



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:06 PM EDT

PDB ID : 1N60 / pdb_00001n60
Title : Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Cyanide-inactivated Form
Authors : Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on : 2002-11-08
Resolution : 1.19 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

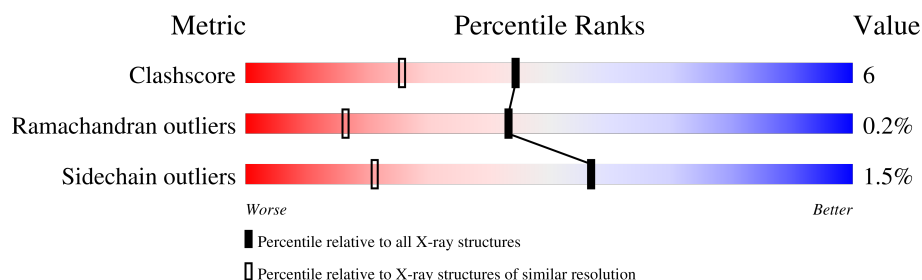
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.19 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	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)

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	86% 10% ..
1	D	166	87% 8% 5%
2	B	809	88% 10% ..
2	E	809	88% 9% ..
3	C	288	86% 12% ..
3	F	288	92% 6% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22712 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	9	7	0
			1230	762	219	231	18			
1	D	158	Total	C	N	O	S	7	6	0
			1200	743	216	223	18			

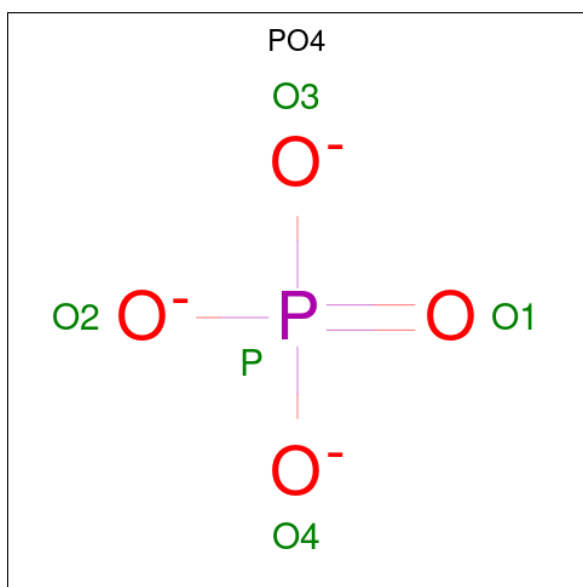
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	803	Total	C	N	O	S	75	17	0
			6257	3976	1068	1165	48			
2	E	796	Total	C	N	O	S	66	16	0
			6201	3947	1058	1149	47			

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

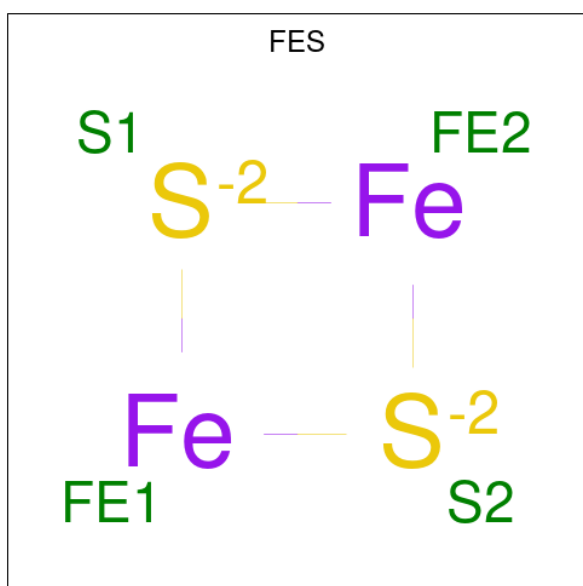
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	33	9	0
			2134	1348	374	400	12			
3	F	286	Total	C	N	O	S	35	7	0
			2123	1341	370	400	12			

- 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		
4	E	1	Total	O	P	0	0
			5	4	1		

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



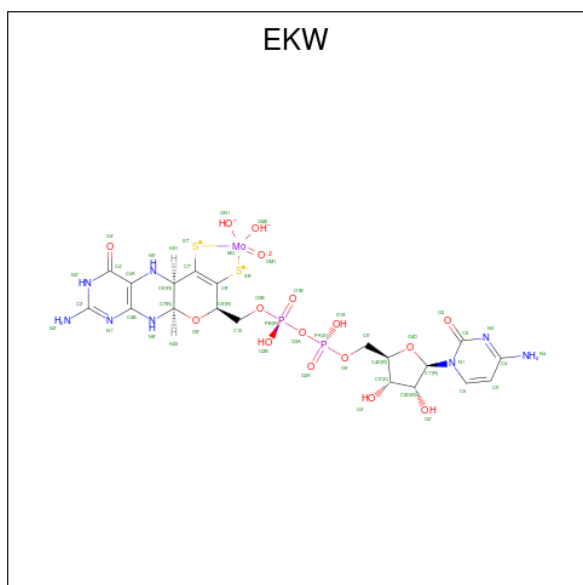
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		

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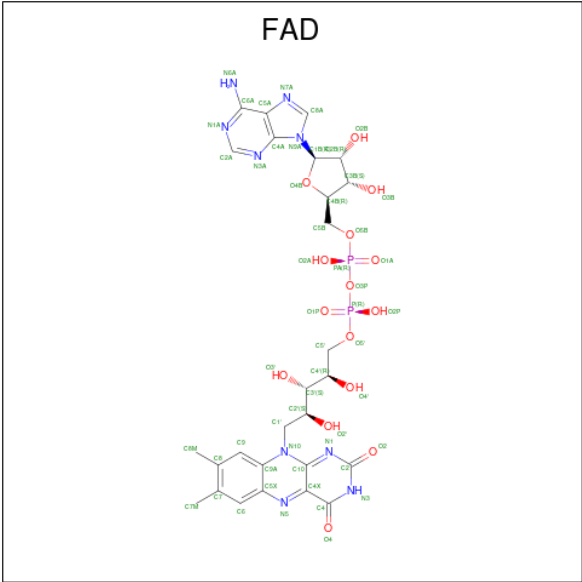
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is Dihydroxo-oxo-molybdopterin (CCD ID: EKW) (formula: $C_{19}H_{26}MoN_8O_{16}P_2S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		
6	E	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		

- 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	C	N	O	P	0	0
			53	27	9	15	2		
7	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	229	Total	O	0	0
			229	229		
8	B	1085	Total	O	0	0
			1085	1085		
8	C	420	Total	O	0	0
			420	420		
8	D	226	Total	O	0	0
			226	226		
8	E	1000	Total	O	0	0
			1000	1000		
8	F	379	Total	O	0	0
			379	379		

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: 



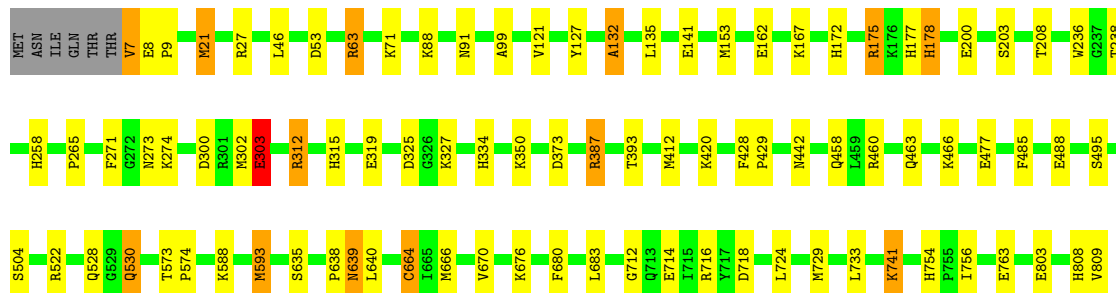
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D: 



