Total O 207 207	0	0
8	B	944	Total O 944 944	0	0
8	C	401	Total O 401 401	0	0
8	D	213	Total O 213 213	0	0
8	E	902	Total O 902 902	0	0
8	F	328	Total O 328 328	0	0

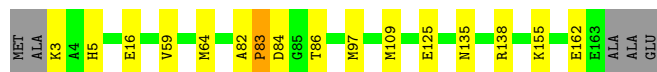
3 Residue-property plots [i](#)

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. 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: 



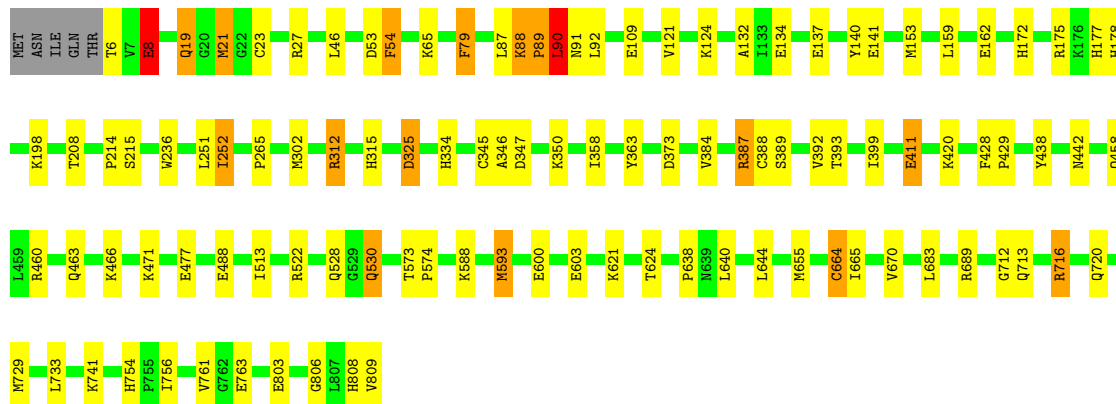
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D: 



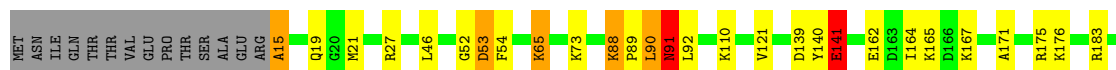
- Molecule 2: Carbon monoxide dehydrogenase large chain

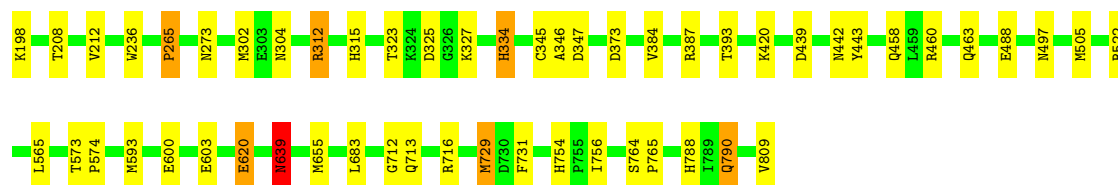
Chain B: 



- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain E: 





- Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain C: 91% 7% •



- Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain F: 91% 6% ••



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	119.16Å 131.38Å 160.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.30	Depositor
% Data completeness (in resolution range)	(Not available) (17.00-1.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.142 , 0.184	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22269	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: DW6, FES, PO4, FAD

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	0.95	2/1253 (0.2%)	0.96	2/1692 (0.1%)
1	D	1.44	8/1218 (0.7%)	1.09	5/1646 (0.3%)
2	B	1.05	18/6421 (0.3%)	1.03	19/8711 (0.2%)
2	E	1.13	19/6374 (0.3%)	0.98	19/8645 (0.2%)
3	C	1.06	5/2191 (0.2%)	1.00	4/2974 (0.1%)
3	F	1.51	5/2167 (0.2%)	1.05	10/2944 (0.3%)
All	All	1.16	57/19624 (0.3%)	1.01	59/26612 (0.2%)

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	4
1	D	0	2
2	B	1	22
2	E	0	12
3	C	0	5
3	F	0	4
All	All	1	49

