



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:39 PM UTC

PDB ID : 1QRD / pdb_00001qrd
Title : QUINONE REDUCTASE/FAD/CIBACRON BLUE/DUROQUINONE COMPLEX
Authors : Li, R.; Bianchet, M.A.; Talalay, P.; Amzel, L.M.
Deposited on : 1995-07-28
Resolution : 2.40 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

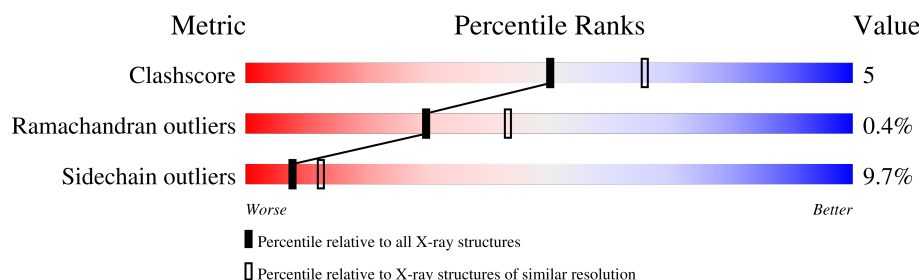
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

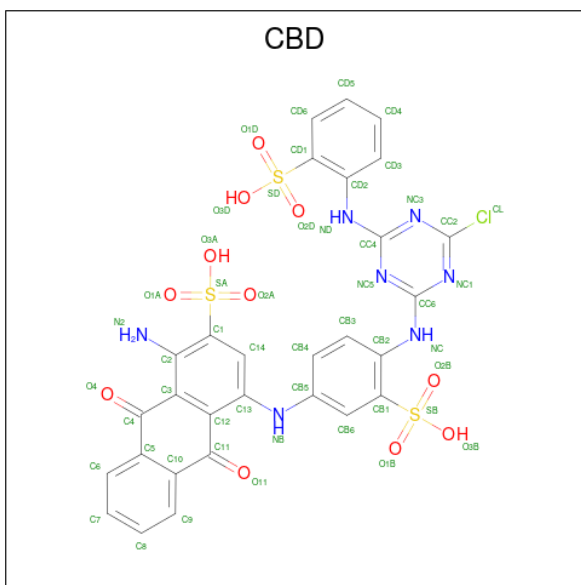
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	273	
1	B	273	

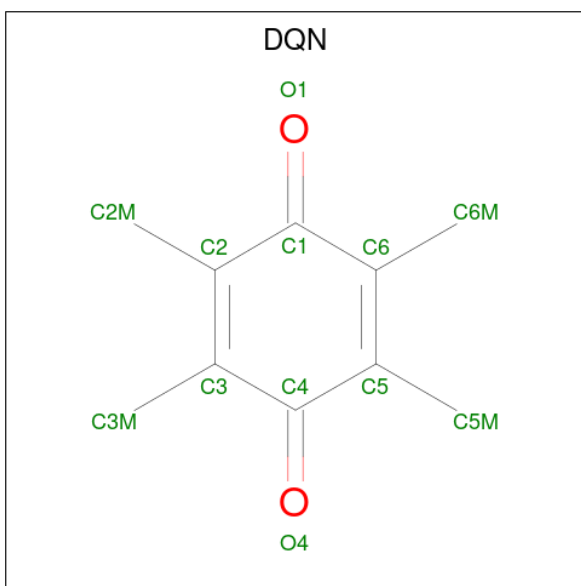
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	274	X	-	-	-
2	FAD	B	274	X	-	-	-



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 51	C 29	Cl 1	N 7	O 11	S 3	0	0
3	B	1	Total 51	C 29	Cl 1	N 7	O 11	S 3	0	0

- Molecule 4 is DUROQUINONE (CCD ID: DQN) (formula: $\text{C}_{10}\text{H}_{12}\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 10 2	0	0
4	B	1	Total C O 12 10 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0
5	B	23	Total 23	O 23	0	0

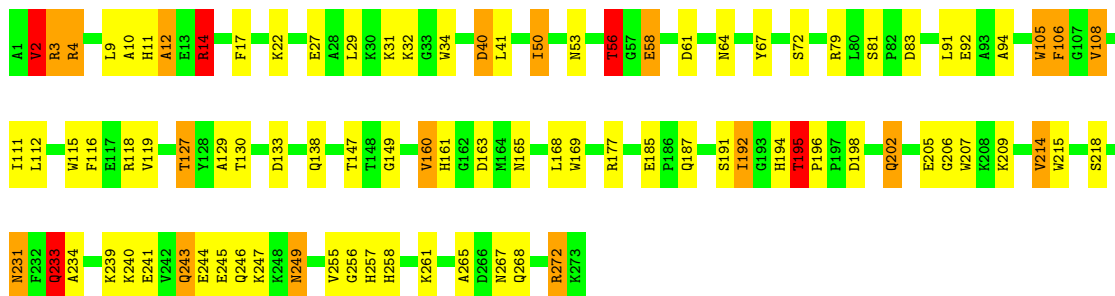
3 Residue-property plots

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.