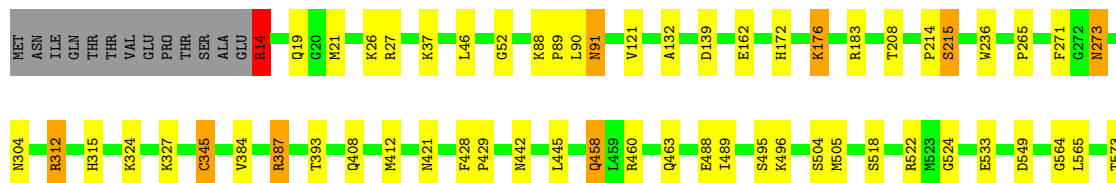
- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain B: 



- Molecule 2: Carbon monoxide dehydrogenase large chain

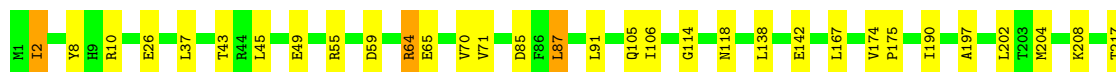
Chain E: 





- Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain C: 86% 12% ..



- Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain F: 92% 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	118.57Å 130.64Å 158.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.80 – 1.19	Depositor
% Data completeness (in resolution range)	(Not available) (17.80-1.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.142 , 0.171	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22712	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: FAD, FES, PO4, EKW

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	1.41	6/1281 (0.5%)	1.14	6/1729 (0.3%)
1	D	1.36	1/1245 (0.1%)	1.00	1/1680 (0.1%)
2	B	1.40	17/6483 (0.3%)	1.08	18/8792 (0.2%)
2	E	1.29	16/6423 (0.2%)	1.07	12/8705 (0.1%)
3	C	1.39	6/2207 (0.3%)	1.09	7/2996 (0.2%)
3	F	1.24	4/2188 (0.2%)	1.05	0/2969
All	All	1.35	50/19827 (0.3%)	1.08	44/26871 (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	3
1	D	0	1
2	B	0	7
2	E	0	4
3	C	0	1
All	All	0	16

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	141	GLU	CD-OE1	26.14	1.75	1.25
2	B	639	ASN	CG-ND2	-24.96	0.80	1.33
3	C	265	GLU	CD-OE2	23.79	1.70	1.25
2	B	200	GLU	CG-CD	18.14	1.97	1.52
1	D	3	LYS	CE-NZ	15.02	1.94	1.49
1	A	97	MET	SD-CE	-13.89	1.44	1.79
1	A	163	GLU	CG-CD	13.76	1.86	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	14	ARG	CD-NE	13.68	1.65	1.46
2	B	200	GLU	CD-OE2	13.40	1.50	1.25
2	B	593	MET	SD-CE	-12.16	1.49	1.79
2	E	620	GLU	CG-CD	11.67	1.81	1.52
2	E	176	LYS	CE-NZ	-11.26	1.15	1.49
2	E	37	LYS	CE-NZ	11.24	1.83	1.49
2	B	741	LYS	CD-CE	11.22	1.86	1.52
1	A	92	GLU	CD-OE2	-10.09	1.06	1.25
1	A	92	GLU	CD-OE1	9.99	1.44	1.25
3	C	65	GLU	CD-OE2	-9.95	1.06	1.25
2	E	664	CYS	CA-CB	9.95	1.71	1.53
1	A	163	GLU	CA-CB	9.32	1.72	1.53
3	C	49	GLU	CD-OE2	-9.02	1.08	1.25
2	E	91	ASN	CG-ND2	8.98	1.52	1.33
2	B	458	GLN	CG-CD	8.89	1.74	1.52
2	B	141	GLU	CG-CD	-8.24	1.31	1.52
2	E	91	ASN	CB-CG	7.72	1.71	1.52
2	B	809	VAL	CB-CG2	-7.52	1.27	1.52
2	B	638	PRO	CA-CB	-7.10	1.43	1.53
2	B	729	MET	SD-CE	-6.84	1.62	1.79
3	F	119	GLY	C-O	-6.72	1.15	1.24
3	F	117	ALA	CA-C	6.36	1.61	1.52
2	E	172	HIS	CA-CB	6.15	1.61	1.53
2	E	273	ASN	CG-ND2	-6.13	1.20	1.33
2	B	132	ALA	CA-CB	-6.00	1.43	1.53
2	E	664	CYS	CB-SG	-5.98	1.61	1.81
3	F	55	ARG	CG-CD	5.96	1.70	1.52
2	E	14	ARG	CA-C	5.88	1.65	1.52
3	C	106	ILE	CG1-CD1	-5.80	1.29	1.51
3	F	190	ILE	CA-CB	5.74	1.61	1.54
2	B	162	GLU	CD-OE2	-5.70	1.14	1.25
2	E	345	CYS	N-CA	-5.63	1.39	1.46
2	E	676	LYS	CE-NZ	5.49	1.65	1.49
2	B	676	LYS	CE-NZ	5.32	1.65	1.49
2	B	88	LYS	CA-C	5.26	1.59	1.52
3	C	190	ILE	C-O	-5.26	1.18	1.24
2	B	635	SER	CA-CB	-5.24	1.46	1.53
1	A	128	ILE	CA-CB	-5.20	1.48	1.54
2	E	621	LYS	CG-CD	-5.19	1.36	1.52
3	C	142	GLU	CG-CD	5.14	1.64	1.52
2	E	215	SER	C-O	-5.13	1.21	1.23
2	B	273	ASN	CG-ND2	-5.03	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	533	GLU	CD-OE2	5.03	1.34	1.25

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	GLU	CB-CA-C	-16.00	79.70	110.10
2	B	8	GLU	CB-CG-CD	14.47	137.19	112.60
2	E	620	GLU	CB-CG-CD	-12.81	90.83	112.60
2	B	200	GLU	CB-CG-CD	-12.61	91.17	112.60
2	E	91	ASN	CA-CB-CG	-12.03	100.57	112.60
2	E	91	ASN	CB-CG-ND2	11.57	133.75	116.40
2	B	639	ASN	OD1-CG-ND2	-10.87	111.73	122.60
3	C	265	GLU	CG-CD-OE2	-10.07	95.25	118.40
3	C	2	ILE	N-CA-C	9.37	116.82	107.55
2	B	458	GLN	OE1-CD-NE2	-9.22	113.38	122.60
2	B	63[A]	ARG	NE-CZ-NH1	-9.13	112.37	121.50
2	B	63[B]	ARG	NE-CZ-NH1	-9.13	112.37	121.50
2	E	91	ASN	OD1-CG-ND2	-8.97	113.62	122.60
2	B	303	GLU	OE1-CD-OE2	-8.90	101.53	122.90
2	E	620	GLU	CG-CD-OE2	-8.69	98.40	118.40
1	A	163	GLU	CA-CB-CG	8.45	130.99	114.10
2	E	620	GLU	CG-CD-OE1	8.25	137.37	118.40
2	E	716	ARG	NE-CZ-NH2	7.26	125.73	119.20
3	C	142	GLU	CB-CG-CD	-7.13	100.48	112.60
1	A	163	GLU	N-CA-CB	7.09	122.55	110.50
2	B	141	GLU	CG-CD-OE2	6.73	133.89	118.40
2	B	63[A]	ARG	CD-NE-CZ	6.62	133.66	124.40
2	B	63[B]	ARG	CD-NE-CZ	6.62	133.66	124.40
1	A	109[A]	MET	CG-SD-CE	6.59	115.41	100.90
1	A	109[B]	MET	CG-SD-CE	6.59	115.41	100.90
2	B	639	ASN	CB-CG-ND2	6.53	126.19	116.40
2	B	141	GLU	CG-CD-OE1	-6.39	103.70	118.40
1	D	3	LYS	CD-CE-NZ	-6.24	91.95	111.90
2	E	176	LYS	CD-CE-NZ	6.22	131.79	111.90
2	E	716	ARG	NE-CZ-NH1	-6.02	115.48	121.50
2	E	716	ARG	CD-NE-CZ	5.90	132.66	124.40
3	C	59	ASP	CA-CB-CG	5.89	118.49	112.60
2	B	485	PHE	CA-CB-CG	-5.71	108.09	113.80
2	E	14	ARG	NE-CZ-NH1	-5.71	115.79	121.50
2	B	741	LYS	CG-CD-CE	-5.66	98.29	111.30
3	C	49	GLU	OE1-CD-OE2	-5.63	109.38	122.90
1	A	47	CYS	N-CA-C	5.61	119.30	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	14	ARG	N-CA-CB	-5.60	100.98	110.50
3	C	37	LEU	CA-C-N	-5.55	116.74	120.24
3	C	37	LEU	C-N-CA	-5.55	116.74	120.24
2	B	63[A]	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	B	63[B]	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	B	303	GLU	CG-CD-OE2	5.21	130.38	118.40
2	B	175	ARG	NE-CZ-NH2	-5.03	114.68	119.20