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	240	LYS	CB-CG	-44.05	0.20	1.52
3	F	240	LYS	CG-CD	27.30	2.34	1.52
1	D	160	PRO	C-O	26.98	1.77	1.23
2	E	162	GLU	CD-OE1	24.07	1.71	1.25
3	F	280	GLU	CD-OE2	21.76	1.66	1.25
2	E	90	LEU	CB-CG	21.73	1.97	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	162	GLU	CD-OE2	-21.28	0.84	1.25
2	B	8	GLU	CD-OE2	19.29	1.61	1.25
2	E	65	LYS	CE-NZ	-17.18	0.97	1.49
2	B	729	MET	SD-CE	-16.01	1.39	1.79
3	C	287	LYS	CB-CG	15.13	1.97	1.52
3	C	142	GLU	CD-OE2	14.95	1.53	1.25
2	B	655	MET	SD-CE	-14.87	1.42	1.79
2	E	65	LYS	CD-CE	14.35	1.95	1.52
1	D	7	GLU	CD-OE1	-14.23	0.98	1.25
1	D	160	PRO	CA-C	-13.26	1.25	1.52
2	E	809	VAL	CB-CG2	11.34	1.90	1.52
1	D	160	PRO	CB-CG	11.16	2.05	1.49
2	E	141	GLU	CG-CD	10.82	1.79	1.52
1	D	159	VAL	CA-CB	10.74	1.60	1.54
2	E	729	MET	SD-CE	-10.34	1.53	1.79
2	B	89	PRO	C-N	9.72	1.47	1.33
2	B	593	MET	SD-CE	-9.01	1.57	1.79
2	B	664	CYS	CA-CB	8.92	1.74	1.53
2	E	639	ASN	CG-ND2	-8.80	1.14	1.33
2	B	664	CYS	N-CA	8.58	1.56	1.46
2	E	171	ALA	CA-CB	8.47	1.67	1.54
2	B	198	LYS	CE-NZ	8.31	1.74	1.49
2	E	620	GLU	CG-CD	8.18	1.72	1.52
2	E	167	LYS	CD-CE	8.17	1.76	1.52
2	B	411	GLU	CD-OE2	7.83	1.40	1.25
2	E	497	ASN	CG-ND2	7.81	1.49	1.33
2	E	73	LYS	CD-CE	7.70	1.75	1.52
2	B	141	GLU	CG-CD	7.69	1.71	1.52
2	B	88	LYS	C-N	-7.66	1.24	1.33
1	D	96	MET	SD-CE	-7.64	1.60	1.79
3	C	55	ARG	CD-NE	7.62	1.56	1.46
2	B	124	LYS	CE-NZ	-7.58	1.26	1.49
3	F	280	GLU	CD-OE1	-7.56	1.10	1.25
1	A	155	LYS	CG-CD	7.18	1.74	1.52
2	B	638	PRO	CG-CD	6.74	1.73	1.50
3	F	280	GLU	CG-CD	6.64	1.68	1.52
2	B	471	LYS	CD-CE	6.45	1.71	1.52
1	D	48	GLY	C-O	-6.41	1.15	1.23
2	B	302	MET	SD-CE	-6.26	1.63	1.79
2	E	458	GLN	CG-CD	-6.15	1.36	1.52
2	E	302	MET	SD-CE	-5.95	1.64	1.79
2	B	655	MET	CG-SD	-5.89	1.66	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	GLU	CD-OE1	-5.80	1.14	1.25
2	B	65	LYS	CG-CD	-5.71	1.35	1.52
2	E	639	ASN	CG-OD1	5.70	1.34	1.23
2	E	420	LYS	CD-CE	5.67	1.69	1.52
2	B	325	ASP	CG-OD2	5.17	1.35	1.25
1	A	97	MET	SD-CE	-5.17	1.66	1.79
1	D	31	GLU	C-O	-5.10	1.18	1.24
2	E	655	MET	SD-CE	5.10	1.92	1.79
3	C	280	GLU	CG-CD	5.04	1.64	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	PRO	O-C-N	-24.72	90.33	122.22
2	B	141	GLU	CA-CB-CG	16.32	146.73	114.10
2	E	15	ALA	N-CA-CB	16.18	134.67	110.40
3	C	287	LYS	CA-CB-CG	-15.55	83.01	114.10
1	D	160	PRO	CB-CA-C	-14.63	82.29	110.10
3	F	240	LYS	CB-CG-CD	14.58	144.84	111.30
3	F	240	LYS	CG-CD-CE	14.23	144.04	111.30
2	B	8	GLU	CG-CD-OE2	-12.34	90.02	118.40
2	E	162	GLU	CG-CD-OE2	11.40	144.63	118.40
3	F	240	LYS	CA-CB-CG	11.14	136.39	114.10
1	D	7	GLU	CG-CD-OE1	10.52	142.60	118.40
1	D	7	GLU	OE1-CD-OE2	-10.45	97.83	122.90
2	B	471	LYS	CD-CE-NZ	-10.11	79.56	111.90
2	E	162	GLU	CG-CD-OE1	-9.83	95.79	118.40
2	E	458	GLN	CB-CG-CD	9.55	128.83	112.60
1	D	160	PRO	N-CD-CG	8.99	116.69	103.20
2	E	809	VAL	CA-CB-CG1	8.96	125.64	110.40
2	B	141	GLU	CG-CD-OE1	-8.66	98.49	118.40
3	F	280	GLU	OE1-CD-OE2	-8.60	102.26	122.90
2	B	141	GLU	CG-CD-OE2	8.47	137.89	118.40
2	B	8	GLU	OE1-CD-OE2	8.45	143.17	122.90
2	E	497	ASN	OD1-CG-ND2	8.28	130.88	122.60
3	F	280	GLU	CG-CD-OE2	8.17	137.19	118.40
2	E	141	GLU	CG-CD-OE1	-7.83	100.39	118.40
2	E	639	ASN	OD1-CG-ND2	7.75	130.35	122.60
2	E	497	ASN	CB-CG-ND2	-7.63	104.96	116.40
1	A	83	PRO	CB-CA-C	-7.55	99.15	111.31
2	B	79	PHE	CZ-CE2-CD2	-7.52	106.47	120.00
2	B	137	GLU	CB-CG-CD	-7.28	100.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	PRO	CA-C-N	6.81	134.55	121.54
2	B	89	PRO	C-N-CA	6.81	134.55	121.54
3	F	240	LYS	CB-CA-C	6.75	123.47	110.17
1	A	109	MET	CG-SD-CE	6.74	115.72	100.90
3	C	45	LEU	CD1-CG-CD2	-6.46	96.60	110.80
2	E	91	ASN	OD1-CG-ND2	-6.45	116.15	122.60
3	C	142	GLU	CG-CD-OE1	6.35	133.00	118.40
2	B	6	THR	N-CA-CB	-6.09	101.15	111.50
2	E	458	GLN	CG-CD-NE2	6.09	125.53	116.40
3	F	158	PHE	CD1-CE1-CZ	-6.08	109.05	120.00
2	E	620	GLU	CG-CD-OE2	-6.05	104.49	118.40
3	F	38	ILE	N-CA-CB	6.04	114.30	110.50
2	B	6	THR	CB-CA-C	-6.00	95.89	109.10
2	E	141	GLU	CB-CG-CD	-5.96	102.47	112.60
1	D	109	MET	CG-SD-CE	5.94	113.96	100.90
2	B	399	ILE	N-CA-C	5.78	116.56	110.72
2	E	439	ASP	N-CA-C	5.75	117.35	111.14
2	E	620	GLU	CG-CD-OE1	5.71	131.53	118.40
2	E	167	LYS	CG-CD-CE	-5.70	98.18	111.30
2	E	90	LEU	CA-CB-CG	-5.57	96.80	116.30
2	B	664	CYS	N-CA-C	-5.53	100.39	109.40
2	B	638	PRO	N-CD-CG	-5.45	95.02	103.20
2	B	638	PRO	CB-CG-CD	-5.24	89.33	106.10
2	E	639	ASN	CB-CG-OD1	-5.16	110.48	120.80
2	E	809	VAL	CA-CB-CG2	-5.14	101.66	110.40
3	F	173	PRO	CA-C-N	-5.12	118.90	122.59
3	F	173	PRO	C-N-CA	-5.12	118.90	122.59
3	C	142	GLU	OE1-CD-OE2	-5.12	110.62	122.90
2	B	471	LYS	CG-CD-CE	-5.11	99.55	111.30
2	B	79	PHE	CE1-CZ-CE2	5.11	129.19	120.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	90	LEU	CA

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	162	GLU	Mainchain
1	A	82	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	83	PRO	Mainchain
2	B	109	GLU	Sidechain
2	B	134	GLU	Sidechain
2	B	140	TYR	Mainchain
2	B	162	GLU	Sidechain
2	B	19	GLN	Sidechain
2	B	27	ARG	Sidechain
2	B	312	ARG	Sidechain
2	B	363	TYR	Sidechain
2	B	387	ARG	Sidechain
2	B	411	GLU	Sidechain
2	B	54	PHE	Peptide
2	B	600	GLU	Sidechain
2	B	689[A]	ARG	Sidechain
2	B	689[B]	ARG	Sidechain
2	B	716	ARG	Sidechain
2	B	79	PHE	Sidechain
2	B	8	GLU	Sidechain
2	B	88	LYS	Mainchain
2	B	89	PRO	Mainchain,Peptide
2	B	90	LEU	Mainchain,Peptide
3	C	10	ARG	Sidechain
3	C	27	ASP	Sidechain
3	C	286	ALA	Peptide
3	C	44	ARG	Sidechain
3	C	59	ASP	Sidechain
1	D	138	ARG	Sidechain
1	D	83	PRO	Mainchain
2	E	140	TYR	Mainchain
2	E	141	GLU	Sidechain
2	E	175	ARG	Sidechain
2	E	27	ARG	Sidechain
2	E	312	ARG	Sidechain
2	E	334	HIS	Sidechain
2	E	387	ARG	Sidechain
2	E	443	TYR	Sidechain
2	E	53	ASP	Mainchain
2	E	600	GLU	Sidechain
2	E	620	GLU	Mainchain
2	E	88	LYS	Mainchain
3	F	141	PRO	Mainchain
3	F	163	PRO	Mainchain