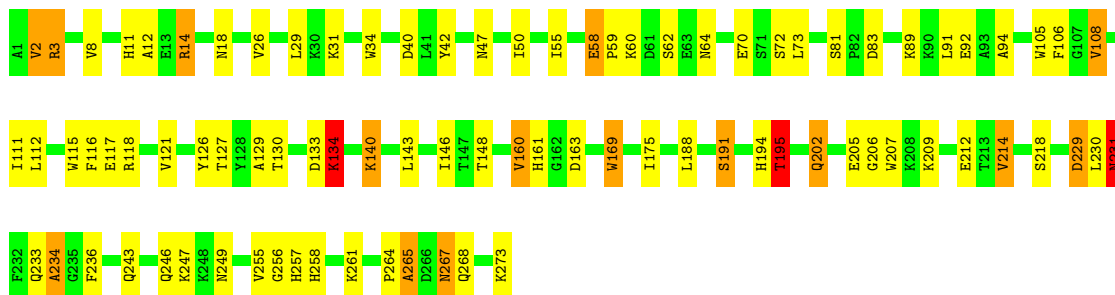
• Molecule 1: QUINONE-REDUCTASE

Chain A: 



• Molecule 1: QUINONE-REDUCTASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.00 Å 107.00 Å 88.40 Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	88.8 (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4642	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: CBD, FAD, DQN

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	1.25	12/2238 (0.5%)	2.01	77/3027 (2.5%)
1	B	1.21	8/2238 (0.4%)	1.94	75/3027 (2.5%)
All	All	1.23	20/4476 (0.4%)	1.98	152/6054 (2.5%)

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	B	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	VAL	CA-CB	10.99	1.69	1.54
1	A	111	ILE	CA-CB	6.92	1.64	1.54
1	A	50	ILE	CA-CB	6.55	1.61	1.54
1	A	161	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	195	THR	CA-CB	6.36	1.63	1.53
1	B	257	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	111	ILE	CA-CB	6.16	1.63	1.54
1	A	257	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	258	HIS	CD2-NE2	-6.02	1.31	1.37
1	B	258	HIS	CD2-NE2	-5.93	1.31	1.37
1	B	2	VAL	CA-CB	5.83	1.62	1.54
1	A	149	GLY	CA-C	5.81	1.58	1.52
1	B	175	ILE	CA-CB	5.78	1.60	1.55
1	B	11	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	50	ILE	CA-CB	5.46	1.61	1.54
1	A	249	ASN	CA-CB	-5.39	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	119	VAL	CA-CB	5.22	1.61	1.54
1	B	194	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	194	HIS	CD2-NE2	-5.06	1.32	1.37