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	HIS	Sidechain
1	A	138	ARG	Sidechain
1	A	163	GLU	Sidechain
2	B	178	HIS	Sidechain
2	B	27	ARG	Sidechain
2	B	303	GLU	Sidechain
2	B	312	ARG	Sidechain
2	B	387	ARG	Sidechain
2	B	63[A]	ARG	Sidechain
2	B	63[B]	ARG	Sidechain
3	C	265	GLU	Sidechain
1	D	138	ARG	Sidechain
2	E	14	ARG	Sidechain
2	E	27	ARG	Sidechain
2	E	312	ARG	Sidechain
2	E	387	ARG	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	1230	0	1208	18	1
1	D	1200	0	1190	19	0
2	B	6257	0	6135	69	0
2	E	6201	0	6101	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2134	0	2187	28	0
3	F	2123	0	2171	25	0
4	A	5	0	0	0	0
4	E	5	0	0	0	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	48	0	0	2	0
6	E	48	0	0	2	0
7	C	53	0	31	1	0
7	F	53	0	31	3	0
8	A	229	0	0	6	0
8	B	1085	0	0	18	3
8	C	420	0	0	6	1
8	D	226	0	0	8	0
8	E	1000	0	0	27	3
8	F	379	0	0	13	0
All	All	22712	0	19054	228	4

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 6.