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Mol	Chain	Res	Type	Group
3	F	29	ARG	Sidechain
3	F	86	PHE	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	1216	0	1189	12	0
1	D	1186	0	1167	14	0
2	B	6232	0	6114	69	1
2	E	6171	0	6049	65	1
3	C	2130	0	2183	19	0
3	F	2114	0	2167	15	0
4	A	5	0	0	1	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	49	0	0	1	0
6	E	49	0	0	0	0
7	C	53	0	31	1	0
7	F	53	0	31	3	0
8	A	207	0	0	2	1
8	B	944	0	0	19	0
8	C	401	0	0	6	0
8	D	213	0	0	4	0
8	E	902	0	0	10	1
8	F	328	0	0	3	0
All	All	22269	0	18931	192	2

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 (192) 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[B]:MET:HG2	2:E:603:GLU:OE1	1.25	1.31
2:E:593[A]:MET:HG2	2:E:603:GLU:OE1	1.25	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:HG11	1:A:64[A]:MET:CE	1.70	1.20
1:D:59:VAL:HG11	1:D:64[A]:MET:HE1	1.24	1.19
2:B:92:LEU:HD21	2:B:252:ILE:HG23	1.25	1.16
2:B:21[A]:MET:HE2	8:B:4470:HOH:O	0.93	1.11
2:E:716:ARG:NE	8:E:5338:HOH:O	1.83	1.09
1:D:59:VAL:HG11	1:D:64[A]:MET:CE	1.84	1.07
2:E:65:LYS:HE2	2:E:141:GLU:OE2	1.55	1.06
2:E:88:LYS:HB2	2:E:89:PRO:HD3	1.41	1.03
1:D:118[A]:GLN:OE1	8:D:5051:HOH:O	1.81	0.99
1:A:59:VAL:HG11	1:A:64[A]:MET:HE1	0.99	0.98
2:E:90:LEU:O	2:E:92:LEU:CD1	2.13	0.96
1:A:59:VAL:CG1	1:A:64[A]:MET:HE1	1.94	0.96
2:B:713:GLN:OE1	8:B:4856:HOH:O	1.85	0.95
2:E:639:ASN:HB3	8:E:5819:HOH:O	1.66	0.94
1:D:3:LYS:N	8:D:5049:HOH:O	2.00	0.93
1:D:92:GLU:HG3	8:D:5072:HOH:O	1.69	0.91
2:B:92:LEU:CD2	2:B:252:ILE:HG23	2.01	0.90
1:D:11:ASN:HD21	1:D:76:THR:H	1.23	0.87
1:A:59:VAL:CG1	1:A:64[A]:MET:CE	2.51	0.87
2:E:21[A]:MET:HE1	2:E:756:ILE:HD12	1.57	0.86
2:B:21[A]:MET:HE1	2:B:756:ILE:HG21	1.57	0.85
3:C:280:GLU:HG3	8:C:4128:HOH:O	1.76	0.85
2:E:334:HIS:ND1	8:E:5775:HOH:O	2.10	0.84
2:B:713:GLN:CD	8:B:4856:HOH:O	2.20	0.83
2:E:208:THR:H	2:E:790:GLN:HE22	1.23	0.83
2:E:65:LYS:CE	2:E:141:GLU:OE2	2.26	0.83
2:B:19:GLN:OE1	2:B:23[A]:CYS:SG	2.37	0.83
2:B:460:ARG:HH11	2:B:463:GLN:HE22	1.28	0.81
2:B:528:GLN:H	2:B:530:GLN:HE22	1.28	0.81
2:E:21[A]:MET:HE1	2:E:756:ILE:CD1	2.12	0.78
2:E:713[A]:GLN:CD	2:E:731:PHE:CZ	2.63	0.77
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.32	0.76
2:E:639:ASN:HB3	8:E:5654:HOH:O	1.86	0.75
2:B:53:ASP:CG	8:B:4860:HOH:O	2.30	0.74
1:D:59:VAL:CG1	1:D:64[A]:MET:CE	2.64	0.73
2:B:21[A]:MET:HE1	2:B:756:ILE:CG2	2.18	0.73
2:E:273:ASN:HD21	2:E:304:ASN:HD21	1.37	0.73
2:E:91:ASN:C	2:E:92:LEU:HD12	2.16	0.70
2:E:90:LEU:CB	2:E:92:LEU:HD13	2.22	0.70
2:E:88:LYS:CB	2:E:89:PRO:HD3	2.20	0.69
1:A:84:ASP:OD1	1:A:86:THR:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:MET:CE	2:B:640:LEU:HD21	2.24	0.68
2:E:141:GLU:CD	2:E:141:GLU:CB	2.67	0.68
2:E:593[B]:MET:HE1	8:E:5546:HOH:O	1.93	0.67
2:B:46:LEU:HD11	2:B:236[B]:TRP:CZ3	2.29	0.67
2:B:87:LEU:O	2:B:90:LEU:HA	1.95	0.67
2:E:90:LEU:O	2:E:92:LEU:HD12	1.94	0.66
2:E:713[A]:GLN:HG2	2:E:731:PHE:CE1	2.32	0.65
3:F:102:ALA:CB	3:F:106[A]:ILE:HG21	2.27	0.65
2:B:803:GLU:OE1	2:B:808:HIS:HD2	1.80	0.63
1:A:125:GLU:OE2	2:B:741[A]:LYS:HD3	1.98	0.63
2:B:528:GLN:H	2:B:530:GLN:NE2	1.95	0.63
2:E:754:HIS:HD2	2:E:756:ILE:H	1.46	0.63
1:D:59:VAL:CG1	1:D:64[A]:MET:HE1	2.15	0.62
2:B:522:ARG:NH1	8:B:4858:HOH:O	2.25	0.61
1:D:159:VAL:N	1:D:160:PRO:HD2	2.14	0.61
1:A:135:ASN:HD21	3:C:105:GLN:HE22	1.46	0.61
3:F:280:GLU:OE2	3:F:280:GLU:OE1	2.18	0.61
1:A:5:HIS:HD2	4:A:3001:PO4:O2	1.85	0.60
2:E:713[A]:GLN:NE2	2:E:731:PHE:CZ	2.69	0.60
1:D:160:PRO:O	1:D:160:PRO:CA	2.50	0.60
2:E:716:ARG:CZ	8:E:5338:HOH:O	2.34	0.60
2:B:530:GLN:HE21	2:B:530:GLN:H	1.48	0.60
2:B:741[B]:LYS:HE3	8:B:4640:HOH:O	2.01	0.60
2:B:593:MET:HE1	2:B:640:LEU:HD21	1.84	0.59
1:D:118[A]:GLN:NE2	8:D:4974:HOH:O	2.36	0.59
2:B:754:HIS:HD2	2:B:756:ILE:H	1.50	0.59
2:E:593[B]:MET:HG2	2:E:603:GLU:CD	2.22	0.58
6:B:810:DW6:OM1	6:B:810:DW6:MO	1.72	0.58
2:B:670:VAL:O	2:B:808:HIS:HE1	1.86	0.58
2:E:90:LEU:HB2	2:E:92:LEU:HD13	1.85	0.58
2:E:593[A]:MET:HE2	8:E:5101:HOH:O	2.04	0.57
2:E:603:GLU:HG3	8:E:5491:HOH:O	2.04	0.57
3:F:106[B]:ILE:HD13	7:F:4931:FAD:C7	2.34	0.57
2:E:90:LEU:C	2:E:92:LEU:CD1	2.77	0.57
2:E:208:THR:OG1	2:E:315:HIS:HD2	1.87	0.57
1:A:5:HIS:HE1	1:A:16:GLU:OE2	1.86	0.57
2:E:88:LYS:HB2	2:E:89:PRO:CD	2.27	0.57
2:E:19:GLN:NE2	8:E:5283:HOH:O	2.37	0.56
2:B:442:ASN:C	2:B:442:ASN:HD22	2.12	0.56
1:D:96:MET:HE2	1:D:96:MET:HA	1.87	0.56
2:E:92:LEU:HD12	2:E:92:LEU:N	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204[A]:MET:HG3	3:C:286:ALA:CB	2.36	0.56
1:A:3:LYS:N	8:A:4040:HOH:O	2.39	0.56