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	N-CA-C	12.10	131.75	113.61
1	B	268	GLN	OE1-CD-NE2	-11.39	111.21	122.60
1	B	202	GLN	OE1-CD-NE2	-11.06	111.54	122.60
1	A	202	GLN	OE1-CD-NE2	-10.77	111.83	122.60
1	A	202	GLN	CG-CD-NE2	10.43	132.04	116.40
1	A	108	VAL	N-CA-CB	-10.19	96.95	111.21
1	B	118	ARG	NE-CZ-NH2	-9.75	110.43	119.20
1	B	108	VAL	N-CA-CB	-9.45	97.98	111.21
1	A	231	ASN	OD1-CG-ND2	-9.43	113.17	122.60
1	A	214	VAL	CB-CA-C	-9.24	99.94	112.04
1	A	61	ASP	CA-CB-CG	9.11	121.71	112.60
1	B	118	ARG	NE-CZ-NH1	8.92	130.42	121.50
1	A	163	ASP	N-CA-C	8.74	122.44	109.59
1	B	202	GLN	CG-CD-NE2	8.64	129.37	116.40
1	B	267	ASN	OD1-CG-ND2	-8.52	114.08	122.60
1	B	3	ARG	N-CA-C	8.07	124.11	113.30
1	B	163	ASP	CA-CB-CG	8.06	120.66	112.60
1	A	56	THR	CA-CB-OG1	-8.00	97.61	109.60
1	A	195	THR	CA-C-N	7.90	125.43	119.66
1	A	195	THR	C-N-CA	7.90	125.43	119.66
1	B	268	GLN	CG-CD-NE2	7.88	128.22	116.40
1	B	34	TRP	CG-CD2-CE3	7.64	141.54	133.90
1	B	160	VAL	CB-CA-C	-7.61	98.81	111.29
1	A	265	ALA	N-CA-C	7.22	120.72	109.96
1	A	160	VAL	CB-CA-C	-7.20	99.48	111.29
1	A	258	HIS	CB-CG-CD2	-7.19	121.86	131.20
1	A	138	GLN	CA-CB-CG	7.16	128.41	114.10
1	A	258	HIS	CB-CG-ND1	7.15	133.42	122.70
1	A	214	VAL	N-CA-C	7.11	118.72	110.62
1	B	207	TRP	CG-CD2-CE3	7.08	140.98	133.90
1	A	261	LYS	CB-CG-CD	-7.08	95.02	111.30
1	B	207	TRP	CB-CG-CD1	-7.05	116.33	126.90
1	A	11	HIS	CB-CG-CD2	-7.04	122.05	131.20
1	B	163	ASP	N-CA-C	7.02	120.49	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASN	CB-CG-ND2	6.99	126.88	116.40
1	A	64	ASN	CA-CB-CG	6.96	119.56	112.60
1	B	26	VAL	CA-C-N	6.55	129.54	120.63
1	B	26	VAL	C-N-CA	6.55	129.54	120.63
1	B	47	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	A	3	ARG	CA-CB-CG	6.46	127.03	114.10
1	B	257	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	A	115	TRP	CG-CD2-CE3	6.46	140.36	133.90
1	B	205	GLU	N-CA-C	6.45	118.31	111.28
1	B	243	GLN	OE1-CD-NE2	-6.45	116.16	122.60
1	A	40	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	138	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	B	83	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	47	ASN	CB-CG-ND2	6.25	125.77	116.40
1	B	188	LEU	CA-C-O	-6.24	113.45	120.32
1	A	243	GLN	CG-CD-NE2	6.23	125.74	116.40
1	A	245	GLU	CB-CG-CD	6.20	123.14	112.60
1	B	34	TRP	CB-CG-CD1	-6.17	117.64	126.90
1	A	81	SER	N-CA-CB	-6.16	100.73	110.03
1	B	261	LYS	CB-CG-CD	-6.12	97.22	111.30
1	B	234	ALA	N-CA-C	6.12	118.75	111.71
1	B	11	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	B	258	HIS	CA-CB-CG	6.10	119.90	113.80
1	A	56	THR	CA-CB-CG2	6.07	120.82	110.50
1	A	105	TRP	CG-CD2-CE3	6.07	139.97	133.90
1	A	56	THR	N-CA-CB	-5.99	101.26	110.85
1	A	163	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	272	ARG	O-C-N	5.99	130.55	122.59
1	A	194	HIS	CA-CB-CG	5.93	119.73	113.80
1	A	81	SER	CA-C-N	5.93	125.47	119.19
1	A	81	SER	C-N-CA	5.93	125.47	119.19
1	A	185	GLU	N-CA-C	5.91	116.40	109.60
1	A	34	TRP	CG-CD2-CE3	5.86	139.76	133.90
1	B	133	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	83	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	257	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	138	GLN	N-CA-C	5.78	119.43	112.38
1	B	267	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	115	TRP	CG-CD2-CE3	5.72	139.62	133.90
1	B	161	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	115	TRP	CB-CG-CD1	-5.70	118.35	126.90
1	A	2	VAL	O-C-N	-5.70	115.45	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	B	212	GLU	CA-CB-CG	-5.67	102.75	114.10
1	B	265	ALA	N-CA-CB	5.67	120.06	110.49
1	A	243	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	B	169	TRP	CG-CD2-CE3	5.64	139.54	133.90
1	A	11	HIS	CB-CG-ND1	5.62	131.14	122.70
1	A	161	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	B	89	LYS	CA-CB-CG	-5.60	102.90	114.10
1	B	207	TRP	O-C-N	-5.59	116.19	122.12
1	A	195	THR	CB-CA-C	5.58	116.40	108.76
1	A	214	VAL	N-CA-CB	5.56	117.42	110.47
1	A	106	PHE	CA-CB-CG	5.56	119.36	113.80
1	B	59	PRO	N-CA-CB	5.55	107.74	103.30
1	B	146	ILE	N-CA-C	5.47	116.36	108.48
1	A	218	SER	CA-C-N	5.47	125.67	120.31
1	A	218	SER	C-N-CA	5.47	125.67	120.31
1	B	134	LYS	N-CA-C	-5.47	106.20	112.92
1	B	231	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	B	34	TRP	CE2-CD2-CG	-5.46	100.64	107.20
1	B	207	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	A	41	LEU	N-CA-C	5.43	116.88	111.07
1	A	12	ALA	N-CA-C	5.43	117.28	111.36
1	B	8	VAL	CA-C-O	-5.37	114.79	120.53
1	A	258	HIS	CA-CB-CG	5.33	119.13	113.80
1	A	92	GLU	CB-CG-CD	-5.32	103.55	112.60
1	B	64	ASN	CA-CB-CG	5.32	117.92	112.60
1	B	70	GLU	N-CA-C	5.32	117.08	111.28