All (228) 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:OE2	1.18	1.28
2:E:593[A]:MET:HG2	2:E:603:GLU:OE2	1.15	1.26
2:B:236[B]:TRP:CZ2	8:B:6002:HOH:O	1.63	1.25
2:B:236[B]:TRP:CH2	8:B:6002:HOH:O	1.73	1.21
1:A:59:VAL:HG11	1:A:64[A]:MET:HE1	1.20	1.12
1:A:59:VAL:HG11	1:A:64[A]:MET:CE	1.80	1.12
3:F:120:ASP:OD2	3:F:121:PRO:HD2	1.55	1.04
1:D:59:VAL:HG11	1:D:64[A]:MET:HE1	1.37	1.03
1:D:59:VAL:HG11	1:D:64[A]:MET:CE	1.89	1.02
1:D:118[A]:GLN:OE1	8:D:6025:HOH:O	1.77	1.02
1:D:32:GLN:HG3	8:D:6114:HOH:O	1.60	0.99
1:D:92:GLU:HG3	8:D:6061:HOH:O	1.61	0.99
1:A:163:GLU:C	8:A:5137:HOH:O	2.06	0.99
1:D:92:GLU:HG3	8:D:6125:HOH:O	1.66	0.95
2:E:593[A]:MET:CG	2:E:603:GLU:OE2	2.12	0.95
1:D:118[A]:GLN:NE2	8:D:5974:HOH:O	1.97	0.95
2:E:327[B]:LYS:NZ	8:E:6499:HOH:O	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ASN:HD21	1:D:76:THR:H	1.19	0.90
3:F:118:ASN:O	8:F:6309:HOH:O	1.90	0.88
2:E:639:ASN:OD1	8:E:6750:HOH:O	1.91	0.88
2:B:460:ARG:HH11	2:B:463:GLN:HE22	1.22	0.88
1:A:3:LYS:N	8:A:5002:HOH:O	2.06	0.87
1:D:3:LYS:N	8:D:6112:HOH:O	2.06	0.87
2:B:528:GLN:H	2:B:530:GLN:HE22	1.21	0.87
2:E:408:GLN:NE2	8:E:6880:HOH:O	2.08	0.85
2:E:208:THR:H	2:E:790:GLN:HE22	1.19	0.85
3:F:120:ASP:OD2	3:F:121:PRO:CD	2.24	0.85
3:C:64[A]:ARG:HD2	3:C:71:VAL:O	1.78	0.84
3:F:119:GLY:HA3	8:F:6309:HOH:O	1.79	0.83
2:E:593[B]:MET:CG	2:E:603:GLU:OE2	2.14	0.81
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.28	0.80
2:B:300:ASP:HB2	2:B:303:GLU:OE1	1.82	0.80
2:B:716:ARG:NH1	8:B:5328:HOH:O	2.11	0.80
1:A:59:VAL:CG1	1:A:64[A]:MET:CE	2.59	0.79
2:E:716:ARG:CZ	8:E:6749:HOH:O	2.30	0.78
2:E:716:ARG:NH1	8:E:6749:HOH:O	2.19	0.75
3:C:55:ARG:HD3	8:C:5133:HOH:O	1.86	0.74
2:E:716:ARG:NE	8:E:6749:HOH:O	2.21	0.74
2:E:327[B]:LYS:HD3	8:E:6247:HOH:O	1.87	0.73
2:E:273:ASN:HD21	2:E:304:ASN:HD21	1.36	0.73
2:B:46:LEU:HD11	2:B:236[B]:TRP:CZ3	2.23	0.72
1:A:68:GLN:HE21	3:C:55:ARG:HH22	1.39	0.70
3:C:85:ASP:OD1	8:C:5329:HOH:O	2.07	0.70
2:B:528:GLN:H	2:B:530:GLN:NE2	1.89	0.69
2:E:88:LYS:HB2	2:E:89:PRO:HD3	1.75	0.69
2:E:754:HIS:HD2	2:E:756:ILE:H	1.41	0.69
1:D:59:VAL:CG1	1:D:64[A]:MET:CE	2.69	0.69
2:B:588:LYS:HD2	8:B:5252:HOH:O	1.92	0.68
1:D:59:VAL:HG11	1:D:64[A]:MET:HE3	1.75	0.68
3:F:221:ASN:ND2	8:F:6097:HOH:O	2.26	0.68
2:B:716:ARG:NH1	8:B:5280:HOH:O	2.27	0.68
2:B:803:GLU:OE1	2:B:808:HIS:HD2	1.78	0.67
2:B:71:LYS:HE3	2:B:135:LEU:O	1.94	0.66
2:B:327:LYS:HG2	2:B:420:LYS:HE3	1.76	0.66
2:E:593[B]:MET:HE1	8:E:6518:HOH:O	1.95	0.66
3:F:120:ASP:CG	3:F:122:GLY:H	2.05	0.64
2:E:458:GLN:HE21	2:E:458:GLN:H	1.45	0.63
2:B:530:GLN:HE21	2:B:530:GLN:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:593[B]:MET:HG2	2:E:603:GLU:CD	2.18	0.63
2:E:495:SER:CB	2:E:504[A]:SER:OG	2.47	0.62
2:B:754:HIS:HD2	2:B:756:ILE:H	1.47	0.62
1:D:159:VAL:HB	1:D:160:PRO:HD3	1.80	0.62
1:A:59:VAL:CG1	1:A:64[A]:MET:HE1	2.13	0.62
2:B:7:VAL:HG13	2:B:9:PRO:HD3	1.83	0.61
6:B:810:EKW:OM1	6:B:810:EKW:MO	1.70	0.61
1:A:84:ASP:OD1	1:A:86:THR:HG23	2.00	0.61
3:C:280:GLU:HG3	8:C:5089:HOH:O	2.00	0.61
2:B:522:ARG:NH1	8:B:6001:HOH:O	2.30	0.60
1:A:118[A]:GLN:NE2	8:A:5128:HOH:O	2.34	0.60
2:E:46:LEU:HD11	2:E:236[B]:TRP:CZ3	2.37	0.60
2:B:236[B]:TRP:HZ2	8:B:6002:HOH:O	1.29	0.60
2:B:670:VAL:O	2:B:808:HIS:HE1	1.84	0.60
6:E:5003:EKW:OM1	6:E:5003:EKW:MO	1.72	0.59
1:A:59:VAL:HG11	1:A:64[A]:MET:HE3	1.82	0.58
2:B:716:ARG:NH2	8:B:5328:HOH:O	2.35	0.58
2:B:236[B]:TRP:HH2	8:B:6002:HOH:O	1.45	0.57
1:A:135:ASN:HD21	3:C:105:GLN:HE22	1.51	0.57
1:D:92:GLU:CG	8:D:6125:HOH:O	2.37	0.57
2:E:754:HIS:CD2	2:E:756:ILE:H	2.22	0.57
1:A:135:ASN:ND2	3:C:105:GLN:HE22	2.03	0.56
2:E:327[B]:LYS:HG2	8:E:6761:HOH:O	2.05	0.56
2:B:334:HIS:HE1	2:B:373:ASP:OD2	1.87	0.56
2:E:593[A]:MET:HG2	2:E:603:GLU:CD	2.21	0.56
2:B:639:ASN:ND2	2:B:639:ASN:CA	2.69	0.56
1:A:163:GLU:CA	8:A:5137:HOH:O	2.50	0.55
2:B:172:HIS:HD2	8:B:5633:HOH:O	1.88	0.55
3:F:120:ASP:OD2	3:F:121:PRO:N	2.40	0.55
2:E:327[B]:LYS:CD	8:E:6761:HOH:O	2.54	0.55
2:B:716:ARG:CZ	8:B:5328:HOH:O	2.52	0.55
2:E:741:LYS:CE	8:E:6574:HOH:O	2.55	0.55
2:B:442:ASN:C	2:B:442:ASN:HD22	2.13	0.54
2:E:741:LYS:NZ	8:E:6574:HOH:O	2.22	0.54
3:C:10:ARG:CZ	3:C:55:ARG:HD2	2.38	0.54
2:E:327[B]:LYS:HD3	8:E:6761:HOH:O	2.07	0.54
3:F:118:ASN:C	8:F:6309:HOH:O	2.44	0.54
3:C:64[A]:ARG:NH1	8:C:5146:HOH:O	2.40	0.54
1:A:68:GLN:HE21	3:C:55:ARG:NH2	2.04	0.53
2:B:754:HIS:CD2	2:B:756:ILE:H	2.26	0.53
2:E:208:THR:OG1	2:E:315:HIS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:VAL:CG1	1:D:64[A]:MET:HE3	2.36	0.53
3:F:10:ARG:CZ	8:F:6047:HOH:O	2.57	0.52
3:F:120:ASP:CG	8:F:6282:HOH:O	2.52	0.52
2:E:327[B]:LYS:HE2	2:E:421:ASN:OD1	2.10	0.52
2:B:302:MET:HB3	8:B:5769:HOH:O	2.10	0.52
2:E:442:ASN:HD22	2:E:442:ASN:C	2.18	0.51
2:E:788:HIS:HE2	2:E:790:GLN:NE2	2.08	0.51
3:F:192:ASP:OD2	8:F:6121:HOH:O	2.19	0.51
3:F:10:ARG:NH1	8:F:6260:HOH:O	2.26	0.50
2:B:350:LYS:HE3	8:B:5658:HOH:O	2.11	0.50
3:C:118:ASN:HD22	7:C:4932:FAD:H4B	1.75	0.49
3:C:138:LEU:HD23	3:C:167:LEU:HA	1.95	0.49
3:F:90:LYS:HE2	8:F:6184:HOH:O	2.12	0.49
2:B:460:ARG:NH1	2:B:463:GLN:HE22	2.01	0.49
2:E:327[B]:LYS:CG	8:E:6761:HOH:O	2.60	0.49
3:F:79:HIS:HD2	8:F:6199:HOH:O	1.95	0.49
2:B:175:ARG:NH2	2:B:178:HIS:O	2.45	0.49
3:F:221:ASN:HD22	3:F:221:ASN:N	2.11	0.49
2:E:593[A]:MET:HE1	8:E:6586:HOH:O	2.13	0.49
1:A:96[A]:MET:HE3	8:A:5126:HOH:O	2.13	0.49
3:C:114:GLY:O	3:C:118:ASN:HB2	2.13	0.48
2:E:445:LEU:C	2:E:445:LEU:HD13	2.38	0.48
2:E:445:LEU:HD22	8:E:6244:HOH:O	2.13	0.48
2:E:593[A]:MET:HE2	8:E:6102:HOH:O	2.14	0.48
2:B:530:GLN:NE2	2:B:530:GLN:H	2.11	0.48
2:E:315:HIS:HE1	8:E:6042:HOH:O	1.97	0.48
2:B:208:THR:OG1	2:B:315:HIS:HD2	1.95	0.48
2:B:428:PHE:HA	2:B:429:PRO:C	2.39	0.48
2:E:495:SER:HB3	2:E:504[A]:SER:OG	2.13	0.48
3:C:10:ARG:NH2	3:C:55:ARG:HD2	2.29	0.48
2:B:593:MET:CE	2:B:640:LEU:HD21	2.44	0.47
3:C:286:ALA:C	8:C:5229:HOH:O	2.57	0.47
2:E:19:GLN:NE2	8:E:6303:HOH:O	2.47	0.47
2:B:495:SER:CB	2:B:504[A]:SER:OG	2.62	0.47
2:E:683:LEU:C	2:E:683:LEU:HD23	2.39	0.47
1:A:59:VAL:CG1	1:A:64[A]:MET:HE3	2.41	0.47
2:B:127:TYR:HA	3:C:2:ILE:HG21	1.97	0.47
3:C:43:THR:HG21	8:C:5088:HOH:O	2.14	0.47
2:E:183:ARG:HD2	8:E:6379:HOH:O	2.13	0.47
2:B:639:ASN:CA	2:B:639:ASN:HD22	2.28	0.47
2:B:387:ARG:HA	2:B:763:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:GLU:CD	8:D:6120:HOH:O	2.58	0.47
2:E:14:ARG:N	8:E:6916:HOH:O	2.48	0.47
3:F:197:ALA:HB3	3:F:217:THR:HB	1.96	0.47
2:B:46:LEU:HD11	2:B:236[B]:TRP:CH2	2.50	0.46
2:B:53:ASP:OD2	8:B:5865:HOH:O	2.20	0.46
2:B:21[A]:MET:HE2	2:B:21[A]:MET:HB3	1.64	0.46
3:C:8:TYR:OH	3:C:10:ARG:HD3	2.15	0.46
2:E:208:THR:H	2:E:790:GLN:NE2	1.99	0.46
2:E:597:HIS:HD2	8:E:6565:HOH:O	1.99	0.46
2:B:258:HIS:HE1	2:E:549:ASP:O	1.98	0.46
2:B:334:HIS:HD2	8:B:5195:HOH:O	1.99	0.46
2:B:714:GLU:OE2	2:B:716:ARG:NH1	2.48	0.46
3:F:118:ASN:HD22	7:F:5931:FAD:H4B	1.80	0.46
2:B:412[B]:MET:HE2	8:B:5930:HOH:O	2.14	0.46
2:B:683:LEU:HD23	2:B:683:LEU:C	2.41	0.46
2:B:803:GLU:OE1	2:B:808:HIS:CD2	2.64	0.46
3:F:120:ASP:CB	8:F:6282:HOH:O	2.64	0.45
2:B:153:MET:HA	2:B:177:HIS:CE1	2.52	0.45
2:E:52:GLY:HA2	2:E:121:VAL:O	2.16	0.45
2:B:99:ALA:O	2:B:172:HIS:HE1	2.00	0.45
3:C:167:LEU:C	3:C:167:LEU:HD23	2.42	0.44
3:C:204[A]:MET:HG3	3:C:286:ALA:CB	2.47	0.44
2:E:714:GLU:CD	2:E:716:ARG:HE	2.25	0.44
2:E:522:ARG:NH1	8:E:6666:HOH:O	2.47	0.44
1:A:54:LEU:C	1:A:54:LEU:HD23	2.43	0.44
2:B:325:ASP:O	2:B:420:LYS:HE2	2.17	0.44
3:F:162:GLU:HB3	3:F:163:PRO:HD2	1.99	0.44
2:B:258:HIS:CD2	2:E:518:SER:HB2	2.52	0.44
2:B:573:THR:HB	2:B:574:PRO:HD3	2.00	0.44
2:E:573:THR:O	2:E:754:HIS:HE1	1.99	0.44
3:F:221:ASN:HD22	3:F:221:ASN:H	1.66	0.44
2:E:26[A]:LYS:NZ	8:E:6672:HOH:O	2.51	0.44
2:B:714:GLU:CD	2:B:716:ARG:HH11	2.25	0.44
2:B:238:THR:HB	2:B:274:LYS:HD3	2.00	0.44
8:A:5132:HOH:O	2:B:741:LYS:HD3	2.18	0.43
2:B:203:SER:O	2:B:319:GLU:HA	2.19	0.43
3:F:276:ARG:NH2	8:F:6142:HOH:O	2.49	0.43
2:B:7:VAL:HA	8:B:5455:HOH:O	2.18	0.43
2:B:315:HIS:HE1	8:B:5008:HOH:O	2.01	0.43
2:E:345:CYS:SG	2:E:384:VAL:HG23	2.59	0.43
2:E:524:GLY:HA3	2:E:564:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:LEU:HD23	2:B:733:LEU:HA	1.83	0.43
3:C:70:VAL:HG23	3:C:174:VAL:HG22	2.00	0.42
2:E:214:PRO:O	2:E:215:SER:C	2.62	0.42
2:E:14:ARG:HH12	2:E:611:ASP:CG	2.27	0.42
2:E:324:LYS:NZ	8:E:6708:HOH:O	2.49	0.42
2:E:505:MET:HA	2:E:565:LEU:HG	2.00	0.42
2:E:573:THR:HB	2:E:574:PRO:HD3	2.01	0.42
1:D:5:HIS:HA	1:D:18:LEU:HD23	2.01	0.42
2:E:21[A]:MET:HE3	2:E:21[A]:MET:HB3	1.90	0.42
2:E:428:PHE:HA	2:E:429:PRO:C	2.44	0.42
2:E:655[A]:MET:HB3	2:E:655[A]:MET:HE3	1.52	0.42
3:C:91:LEU:HD21	3:C:175:PRO:HD3	2.00	0.42
3:C:197:ALA:HB3	3:C:217:THR:HB	2.02	0.42
2:E:764:SER:N	2:E:765:PRO:HD2	2.33	0.42
2:E:271:PHE:HA	6:E:5003:EKW:S7'	2.60	0.42
2:E:489:ILE:HD11	2:E:655[A]:MET:HG3	2.01	0.42
2:E:489:ILE:HG12	2:E:655[A]:MET:HE2	2.02	0.42
2:E:21[B]:MET:HE2	8:E:6262:HOH:O	2.18	0.42
2:E:162:GLU:OE2	8:E:6442:HOH:O	2.21	0.42
2:E:412[A]:MET:HE3	2:E:412[A]:MET:HB2	1.67	0.42
2:E:718:ASP:HB3	2:E:724:LEU:HD11	2.02	0.42
2:B:714:GLU:OE1	2:B:716:ARG:HD3	2.19	0.42
3:F:10:ARG:NE	8:F:6047:HOH:O	2.52	0.42
2:B:271:PHE:HA	6:B:810:EKW:S7'	2.60	0.41
3:F:106:ILE:HD13	7:F:5931:FAD:C7	2.50	0.41
3:F:106:ILE:HD13	7:F:5931:FAD:C8	2.49	0.41
3:F:120:ASP:OD2	3:F:120:ASP:C	2.60	0.41
2:B:593:MET:HB3	2:B:593:MET:HE2	1.78	0.41
2:B:664[A]:CYS:HB2	2:B:680:PHE:CD2	2.54	0.41
1:D:18:LEU:HD23	1:D:18:LEU:HA	1.92	0.41
2:B:466:LYS:NZ	2:B:477:GLU:OE2	2.47	0.41
2:B:495:SER:HB3	2:B:504[A]:SER:OG	2.21	0.41
2:E:327[B]:LYS:CE	2:E:327[B]:LYS:HA	2.50	0.41
3:C:202:LEU:C	3:C:202:LEU:HD12	2.46	0.41
2:E:387:ARG:HA	2:E:763:GLU:HG2	2.02	0.41
2:E:121:VAL:HG11	2:E:132:ALA:HB3	2.03	0.41
2:B:666[B]:MET:HE3	2:B:666[B]:MET:HB2	1.90	0.40
3:C:221[A]:ASN:OD1	3:C:222:THR:HG23	2.21	0.40
2:B:121:VAL:HG11	2:B:132:ALA:HB3	2.04	0.40
2:B:718:ASP:HB3	2:B:724:LEU:HD11	2.03	0.40
3:C:204[A]:MET:HG3	3:C:286:ALA:HB1	2.04	0.40