1:A:135:ASN:ND2	3:C:105:GLN:HE22	2.03	0.55
2:B:588:LYS:HD2	8:B:4246:HOH:O	2.06	0.55
2:E:713[A]:GLN:CG	2:E:731:PHE:CE1	2.89	0.55
2:E:90:LEU:O	2:E:92:LEU:HD11	2.06	0.55
2:E:90:LEU:C	2:E:92:LEU:HD13	2.32	0.55
2:B:720:GLN:HG3	8:B:4723:HOH:O	2.07	0.54
3:C:240:LYS:HB3	3:C:241:PRO:HD3	1.89	0.54
2:E:46:LEU:HD11	2:E:236[B]:TRP:CZ3	2.42	0.54
2:B:593:MET:HE2	2:B:640:LEU:HD21	1.90	0.54
3:C:118:ASN:HD22	7:C:3932:FAD:H4B	1.73	0.54
3:C:158:PHE:HB2	8:C:4252:HOH:O	2.08	0.54
2:B:573:THR:HB	2:B:574:PRO:HD3	1.90	0.53
2:B:716:ARG:CZ	8:B:4268:HOH:O	2.56	0.53
2:B:325:ASP:O	2:B:420:LYS:HE2	2.09	0.53
2:E:754:HIS:CD2	2:E:756:ILE:H	2.26	0.53
2:E:442:ASN:HD22	2:E:442:ASN:C	2.16	0.53
3:F:45:LEU:HD12	8:F:5161:HOH:O	2.09	0.53
2:B:716:ARG:NE	8:B:4268:HOH:O	2.42	0.52
3:F:118:ASN:HD22	7:F:4931:FAD:H4B	1.75	0.52
2:E:90:LEU:O	2:E:92:LEU:HD13	2.06	0.52
2:B:806:GLY:O	2:B:809:VAL:HG22	2.10	0.52
3:C:204[A]:MET:HG3	3:C:286:ALA:HB1	1.92	0.51
2:B:754:HIS:CD2	2:B:756:ILE:H	2.28	0.51
2:B:664:CYS:C	2:B:665:ILE:HD12	2.35	0.51
2:B:713:GLN:NE2	2:B:733:LEU:HD23	2.24	0.51
2:B:741[A]:LYS:CD	8:B:4308:HOH:O	2.58	0.51
2:E:593[A]:MET:HG2	2:E:603:GLU:CD	2.28	0.51
2:B:665:ILE:HD12	2:B:665:ILE:N	2.25	0.51
2:B:334:HIS:HE1	2:B:373:ASP:OD2	1.93	0.51
2:B:53:ASP:CB	8:B:4860:HOH:O	2.60	0.50
2:B:458:GLN:HG2	8:B:4236:HOH:O	2.10	0.50
2:B:466:LYS:HE2	2:B:477:GLU:HG2	1.93	0.50
2:B:53:ASP:HB2	8:B:4860:HOH:O	2.11	0.50
2:B:350:LYS:HE3	8:B:4657:HOH:O	2.12	0.50
2:B:593:MET:HG2	2:B:603:GLU:OE2	2.12	0.50
2:E:53:ASP:CG	2:E:54:PHE:H	2.21	0.49
3:F:79:HIS:HD2	8:F:5192:HOH:O	1.94	0.49
2:E:788:HIS:HE2	2:E:790:GLN:NE2	2.10	0.49
3:C:221[A]:ASN:ND2	8:C:4132:HOH:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:522:ARG:NH1	8:E:5403:HOH:O	2.44	0.49
2:B:153:MET:HA	2:B:177:HIS:CE1	2.49	0.48
3:F:137:GLU:HG2	3:F:146:ILE:CD1	2.44	0.48
2:B:513:ILE:HD12	2:B:644:LEU:HD23	1.96	0.48
1:D:59:VAL:HG11	1:D:64[A]:MET:HE3	1.85	0.48
2:B:741[A]:LYS:HD2	8:B:4308:HOH:O	2.11	0.48
2:B:53:ASP:CG	2:B:54:PHE:H	2.23	0.47
3:F:102:ALA:CB	3:F:106[A]:ILE:CG2	2.92	0.47
3:F:106[B]:ILE:HD13	7:F:4931:FAD:C8	2.45	0.47
3:C:222:THR:HB	3:C:223:PRO:HD2	1.97	0.46
1:D:5:HIS:HA	1:D:18:LEU:HD12	1.97	0.46
2:E:683:LEU:C	2:E:683:LEU:HD23	2.40	0.46
2:B:428:PHE:HA	2:B:429:PRO:C	2.41	0.46
2:B:624:THR:HB	8:B:4150:HOH:O	2.15	0.46
2:E:92:LEU:CD1	2:E:92:LEU:N	2.79	0.46
3:C:204[A]:MET:CE	3:C:238:LEU:HD12	2.46	0.46
2:E:21[A]:MET:HE1	2:E:756:ILE:HD13	1.93	0.45
3:C:285:ARG:CZ	8:C:4141:HOH:O	2.65	0.45
2:E:88:LYS:CB	2:E:89:PRO:CD	2.88	0.45
3:C:221[A]:ASN:ND2	8:C:4117:HOH:O	2.50	0.45
2:E:212:VAL:HB	2:E:713[A]:GLN:NE2	2.32	0.45
2:B:208:THR:OG1	2:B:315:HIS:HD2	1.99	0.45
2:B:683:LEU:HD23	2:B:683:LEU:C	2.42	0.45
2:E:764:SER:N	2:E:765:PRO:HD2	2.31	0.44
2:B:175:ARG:NH2	2:B:178:HIS:O	2.50	0.44
2:B:809:VAL:O	2:B:809:VAL:HG23	2.17	0.44
3:F:137:GLU:HG2	3:F:146:ILE:HD13	1.98	0.44
2:B:334:HIS:HD2	8:B:4196:HOH:O	2.01	0.44
2:B:460:ARG:NH1	2:B:463:GLN:HE22	2.06	0.44
2:B:530:GLN:NE2	2:B:530:GLN:H	2.16	0.43
2:B:803:GLU:OE1	2:B:808:HIS:CD2	2.66	0.43
3:F:28:ALA:O	3:F:29:ARG:HD2	2.17	0.43
2:B:121:VAL:HG11	2:B:132:ALA:HB3	2.00	0.43
3:F:221:ASN:ND2	8:F:5112:HOH:O	2.50	0.43
3:C:138:LEU:HD23	3:C:167:LEU:HA	1.99	0.43
2:B:384:VAL:HG13	2:B:388:CYS:SG	2.59	0.43
3:C:287:LYS:CA	8:C:4089:HOH:O	2.66	0.43
2:E:505:MET:HA	2:E:565:LEU:HG	1.99	0.43
1:A:3:LYS:CA	8:A:4040:HOH:O	2.67	0.43
3:C:204[A]:MET:HE1	3:C:238:LEU:HD12	2.01	0.43
2:E:52:GLY:HA2	2:E:121:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:ILE:HG13	2:E:165:LYS:HG2	2.01	0.43
2:E:208:THR:H	2:E:790:GLN:NE2	2.02	0.43
2:E:345:CYS:SG	2:E:384:VAL:HG23	2.59	0.43
2:E:713[A]:GLN:NE2	2:E:731:PHE:HZ	2.16	0.42
2:E:346:ALA:O	2:E:347:ASP:CG	2.62	0.42
3:F:202:LEU:C	3:F:202:LEU:HD12	2.45	0.42
3:F:222:THR:HB	3:F:223:PRO:HD2	2.01	0.42
2:B:389:SER:HB2	2:B:392:VAL:HB	2.01	0.42
2:B:593:MET:HE2	2:B:593:MET:HB3	1.77	0.41
2:E:573:THR:HB	2:E:574:PRO:HD3	2.02	0.41
2:B:172:HIS:HD2	8:B:4630:HOH:O	2.02	0.41
2:E:593[B]:MET:HE3	2:E:603:GLU:OE1	2.21	0.41
2:E:729:MET:HB2	2:E:729:MET:HE2	1.88	0.41
2:B:345:CYS:SG	2:B:384:VAL:HG23	2.60	0.41
2:B:346:ALA:O	2:B:347:ASP:CG	2.64	0.41
2:E:183:ARG:HD2	2:E:373:ASP:OD1	2.21	0.41
2:B:387:ARG:HA	2:B:763:GLU:HG2	2.03	0.41
3:F:243:LEU:HD13	3:F:243:LEU:HA	1.93	0.41
2:E:323:THR:OG1	2:E:325:ASP:OD2	2.36	0.40
2:E:713[A]:GLN:CG	2:E:731:PHE:CZ	3.04	0.40
2:B:621:LYS:HA	2:B:621:LYS:HD2	1.93	0.40
2:B:214:PRO:O	2:B:215:SER:C	2.65	0.40
2:B:358:ILE:HD11	2:B:438:TYR:CE1	2.57	0.40