1	A	58	GLU	CB-CG-CD	5.32	121.64	112.60
1	B	195	THR	CA-C-N	5.31	125.85	120.38
1	B	195	THR	C-N-CA	5.31	125.85	120.38
1	B	230	LEU	N-CA-C	5.31	117.80	108.56
1	A	168	LEU	N-CA-C	5.31	118.92	112.23
1	A	147	THR	N-CA-C	-5.30	101.93	110.14
1	A	34	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	A	53	ASN	O-C-N	-5.28	115.57	122.59
1	B	264	PRO	N-CA-C	5.28	121.62	113.75
1	B	50	ILE	N-CA-CB	-5.27	103.03	110.26
1	A	177	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	B	31	LYS	CA-CB-CG	-5.27	103.55	114.10
1	B	140	LYS	CG-CD-CE	-5.26	99.19	111.30
1	A	118	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	14	ARG	N-CA-C	-5.24	106.88	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	GLU	CB-CG-CD	5.24	121.51	112.60
1	B	218	SER	CA-C-N	5.24	125.71	120.52
1	B	218	SER	C-N-CA	5.24	125.71	120.52
1	B	265	ALA	CB-CA-C	-5.24	100.00	110.42
1	B	258	HIS	CB-CG-ND1	5.22	130.53	122.70
1	B	60	LYS	CB-CG-CD	-5.19	99.36	111.30
1	B	117	GLU	CB-CG-CD	5.19	121.42	112.60
1	B	81	SER	N-CA-CB	-5.19	102.13	109.75
1	A	187	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	257	HIS	CB-CG-ND1	5.18	130.47	122.70
1	A	116	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	258	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	B	58	GLU	N-CA-C	5.14	121.17	109.81
1	A	207	TRP	CB-CG-CD1	-5.12	119.22	126.90
1	B	62	SER	N-CA-C	5.12	118.30	111.75
1	A	161	HIS	CB-CG-ND1	5.11	130.37	122.70
1	B	18	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	B	40	ASP	CA-CB-CG	5.11	117.70	112.60
1	A	10	ALA	N-CA-C	5.10	115.73	108.54
1	B	126	TYR	CA-C-N	5.09	130.55	121.75
1	B	126	TYR	C-N-CA	5.09	130.55	121.75
1	A	12	ALA	CB-CA-C	-5.09	102.20	110.85
1	B	121	VAL	N-CA-CB	-5.08	103.54	110.56
1	B	11	HIS	CB-CG-ND1	5.08	130.32	122.70
1	A	192	ILE	CB-CG1-CD1	-5.07	103.16	113.80
1	A	165	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	196	PRO	CA-C-N	5.06	125.09	119.32
1	A	196	PRO	C-N-CA	5.06	125.09	119.32
1	B	116	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	148	THR	N-CA-CB	-5.02	102.14	111.13
1	B	214	VAL	N-CA-C	5.01	119.77	109.34
1	A	205	GLU	CA-C-N	5.01	125.50	119.94
1	A	205	GLU	C-N-CA	5.01	125.50	119.94
1	A	233	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	42	TYR	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	2181	0	2182	27	0
1	B	2181	0	2182	18	0
2	A	53	0	30	0	0
2	B	53	0	29	0	0
3	A	51	0	20	3	0
3	B	51	0	20	3	0
4	A	12	0	12	4	0
4	B	12	0	12	4	0
5	A	25	0	0	0	0
5	B	23	0	0	0	0
All	All	4642	0	4487	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TRP:CE3	4:A:276:DQN:H3M1	2.21	0.76
1:B:127:THR:HG22	1:B:129:ALA:H	1.50	0.75
1:B:105:TRP:CE3	4:B:276:DQN:H3M1	2.24	0.71
1:B:127:THR:HB	1:B:130:THR:OG1	1.90	0.71
1:A:231:ASN:ND2	1:A:234:ALA:H	1.91	0.69
1:B:231:ASN:ND2	1:B:234:ALA:H	1.91	0.68
1:B:106:PHE:HE1	4:B:276:DQN:O4	1.84	0.60
1:A:127:THR:HB	1:A:130:THR:OG1	2.03	0.58
1:A:3:ARG:HG3	1:A:4:ARG:HH21	1.69	0.58
1:B:191:SER:O	1:B:195:THR:HG22	2.04	0.57
1:A:255:VAL:HG23	1:A:267:ASN:HD22	1.71	0.55
1:A:4:ARG:HB3	1:A:94:ALA:HA	1.91	0.52
1:A:106:PHE:HE1	4:A:276:DQN:O4	1.94	0.51
1:A:2:VAL:HB	1:A:215:TRP:CD1	2.45	0.51
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.75	0.50
1:B:246:GLN:HA	1:B:249:ASN:ND2	2.27	0.50
1:A:12:ALA:O	1:A:14:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLY:HA3	1:B:202:GLN:HE21	1.77	0.48
1:A:127:THR:HG22	1:A:129:ALA:H	1.78	0.48
3:B:275:CBD:HB3	3:B:275:CBD:NC1	2.29	0.47
3:A:275:CBD:CL	4:A:276:DQN:C5M	3.00	0.47
1:B:229:ASP:HB3	1:B:234:ALA:CB	2.45	0.47
1:A:50:ILE:HD11	1:A:67:TYR:CD2	2.50	0.46
1:A:202:GLN:HE21	1:B:206:GLY:HA3	1.81	0.46
1:A:246:GLN:HA	1:A:249:ASN:ND2	2.31	0.46
3:B:275:CBD:CL	4:B:276:DQN:H6M2	2.53	0.46
1:A:9:LEU:HD22	1:A:22:LYS:HG3	1.97	0.46
1:A:17:PHE:CB	1:A:192:ILE:HD11	2.46	0.46
1:A:17:PHE:CG	1:A:192:ILE:HD11	2.52	0.45
1:A:239:LYS:O	1:A:243:GLN:HG3	2.17	0.45
1:A:191:SER:O	1:A:195:THR:HG22	2.17	0.44
1:B:169:TRP:CZ2	1:B:256:GLY:HA3	2.52	0.44
1:B:94:ALA:O	1:B:140:LYS:HE2	2.17	0.44
1:B:231:ASN:HD22	1:B:234:ALA:H	1.63	0.44
1:A:56:THR:HB	1:A:79:ARG:O	2.18	0.43
1:A:231:ASN:HD22	1:A:233:GLN:N	2.16	0.43
3:A:275:CBD:CL	4:A:276:DQN:H5M2	2.56	0.43
1:A:209:LYS:HD2	1:B:209:LYS:HB2	2.00	0.43
1:A:3:ARG:NH1	1:A:4:ARG:NH2	2.67	0.43
1:B:229:ASP:O	1:B:236:PHE:HA	2.19	0.42
3:B:275:CBD:CL	4:B:276:DQN:C6M	3.04	0.42
1:B:12:ALA:O	1:B:14:ARG:NH1	2.53	0.42
1:B:134:LYS:HE2	1:B:134:LYS:HB3	1.83	0.42
1:A:14:ARG:NH2	1:A:40:ASP:OD1	2.52	0.42
1:A:27:GLU:HG2	1:A:31:LYS:HE3	2.01	0.42
1:A:50:ILE:HG12	1:A:67:TYR:CE1	2.56	0.41
1:A:169:TRP:CZ2	1:A:256:GLY:HA3	2.55	0.41
3:A:275:CBD:O2A	3:A:275:CBD:N2	2.53	0.41