All (4) 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)
8:B:5459:HOH:O	8:E:6649:HOH:O[4_477]	1.91	0.29
8:B:5809:HOH:O	8:E:6654:HOH:O[4_477]	2.03	0.17
8:B:6005:HOH:O	8:C:5179:HOH:O[2_675]	2.03	0.17
1:A:163:GLU:CG	8:E:6562:HOH:O[4_477]	2.19	0.01

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	166/166 (100%)	162 (98%)	4 (2%)	0	100	100
1	D	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
2	B	818/809 (101%)	791 (97%)	24 (3%)	3 (0%)	30	10
2	E	809/809 (100%)	784 (97%)	22 (3%)	3 (0%)	30	10
3	C	293/288 (102%)	290 (99%)	3 (1%)	0	100	100
3	F	290/288 (101%)	287 (99%)	3 (1%)	0	100	100
All	All	2538/2526 (100%)	2473 (97%)	59 (2%)	6 (0%)	43	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	312	ARG
2	E	312	ARG
2	B	712	GLY
2	E	712	GLY
2	B	265	PRO
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	136/131 (104%)	135 (99%)	1 (1%)	76	47
1	D	132/131 (101%)	132 (100%)	0	100	100
2	B	664/653 (102%)	654 (98%)	10 (2%)	57	21
2	E	657/653 (101%)	647 (98%)	10 (2%)	57	21
3	C	219/212 (103%)	211 (96%)	8 (4%)	30	3
3	F	216/212 (102%)	212 (98%)	4 (2%)	50	13
All	All	2024/1992 (102%)	1991 (98%)	33 (2%)	57	19