All (2) 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:458:GLN:NE2	8:E:5418:HOH:O[4_477]	1.23	0.97
2:E:15:ALA:N	8:A:4033:HOH:O[4_577]	1.69	0.51

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	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
1	D	159/166 (96%)	156 (98%)	3 (2%)	0	100	100
2	B	810/809 (100%)	783 (97%)	22 (3%)	5 (1%)	21	4
2	E	804/809 (99%)	772 (96%)	29 (4%)	3 (0%)	30	9
3	C	291/288 (101%)	288 (99%)	3 (1%)	0	100	100
3	F	288/288 (100%)	283 (98%)	5 (2%)	0	100	100
All	All	2514/2526 (100%)	2441 (97%)	65 (3%)	8 (0%)	36	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	LEU
2	B	312	ARG
2	B	265	PRO
2	B	712	GLY
2	E	312	ARG
2	E	712	GLY
2	E	265	PRO
2	B	761	VAL

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	133/131 (102%)	133 (100%)	0	100	100
1	D	129/131 (98%)	128 (99%)	1 (1%)	73	45
2	B	656/653 (100%)	645 (98%)	11 (2%)	53	17
2	E	651/653 (100%)	639 (98%)	12 (2%)	51	16
3	C	217/212 (102%)	209 (96%)	8 (4%)	30	3
3	F	214/212 (101%)	210 (98%)	4 (2%)	50	14
All	All	2000/1992 (100%)	1964 (98%)	36 (2%)	53	16

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	GLU
2	B	21[A]	MET
2	B	21[B]	MET
2	B	90	LEU
2	B	91	ASN
2	B	159	LEU
2	B	251	LEU
2	B	252	ILE
2	B	393	THR
2	B	488	GLU
2	B	530	GLN
3	C	20	LEU
3	C	26	GLU
3	C	45	LEU
3	C	59	ASP
3	C	106	ILE
3	C	221[A]	ASN
3	C	221[B]	ASN
3	C	287	LYS
1	D	18	LEU
2	E	91	ASN
2	E	110	LYS
2	E	139	ASP
2	E	141	GLU
2	E	176	LYS
2	E	198	LYS
2	E	265	PRO
2	E	327	LYS
2	E	393	THR
2	E	488	GLU
2	E	639	ASN
2	E	790	GLN
3	F	87	LEU
3	F	146	ILE
3	F	221	ASN
3	F	240	LYS

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

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Mol	Chain	Res	Type
1	A	13	HIS
1	A	33	GLN
1	A	34	ASN
1	A	135	ASN
2	B	115	ASN
2	B	172	HIS
2	B	258	HIS
2	B	315	HIS
2	B	334	HIS
2	B	442	ASN
2	B	463	GLN
2	B	530	GLN
2	B	592	GLN
2	B	597	HIS
2	B	634	ASN
2	B	639	ASN
2	B	713	GLN
2	B	754	HIS
2	B	808	HIS
3	C	118	ASN
3	C	154	GLN
1	D	11	ASN
1	D	32	GLN
2	E	19	GLN
2	E	59	HIS
2	E	91	ASN
2	E	103	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	592	GLN
2	E	597	HIS
2	E	754	HIS
2	E	790	GLN
2	E	804	GLN
3	F	79	HIS
3	F	118	ASN
3	F	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	-	-	-		
5	FES	D	4908	1	0,4,4	-	-	-		
6	DW6	E	810	2	46,54,54	2.18	14 (30%)	54,87,87	2.07	11 (20%)
6	DW6	B	810	2	46,54,54	1.70	5 (10%)	54,87,87	1.33	5 (9%)
5	FES	A	3908	1	0,4,4	-	-	-		
4	PO4	A	3001	-	4,4,4	0.92	0	6,6,6	1.50	1 (16%)
7	FAD	F	4931	-	58,58,58	1.11	2 (3%)	85,89,89	1.28	10 (11%)
5	FES	D	4907	1	0,4,4	-	-	-		
7	FAD	C	3932	-	58,58,58	1.02	3 (5%)	85,89,89	1.08	7 (8%)