There are no symmetry-related clashes.

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	271/273 (99%)	258 (95%)	12 (4%)	1 (0%)	30	43
1	B	271/273 (99%)	256 (94%)	14 (5%)	1 (0%)	30	43
All	All	542/546 (99%)	514 (95%)	26 (5%)	2 (0%)	30	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ALA
1	A	272	ARG

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	231/231 (100%)	209 (90%)	22 (10%)	8	13
1	B	231/231 (100%)	208 (90%)	23 (10%)	7	11
All	All	462/462 (100%)	417 (90%)	45 (10%)	8	12

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	4	ARG
1	A	14	ARG
1	A	29	LEU
1	A	32	LYS
1	A	56	THR
1	A	58	GLU
1	A	72	SER
1	A	91	LEU
1	A	108	VAL
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	127	THR
1	A	133	ASP
1	A	160	VAL
1	A	195	THR
1	A	198	ASP
1	A	214	VAL
1	A	233	GLN
1	A	240	LYS
1	A	241	GLU
1	A	244	GLU
1	A	247	LYS
1	B	2	VAL
1	B	3	ARG
1	B	14	ARG
1	B	29	LEU
1	B	55	ILE
1	B	58	GLU
1	B	72	SER
1	B	73	LEU
1	B	91	LEU
1	B	92	GLU
1	B	108	VAL
1	B	112	LEU
1	B	134	LYS
1	B	143	LEU
1	B	160	VAL
1	B	191	SER
1	B	195	THR
1	B	214	VAL
1	B	229	ASP
1	B	231	ASN
1	B	233	GLN
1	B	247	LYS
1	B	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	47	ASN
1	A	64	ASN
1	A	66	GLN

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	161	HIS
1	A	172	GLN
1	A	202	GLN
1	A	231	ASN
1	A	249	ASN
1	A	267	ASN
1	A	268	GLN
1	B	138	GLN
1	B	161	HIS
1	B	172	GLN
1	B	182	GLN
1	B	202	GLN
1	B	231	ASN
1	B	249	ASN
1	B	267	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](#)