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
2	B	7	VAL
2	B	21[A]	MET
2	B	21[B]	MET
2	B	91	ASN
2	B	167	LYS
2	B	393	THR
2	B	488	GLU
2	B	530	GLN
2	B	664[A]	CYS
2	B	664[B]	CYS
3	C	26	GLU
3	C	45	LEU
3	C	64[A]	ARG
3	C	64[B]	ARG
3	C	87[A]	LEU
3	C	87[B]	LEU
3	C	208	LYS
3	C	240	LYS
2	E	90	LEU
2	E	91	ASN
2	E	139	ASP

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Mol	Chain	Res	Type
2	E	176	LYS
2	E	393	THR
2	E	458	GLN
2	E	488	GLU
2	E	496	LYS
2	E	620	GLU
2	E	790	GLN
3	F	55	ARG
3	F	142	GLU
3	F	221	ASN
3	F	231	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	34	ASN
1	A	68	GLN
1	A	135	ASN
2	B	35	GLN
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	457	HIS
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	720	GLN
2	B	754	HIS
2	B	808	HIS
3	C	118	ASN
3	C	130	GLN
1	D	11	ASN

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Mol	Chain	Res	Type
1	D	13	HIS
1	D	32	GLN
2	E	19	GLN
2	E	59	HIS
2	E	115	ASN
2	E	273	ASN
2	E	315	HIS
2	E	442	ASN
2	E	458	GLN
2	E	463	GLN
2	E	497	ASN
2	E	597	HIS
2	E	713	GLN
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 ⓘ

10 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	4907	1	0,4,4	-	-	-		
6	EKW	B	810	-	44,53,53	1.31	6 (13%)	54,86,86	1.33	7 (12%)
5	FES	A	4908	1	0,4,4	-	-	-		
6	EKW	E	5003	-	44,53,53	1.69	8 (18%)	54,86,86	1.65	9 (16%)
5	FES	D	5907	1	0,4,4	-	-	-		
4	PO4	A	4001	-	4,4,4	0.51	0	6,6,6	1.24	1 (16%)
4	PO4	E	5002	-	4,4,4	1.39	0	6,6,6	2.12	2 (33%)
5	FES	D	5908	1	0,4,4	-	-	-		
7	FAD	F	5931	-	58,58,58	1.26	6 (10%)	85,89,89	1.27	11 (12%)
7	FAD	C	4932	-	58,58,58	1.13	3 (5%)	85,89,89	1.15	8 (9%)

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	4907	1	-	-	0/1/1/1
6	EKW	B	810	-	-	0/22/78/78	0/6/6/6
5	FES	A	4908	1	-	-	0/1/1/1
6	EKW	E	5003	-	-	0/22/78/78	0/6/6/6
5	FES	D	5907	1	-	-	0/1/1/1
5	FES	D	5908	1	-	-	0/1/1/1
7	FAD	F	5931	-	-	2/34/50/50	0/6/6/6
7	FAD	C	4932	-	-	0/34/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5003	EKW	OM1-MO	4.94	1.72	1.68
7	C	4932	FAD	C4X-N5	4.48	1.40	1.30
6	E	5003	EKW	C7-C6'	-4.44	1.50	1.53
7	F	5931	FAD	C4X-N5	4.06	1.39	1.30
6	B	810	EKW	O4D-C1'	-3.36	1.34	1.42
6	E	5003	EKW	C4A-C4B	3.21	1.44	1.38
7	F	5931	FAD	O4B-C4B	-3.02	1.38	1.45
6	E	5003	EKW	O4'-C4'	2.91	1.29	1.23
7	F	5931	FAD	O4-C4	2.90	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	810	EKW	C4A-C4B	2.90	1.43	1.38
6	E	5003	EKW	C4'-N3'	-2.82	1.33	1.38
7	C	4932	FAD	O4B-C4B	-2.76	1.38	1.45
6	B	810	EKW	C5-C4	-2.60	1.36	1.42
6	B	810	EKW	OM1-MO	2.60	1.70	1.68
6	E	5003	EKW	O9'-C9'	-2.58	1.38	1.43
7	F	5931	FAD	C4X-C10	-2.46	1.37	1.44
7	F	5931	FAD	C8A-N9A	-2.44	1.33	1.37
6	B	810	EKW	C7-N8'	-2.37	1.41	1.45
6	E	5003	EKW	C10-C9'	-2.31	1.48	1.51
6	B	810	EKW	C4B-N8'	2.25	1.37	1.35
6	E	5003	EKW	C1'-N1	-2.20	1.41	1.47
7	C	4932	FAD	C9-C8	-2.08	1.36	1.39
7	F	5931	FAD	C4A-N9A	-2.02	1.33	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	5003	EKW	C7'-C8'-S8'	-5.16	117.22	120.15
6	E	5003	EKW	C7-C6'-N5'	4.80	112.58	107.87
4	E	5002	PO4	O4-P-O2	3.89	120.03	107.91
7	F	5931	FAD	C5X-C9A-N10	3.65	121.27	117.97
6	E	5003	EKW	O9'-C9'-C8'	3.46	113.98	109.09
7	F	5931	FAD	C9A-C5X-N5	-3.46	118.78	122.45
6	E	5003	EKW	O4'-C4'-C4A	-3.46	118.92	127.26
6	B	810	EKW	C7-C6'-N5'	3.26	111.07	107.87
6	E	5003	EKW	C8'-C7'-S7'	3.19	121.96	120.15
6	B	810	EKW	O2-C2-N3	-3.12	117.40	122.33
7	C	4932	FAD	N9A-C8A-N7A	-3.10	109.53	113.94
4	E	5002	PO4	O3-P-O1	-3.03	100.25	110.95
6	E	5003	EKW	C4'-C4A-N5'	2.97	124.36	116.27
7	F	5931	FAD	C4X-C4-N3	2.80	120.39	113.25
7	C	4932	FAD	C5A-N7A-C8A	2.71	107.70	103.45
7	F	5931	FAD	O4B-C4B-C5B	2.65	117.81	109.33
6	B	810	EKW	C7'-C8'-S8'	-2.57	118.69	120.15
7	C	4932	FAD	C4X-C10-N10	2.57	120.15	116.48
7	C	4932	FAD	N3A-C2A-N1A	-2.51	124.79	128.58
6	E	5003	EKW	O9'-C7-N8'	-2.47	106.37	108.61
7	C	4932	FAD	O4B-C1B-N9A	-2.45	103.38	108.09
6	E	5003	EKW	O9'-C7-C6'	2.44	110.59	108.96
7	F	5931	FAD	O3'-C3'-C2'	-2.43	103.41	108.93
7	C	4932	FAD	C4A-C5A-N7A	-2.43	107.81	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4001	PO4	O4-P-O2	2.38	115.31	107.91
6	B	810	EKW	O9'-C9'-C8'	2.37	112.43	109.09
7	F	5931	FAD	C4X-C10-N10	2.34	119.84	116.48
6	B	810	EKW	C2'-N1'-C4B	2.34	117.49	113.36
6	E	5003	EKW	O2-C2-N3	-2.25	118.79	122.33
7	F	5931	FAD	C9A-C9-C8	2.21	123.67	119.22
7	F	5931	FAD	O3B-C3B-C2B	-2.12	105.03	111.82
7	F	5931	FAD	C4-N3-C2	-2.12	121.89	125.64
6	B	810	EKW	O4'-C4'-C4A	-2.10	122.19	127.26
7	F	5931	FAD	C10-N1-C2	2.10	121.39	116.85
7	C	4932	FAD	C4A-N9A-C8A	2.08	107.92	105.74
6	B	810	EKW	C2D-C1'-N1	-2.07	107.50	113.25
7	C	4932	FAD	O4B-C4B-C5B	2.03	115.83	109.33
7	F	5931	FAD	C2B-C1B-N9A	2.01	118.30	113.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	5931	FAD	C3'-C4'-C5'-O5'
7	F	5931	FAD	PA-O3P-P-O2P