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	-	-	0/1/1/1
6	DW6	E	810	2	-	1/22/82/82	0/6/6/6
5	FES	D	4908	1	-	-	0/1/1/1
6	DW6	B	810	2	-	1/22/82/82	0/6/6/6
5	FES	A	3908	1	-	-	0/1/1/1
7	FAD	F	4931	-	-	2/34/50/50	0/6/6/6
7	FAD	C	3932	-	-	2/34/50/50	0/6/6/6
5	FES	D	4907	1	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	810	DW6	C10-C9'	7.95	1.62	1.51
6	E	810	DW6	C7-C6'	-7.29	1.47	1.53
6	E	810	DW6	O4'-C4'	4.68	1.32	1.23
7	F	4931	FAD	C4X-N5	4.46	1.40	1.30
7	C	3932	FAD	C4X-N5	4.10	1.39	1.30
6	E	810	DW6	C2-N3	3.91	1.44	1.36
6	E	810	DW6	C4B-N8'	3.80	1.39	1.35
6	B	810	DW6	PA-O3A	3.68	1.63	1.59
6	E	810	DW6	OM1-MO	3.55	1.78	1.69
6	E	810	DW6	O2-C2	3.11	1.29	1.23
6	E	810	DW6	O9'-C9'	-3.11	1.37	1.43
7	F	4931	FAD	C5'-C4'	3.10	1.56	1.51
6	E	810	DW6	C6'-N5'	3.06	1.49	1.46
6	E	810	DW6	MO-S8'	2.99	2.43	2.39
6	E	810	DW6	C4'-N3'	-2.79	1.33	1.38
6	E	810	DW6	C10-C9'	-2.71	1.48	1.51
6	E	810	DW6	C6-C5	2.71	1.41	1.35
6	B	810	DW6	MO-S7'	-2.55	2.35	2.39
6	E	810	DW6	C2-N1	-2.40	1.35	1.40
7	C	3932	FAD	P-O3P	2.34	1.62	1.59
6	B	810	DW6	O4D-C1'	-2.31	1.36	1.42
6	B	810	DW6	MO-S8'	2.22	2.42	2.39
7	C	3932	FAD	C10-N1	2.18	1.37	1.33
6	E	810	DW6	PA-O3A	2.17	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	810	DW6	C7-C6'-N5'	8.51	116.23	107.87
6	E	810	DW6	C8'-C7'-S7'	7.22	124.25	120.15
6	B	810	DW6	O9'-C9'-C8'	4.65	115.65	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	810	DW6	C2'-N1'-C4B	4.07	120.54	113.36
7	F	4931	FAD	C9A-C5X-N5	-3.89	118.33	122.45
6	E	810	DW6	O4'-C4'-C4A	-3.52	118.77	127.26
7	F	4931	FAD	N3A-C2A-N1A	-3.46	123.34	128.58
4	A	3001	PO4	O3-P-O2	3.09	117.53	107.91
7	F	4931	FAD	C4X-C10-N10	3.07	120.88	116.48
7	F	4931	FAD	C5X-C9A-N10	3.01	120.69	117.97
6	E	810	DW6	O2-C2-N3	-2.74	118.02	122.33
6	E	810	DW6	C4A-C4'-N3'	2.70	119.54	112.13
6	B	810	DW6	C7-C6'-N5'	2.63	110.45	107.87
7	C	3932	FAD	N3A-C2A-N1A	-2.61	124.63	128.58
6	E	810	DW6	C2'-N1'-C4B	2.60	117.95	113.36
7	F	4931	FAD	C4A-C5A-N7A	-2.55	107.67	110.58
7	C	3932	FAD	N9A-C8A-N7A	-2.51	110.38	113.94
7	F	4931	FAD	C10-C4X-N5	-2.44	119.82	124.81
6	E	810	DW6	C5-C6-N1	-2.43	117.89	121.84
7	C	3932	FAD	C5A-N7A-C8A	2.43	107.27	103.45
6	B	810	DW6	C8'-C7'-S7'	2.35	121.49	120.15
7	C	3932	FAD	C4X-C4-N3	2.35	119.23	113.25
6	E	810	DW6	O9'-C9'-C8'	2.31	112.35	109.09
7	C	3932	FAD	C4A-C5A-N7A	-2.30	107.95	110.58
7	F	4931	FAD	C6-C5X-N5	2.30	122.26	118.44
7	C	3932	FAD	C4X-C10-N10	2.25	119.70	116.48
7	F	4931	FAD	O4'-C4'-C5'	-2.23	105.07	109.99
6	E	810	DW6	C6-N1-C2	2.10	124.01	120.46
7	F	4931	FAD	C5A-C4A-N3A	-2.09	123.83	126.72
6	B	810	DW6	O5'-PA-O2A	-2.09	100.65	108.94
7	C	3932	FAD	C6A-C5A-C4A	2.06	119.99	117.18
6	E	810	DW6	C4'-C4A-N5'	2.02	121.78	116.27
7	F	4931	FAD	C4-N3-C2	-2.02	122.06	125.64
6	E	810	DW6	C3'-C2D-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