6 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
3	CBD	B	275	-	56,56,56	2.06	12 (21%)	81,87,87	3.28	32 (39%)
3	CBD	A	275	-	56,56,56	1.87	12 (21%)	81,87,87	3.04	33 (40%)
2	FAD	A	274	-	58,58,58	1.56	8 (13%)	85,89,89	2.25	30 (35%)
4	DQN	A	276	-	12,12,12	0.94	0	18,18,18	1.06	0
4	DQN	B	276	-	12,12,12	1.10	0	18,18,18	1.08	1 (5%)
2	FAD	B	274	-	58,58,58	1.45	5 (8%)	85,89,89	2.31	31 (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
3	CBD	B	275	-	-	3/30/46/46	0/6/6/6
3	CBD	A	275	-	-	7/30/46/46	0/6/6/6
2	FAD	A	274	-	3/3/9/9	13/34/50/50	0/6/6/6
4	DQN	A	276	-	-	-	0/1/1/1
4	DQN	B	276	-	-	-	0/1/1/1
2	FAD	B	274	-	3/3/9/9	11/34/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	275	CBD	CC4-ND	5.47	1.48	1.36
3	B	275	CBD	C2-N2	5.38	1.54	1.37
3	B	275	CBD	CC6-NC	5.29	1.47	1.36
2	A	274	FAD	C1'-N10	-5.19	1.35	1.47
3	A	275	CBD	C2-N2	4.97	1.53	1.37
3	B	275	CBD	CD6-CD1	4.91	1.44	1.39
3	A	275	CBD	CC6-NC	4.88	1.46	1.36
2	B	274	FAD	C1'-N10	-4.86	1.36	1.47
3	A	275	CBD	CC4-ND	4.81	1.46	1.36
3	B	275	CBD	CC2-CL	4.62	1.87	1.73
2	A	274	FAD	C10-N1	4.44	1.42	1.33
3	A	275	CBD	CD6-CD1	4.22	1.44	1.39
2	A	274	FAD	C8M-C8	4.10	1.58	1.51
2	B	274	FAD	C10-N1	4.05	1.41	1.33
2	B	274	FAD	C5A-N7A	-3.83	1.32	1.39
3	A	275	CBD	CC2-CL	3.83	1.85	1.73
2	A	274	FAD	C5A-N7A	-3.74	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	274	FAD	C5'-C4'	3.73	1.56	1.51
3	B	275	CBD	CC2-NC3	3.67	1.39	1.32
3	B	275	CBD	C13-NB	3.21	1.48	1.39
2	B	274	FAD	C4X-N5	3.16	1.37	1.30
3	A	275	CBD	CC2-NC3	3.10	1.37	1.32
3	B	275	CBD	CB5-NB	3.06	1.47	1.40
3	A	275	CBD	C13-NB	2.85	1.47	1.39
3	B	275	CBD	CB2-NC	2.62	1.47	1.39
2	A	274	FAD	C4X-N5	2.59	1.36	1.30
3	B	275	CBD	CC2-NC1	2.53	1.36	1.32
3	B	275	CBD	C10-C11	-2.51	1.43	1.48
3	B	275	CBD	CD2-ND	2.41	1.46	1.39
3	A	275	CBD	CD3-CD2	2.28	1.43	1.39
3	A	275	CBD	CB5-NB	2.23	1.45	1.40
3	A	275	CBD	CD2-ND	2.20	1.45	1.39
3	A	275	CBD	CB2-NC	2.11	1.45	1.39
3	A	275	CBD	CC2-NC1	2.10	1.36	1.32
2	B	274	FAD	C8M-C8	2.06	1.54	1.51
2	A	274	FAD	C8A-N7A	2.05	1.35	1.31
2	A	274	FAD	C4-N3	2.01	1.42	1.38