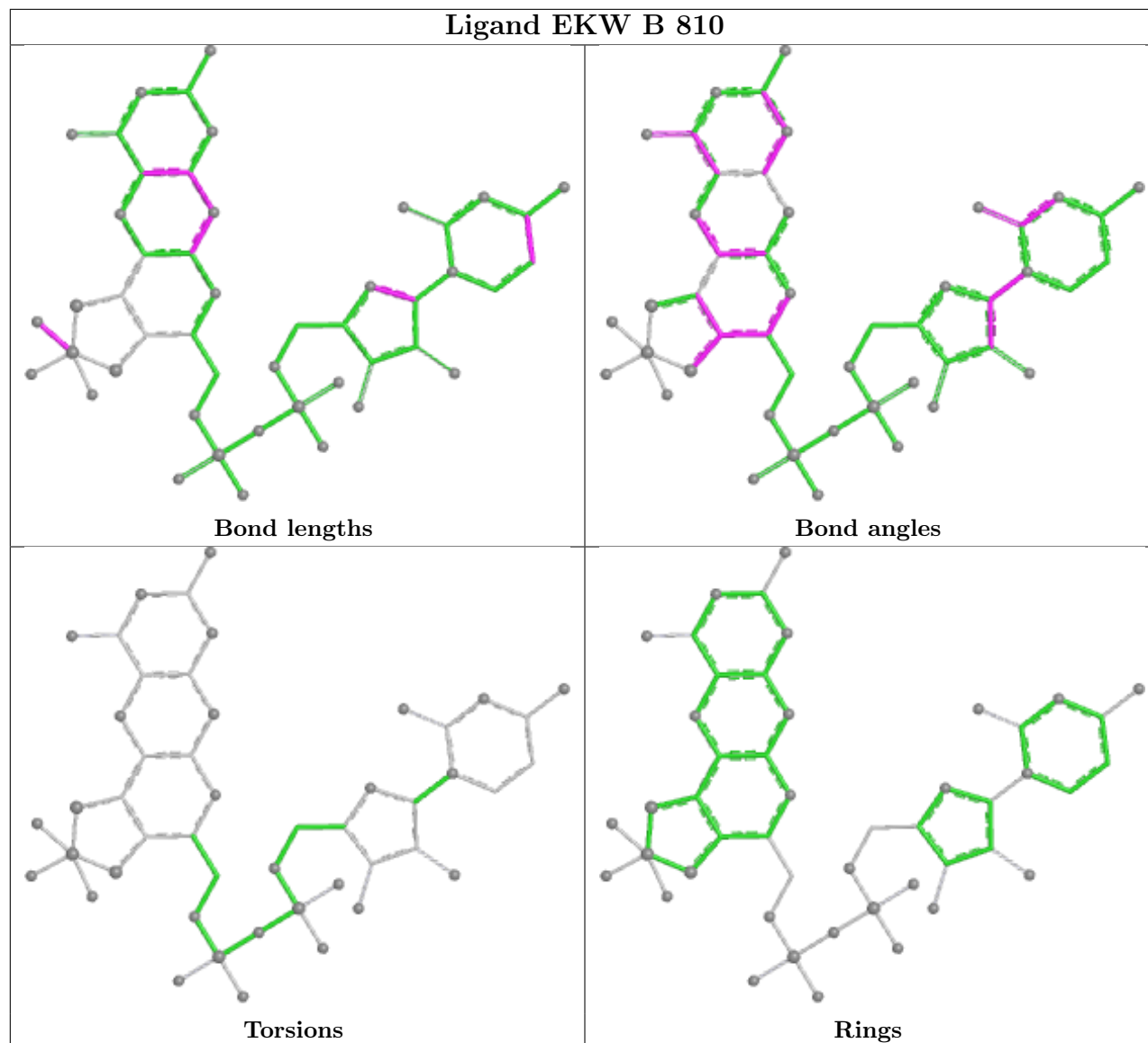
There are no ring outliers.

4 monomers are involved in 8 short contacts:

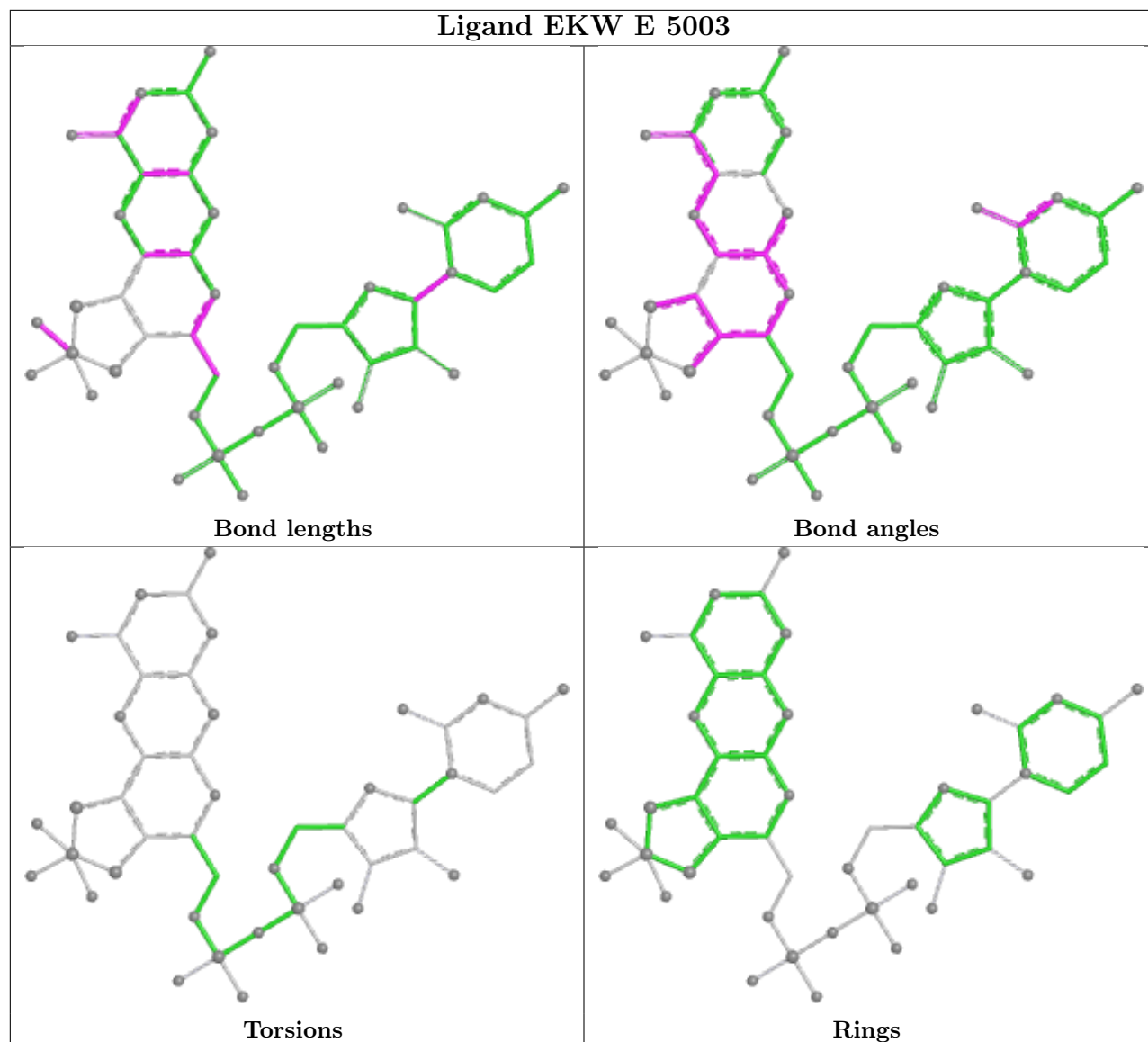
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	810	EKW	2	0
6	E	5003	EKW	2	0
7	F	5931	FAD	3	0
7	C	4932	FAD	1	0