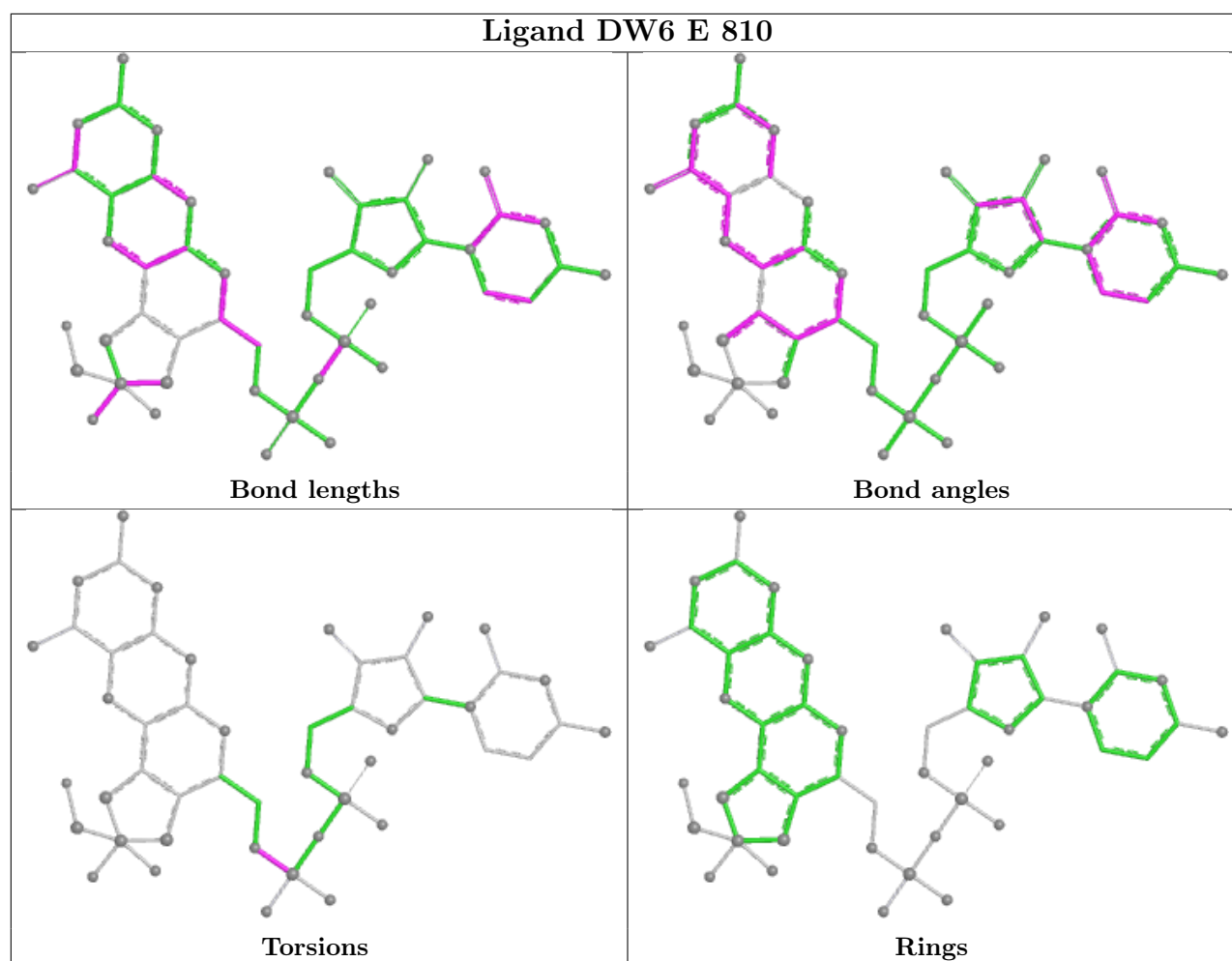
Mol	Chain	Res	Type	Atoms
6	B	810	DW6	C10-O3B-PB-O1B
6	E	810	DW6	C10-O3B-PB-O1B
7	C	3932	FAD	PA-O3P-P-O1P
7	C	3932	FAD	PA-O3P-P-O2P
7	F	4931	FAD	PA-O3P-P-O2P
7	F	4931	FAD	PA-O3P-P-O1P

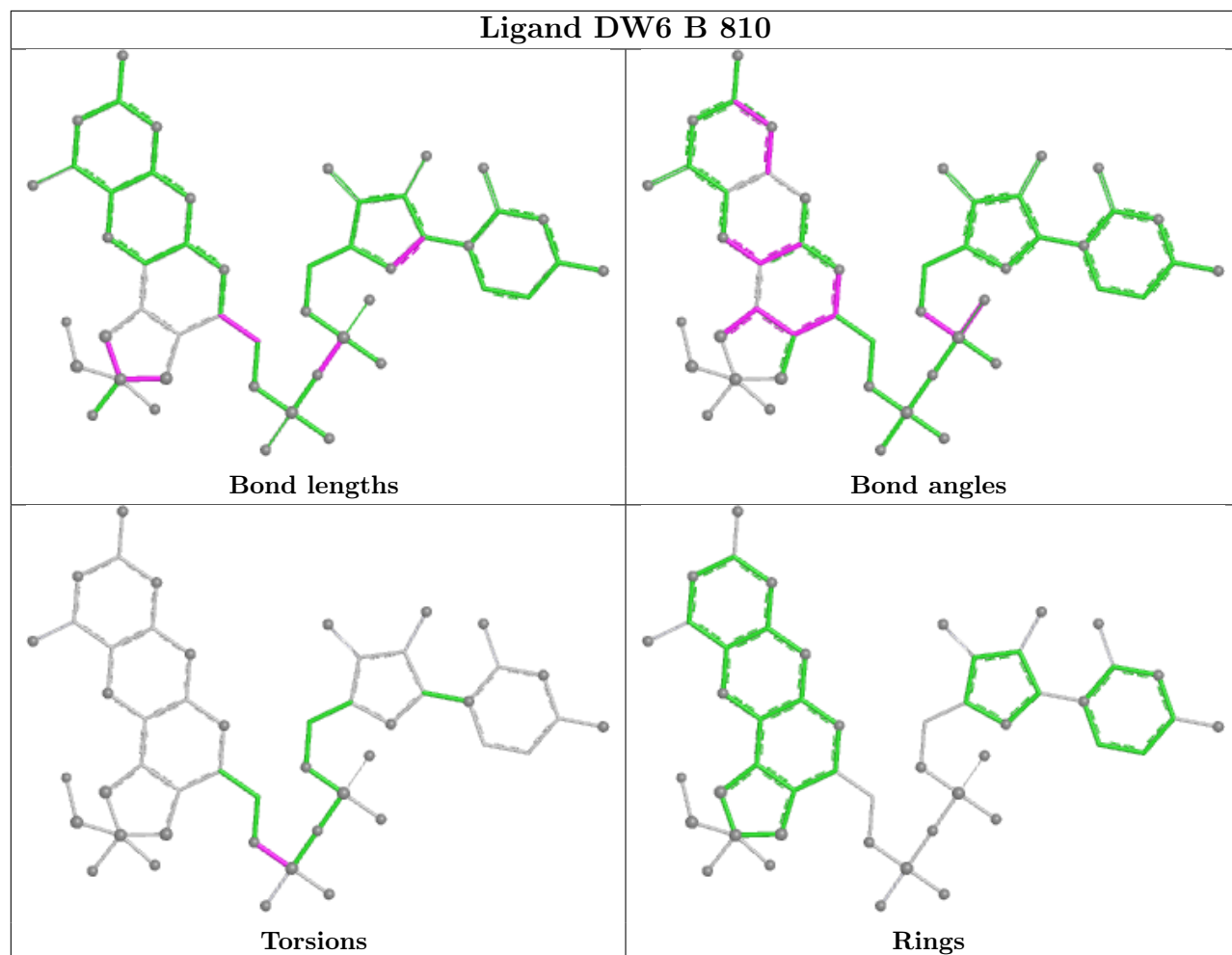
There are no ring outliers.