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	275	CBD	CC6-NC1-CC2	10.80	123.79	112.41
3	B	275	CBD	CC4-NC3-CC2	10.43	123.40	112.41
3	A	275	CBD	CC4-NC3-CC2	10.07	123.02	112.41
3	B	275	CBD	NC3-CC2-NC1	-8.59	113.82	129.52
3	A	275	CBD	CB1-CB2-NC	-8.01	114.11	121.50
3	B	275	CBD	CL-CC2-NC3	7.94	126.35	115.17
3	B	275	CBD	CB1-CB2-NC	-7.59	114.49	121.50
3	A	275	CBD	CC6-NC1-CC2	7.40	120.20	112.41
3	A	275	CBD	CD1-CD2-ND	-7.37	114.70	121.50
3	A	275	CBD	NC3-CC2-NC1	-6.97	116.77	129.52
3	B	275	CBD	C1-C2-N2	-6.92	115.64	122.64
3	B	275	CBD	CD1-CD2-ND	-6.61	115.40	121.50
3	B	275	CBD	C10-C11-C12	6.44	128.40	117.97
2	B	274	FAD	C5A-C4A-N3A	-6.43	117.86	126.72
3	A	275	CBD	C10-C11-C12	6.29	128.16	117.97
3	A	275	CBD	CL-CC2-NC3	6.28	124.01	115.17
2	A	274	FAD	C5A-C4A-N3A	-6.17	118.23	126.72
2	B	274	FAD	C4'-C3'-C2'	6.11	123.74	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	274	FAD	N3A-C4A-N9A	5.95	137.29	127.17
2	A	274	FAD	N3A-C4A-N9A	5.68	136.82	127.17
2	B	274	FAD	C10-N1-C2	5.43	128.60	116.85
2	A	274	FAD	N3A-C2A-N1A	-5.23	120.67	128.58
3	A	275	CBD	C5-C4-C3	5.14	126.28	117.97
2	A	274	FAD	C10-N1-C2	5.11	127.91	116.85
2	A	274	FAD	C4'-C3'-C2'	5.02	121.92	113.57
3	B	275	CBD	O11-C11-C10	-4.99	113.79	120.99
2	B	274	FAD	N3A-C2A-N1A	-4.98	121.05	128.58
2	B	274	FAD	C4X-C10-N1	-4.83	112.75	124.59
3	A	275	CBD	CD2-CD1-SD	-4.77	117.62	121.90
3	B	275	CBD	C5-C4-C3	4.75	125.66	117.97
3	B	275	CBD	C5-C10-C11	-4.70	115.80	120.86
2	A	274	FAD	O3'-C3'-C2'	4.63	119.46	108.93
3	A	275	CBD	O3D-SD-CD1	4.52	114.91	106.12
3	A	275	CBD	NC5-CC4-NC3	-4.52	118.85	126.26
2	A	274	FAD	C4X-C10-N1	-4.33	113.97	124.59
3	A	275	CBD	C10-C5-C4	-4.32	116.21	120.86
3	B	275	CBD	CB2-CB1-SB	-4.29	118.06	121.90
2	A	274	FAD	O3'-C3'-C4'	4.27	118.62	108.93
3	A	275	CBD	O11-C11-C12	-4.24	114.37	121.44
2	B	274	FAD	O3'-C3'-C4'	4.22	118.52	108.93
3	B	275	CBD	NC5-CC4-NC3	-4.11	119.52	126.26
3	A	275	CBD	C5-C10-C11	-4.09	116.46	120.86
2	B	274	FAD	C4-C4X-C10	4.03	123.85	116.93
2	A	274	FAD	C4-C4X-C10	3.95	123.70	116.93
3	A	275	CBD	C1-C2-N2	-3.91	118.69	122.64
2	B	274	FAD	O3'-C3'-C2'	3.87	117.73	108.93
3	B	275	CBD	NC5-CC6-NC1	-3.84	119.97	126.26
2	B	274	FAD	C6A-C5A-C4A	3.83	122.40	117.18
3	A	275	CBD	C3-C12-C11	-3.75	114.93	120.00
2	B	274	FAD	C6A-C5A-N7A	-3.73	124.91	132.09
2	A	274	FAD	C6A-C5A-C4A	3.69	122.22	117.18
2	A	274	FAD	C6A-C5A-N7A	-3.62	125.12	132.09
3	A	275	CBD	O4-C4-C3	-3.60	115.43	121.44
2	B	274	FAD	C2A-N3A-C4A	3.48	120.33	111.83
2	A	274	FAD	C2A-N3A-C4A	3.48	120.33	111.83
3	B	275	CBD	C10-C5-C4	-3.39	117.22	120.86
3	B	275	CBD	O4-C4-C3	-3.31	115.92	121.44
2	B	274	FAD	C4X-C10-N10	3.29	121.20	116.48
2	B	274	FAD	C2B-C3B-C4B	3.27	108.92	102.61
2	A	274	FAD	O2-C2-N3	3.24	124.80	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	274	FAD	C5X-C9A-N10	3.23	120.89	117.97
3	B	275	CBD	CL-CC2-NC1	3.16	119.62	115.17
3	B	275	CBD	CD2-CD1-SD	-3.15	119.08	121.90
3	B	275	CBD	CC6-NC5-CC4	3.15	119.50	113.85
3	B	275	CBD	C3-C12-C11	-3.14	115.76	120.00
2	B	274	FAD	C1'-C2'-C3'	3.12	118.13	109.66
3	A	275	CBD	CC6-NC5-CC4	3.09	119.39	113.85
3	A	275	CBD	O11-C11-C10	-3.07	116.56	120.99
3	A	275	CBD	CB6-CB1-CB2	-3.07	117.79	120.85