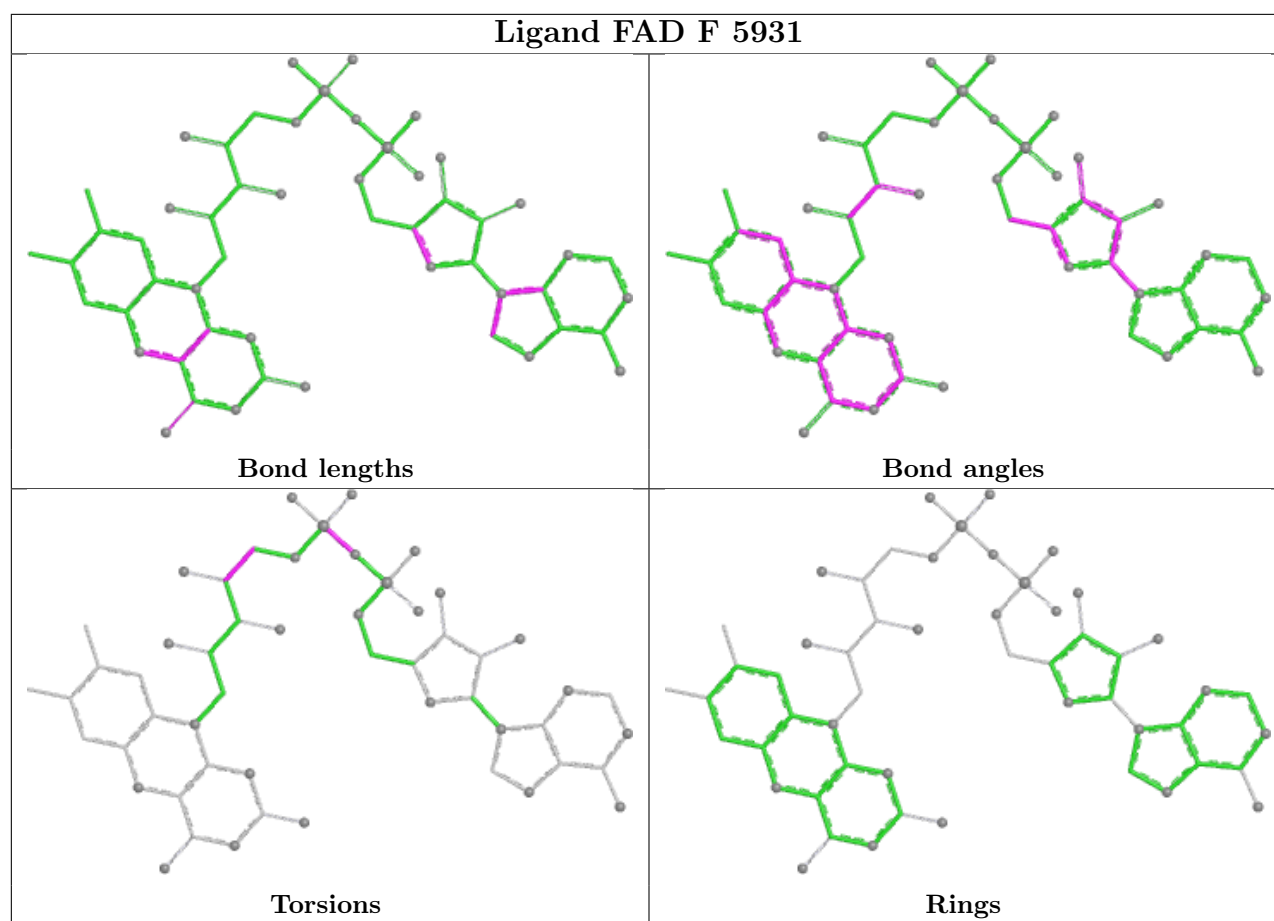
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

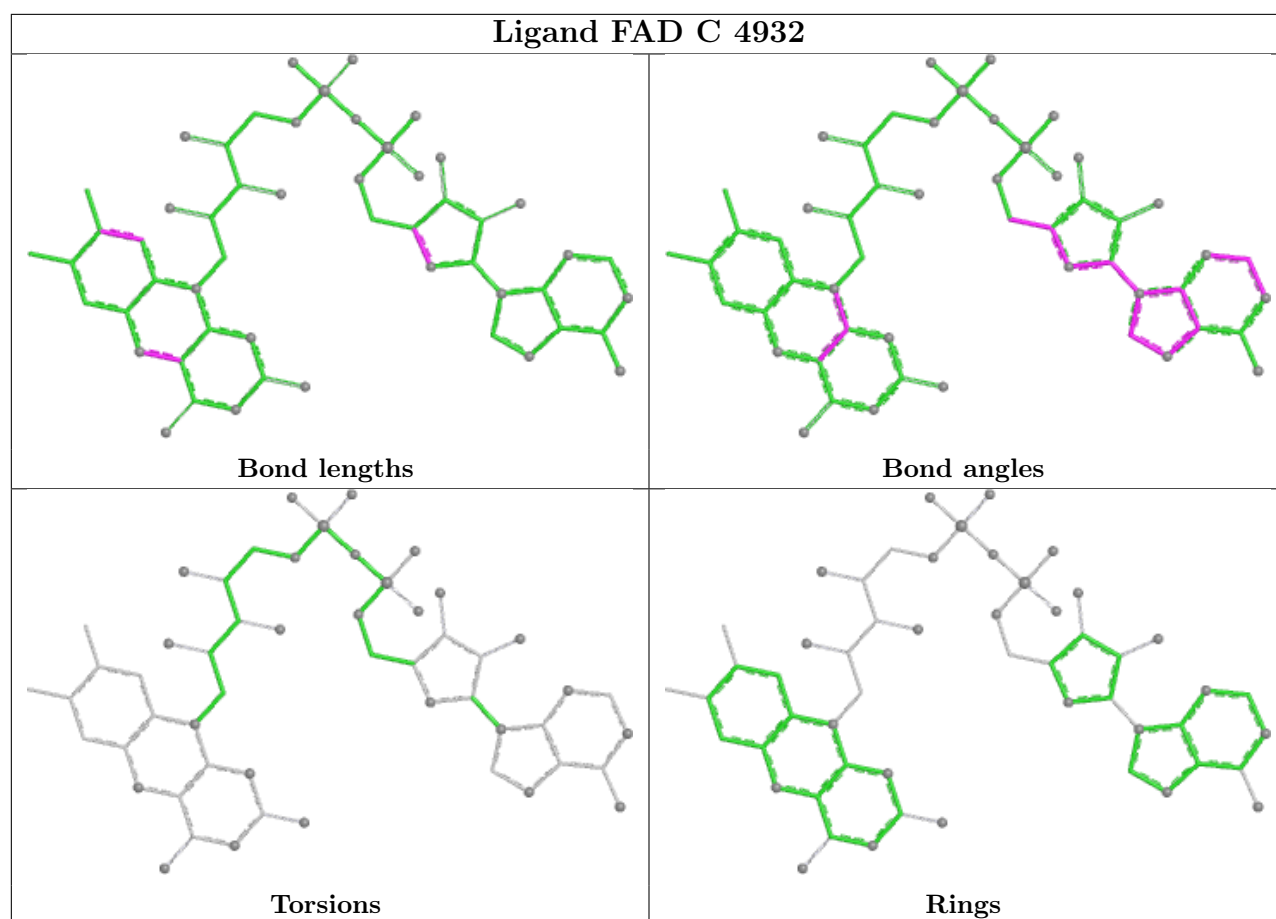
equivalents in the CSD to analyse the geometry.



Ligand EKW E 5003







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.