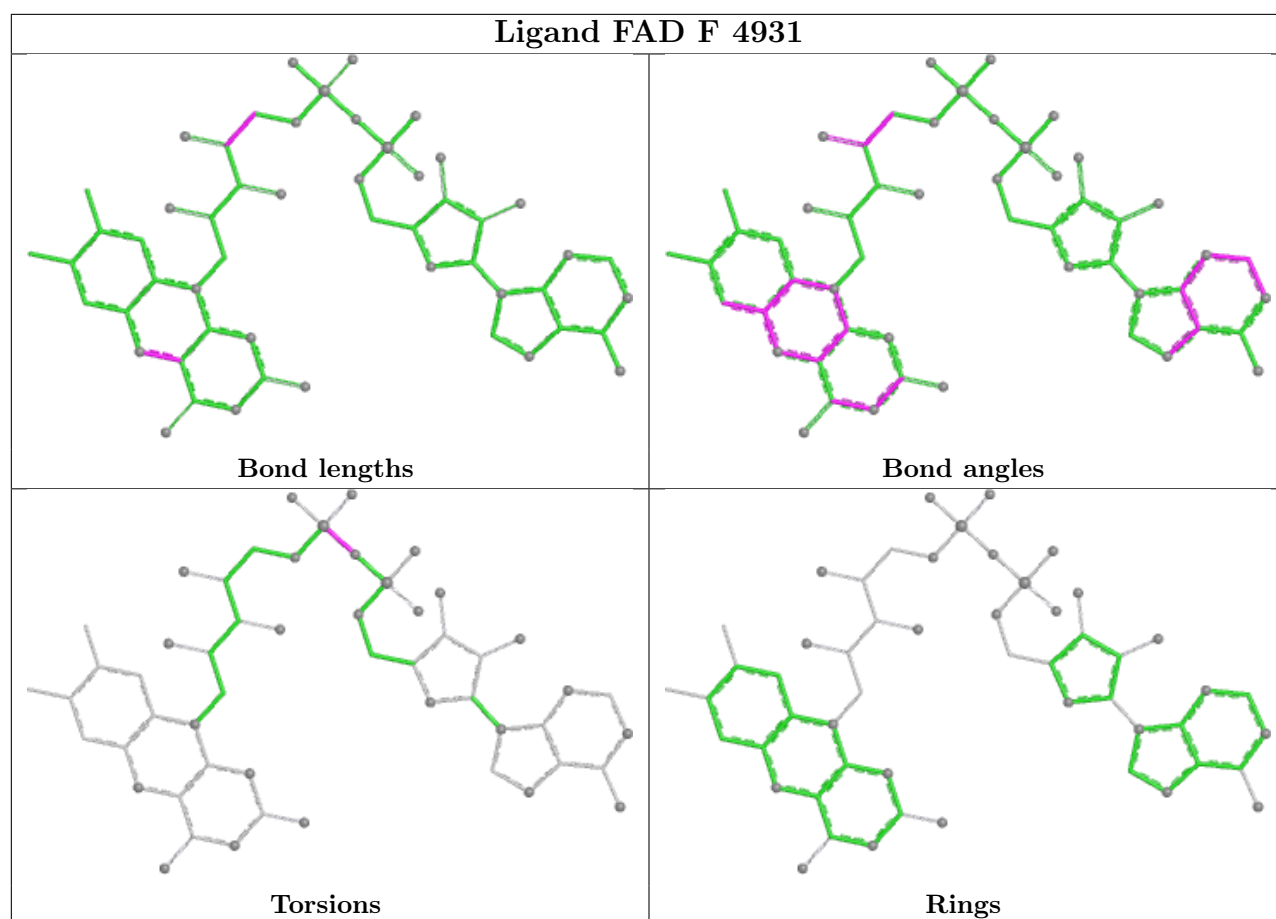
4 monomers are involved in 6 short contacts:

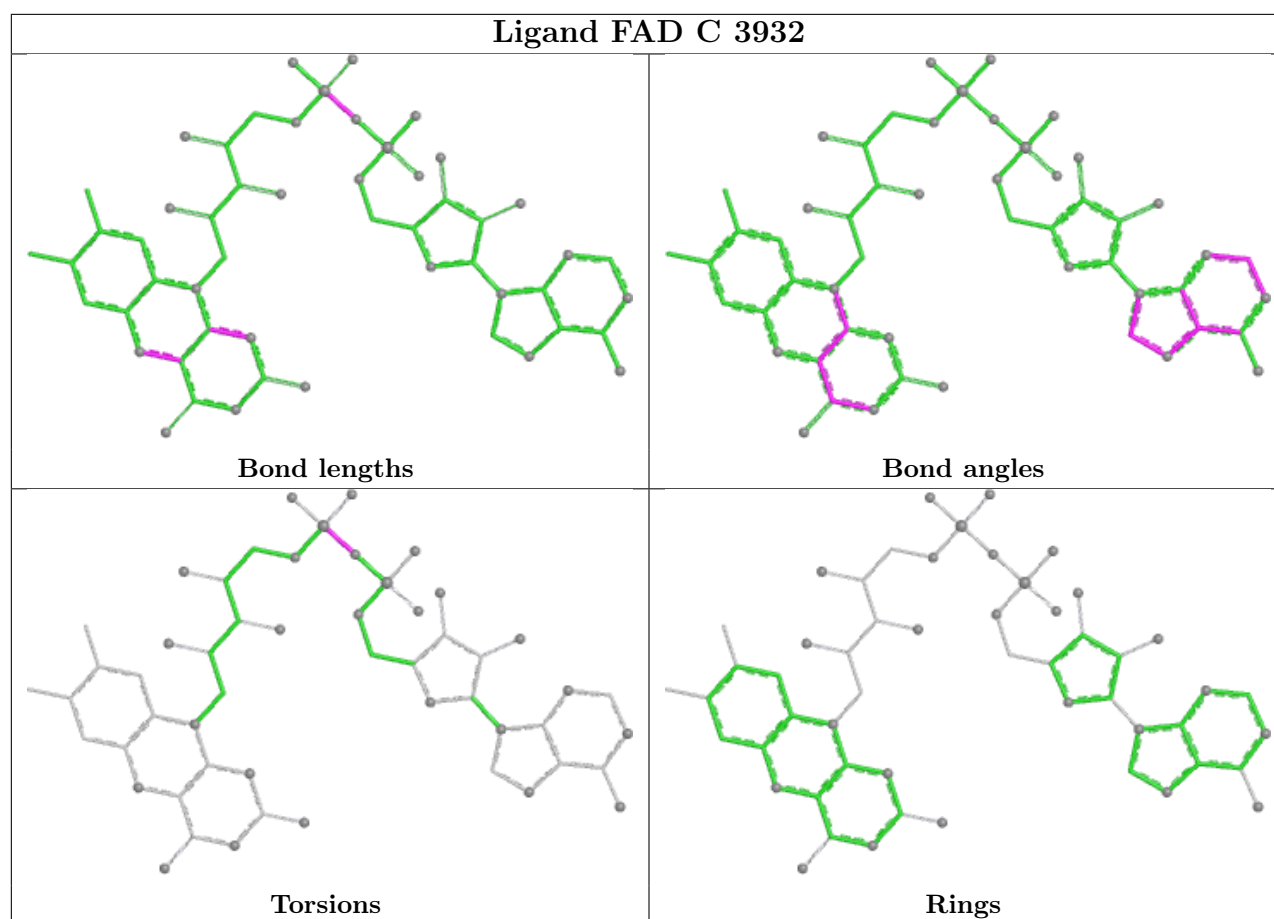
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	810	DW6	1	0
4	A	3001	PO4	1	0
7	F	4931	FAD	3	0
7	C	3932	FAD	1	0

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.