3	A	275	CBD	C6-C5-C4	3.03	123.98	119.26
3	B	275	CBD	O3D-SD-CD1	3.00	111.96	106.12
2	A	274	FAD	C4-C4X-N5	-2.99	114.07	118.21
2	B	274	FAD	O2'-C2'-C1'	2.99	122.50	110.20
2	A	274	FAD	C4X-C10-N10	2.97	120.74	116.48
2	A	274	FAD	O4B-C1B-N9A	2.96	113.78	108.09
2	A	274	FAD	N3-C2-N1	-2.96	113.21	119.50
3	A	275	CBD	CL-CC2-NC1	2.87	119.21	115.17
3	B	275	CBD	C6-C5-C4	2.87	123.73	119.26
3	A	275	CBD	C13-C12-C11	2.78	124.83	121.05
3	A	275	CBD	O3D-SD-O1D	-2.77	98.70	111.55
2	B	274	FAD	O5'-C5'-C4'	2.76	116.73	109.36
3	A	275	CBD	NC5-CC6-NC1	-2.74	121.76	126.26
3	B	275	CBD	C2-C3-C4	2.72	123.06	120.62
3	B	275	CBD	O3B-SB-CB1	-2.70	100.87	106.12
2	B	274	FAD	O2-C2-N3	2.69	123.74	118.58
3	B	275	CBD	CB3-CB2-NC	2.65	126.63	121.32
3	B	275	CBD	C3-C2-N2	2.64	126.19	122.59
2	B	274	FAD	N3-C2-N1	-2.63	113.92	119.50
2	A	274	FAD	N9A-C8A-N7A	-2.62	110.21	113.94
3	B	275	CBD	CB2-NC-CC6	-2.60	121.28	129.22
2	A	274	FAD	C4A-N9A-C8A	2.57	108.43	105.74
2	B	274	FAD	N10-C10-N1	2.56	126.04	118.51
3	B	275	CBD	C12-C3-C4	-2.54	116.56	120.00
3	B	275	CBD	O11-C11-C12	-2.54	117.20	121.44
2	B	274	FAD	N9A-C8A-N7A	-2.52	110.36	113.94
2	B	274	FAD	C4A-N9A-C8A	2.50	108.37	105.74
2	B	274	FAD	O4B-C4B-C5B	-2.47	101.44	109.33
3	A	275	CBD	CB3-CB2-CB1	2.46	121.25	117.81
3	B	275	CBD	CD3-CD2-ND	2.45	126.21	121.32
4	B	276	DQN	O4-C4-C5	-2.42	113.96	120.73
3	B	275	CBD	C13-C12-C11	2.37	124.27	121.05
2	B	274	FAD	O4'-C4'-C5'	2.37	115.20	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	274	FAD	C5X-C9A-N10	2.34	120.09	117.97
2	A	274	FAD	O2'-C2'-C1'	2.33	119.79	110.20
2	B	274	FAD	O4'-C4'-C3'	2.32	114.69	109.25
3	A	275	CBD	C9-C10-C11	2.31	122.86	119.26
2	A	274	FAD	C2B-C3B-C4B	2.31	107.07	102.61
2	A	274	FAD	C9A-N10-C10	-2.30	117.24	120.75
3	A	275	CBD	O2A-SA-C1	-2.30	101.20	106.52
2	A	274	FAD	N10-C10-N1	2.30	125.29	118.51
2	B	274	FAD	O2A-PA-O3P	2.29	113.47	107.27
3	A	275	CBD	CB2-NC-CC6	-2.26	122.32	129.22
2	A	274	FAD	C2A-N1A-C6A	2.26	122.45	118.73
2	A	274	FAD	O5'-C5'-C4'	2.22	115.28	109.36
3	A	275	CBD	C2-C3-C4	2.21	122.61	120.62
2	A	274	FAD	C1'-C2'-C3'	2.19	115.61	109.66
2	A	274	FAD	O2P-P-O3P	2.19	113.20	107.27
2	B	274	FAD	C4A-N9A-C1B	-2.17	121.55	126.63
2	B	274	FAD	C9A-N10-C10	-2.15	117.48	120.75
3	A	275	CBD	O3A-SA-O2A	2.12	121.40	111.55
3	B	275	CBD	C9-C10-C5	2.12	121.64	119.26
2	A	274	FAD	C4A-N9A-C1B	-2.11	121.70	126.63
3	A	275	CBD	O3A-SA-C1	-2.10	102.04	106.12
3	A	275	CBD	O3B-SB-CB1	2.09	110.19	106.12
2	A	274	FAD	O3P-PA-O1A	-2.03	104.60	110.70
2	B	274	FAD	C10-C4X-N5	-2.01	120.71	124.81
2	B	274	FAD	C4-C4X-N5	-2.00	115.44	118.21

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	274	FAD	C3'
2	A	274	FAD	C2'
2	A	274	FAD	C4'
2	B	274	FAD	C3'
2	B	274	FAD	C2'
2	B	274	FAD	C4'

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	274	FAD	N10-C1'-C2'-O2'
2	A	274	FAD	C1'-C2'-C3'-O3'
2	A	274	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	A	274	FAD	O3'-C3'-C4'-O4'
2	A	274	FAD	O3'-C3'-C4'-C5'
2	A	274	FAD	C3'-C4'-C5'-O5'
2	A	274	FAD	O4'-C4'-C5'-O5'
2	B	274	FAD	N10-C1'-C2'-O2'
2	B	274	FAD	C1'-C2'-C3'-O3'
2	B	274	FAD	O3'-C3'-C4'-O4'
2	B	274	FAD	O3'-C3'-C4'-C5'
2	B	274	FAD	O4'-C4'-C5'-O5'
3	A	275	CBD	C14-C1-SA-O1A
3	A	275	CBD	C14-C1-SA-O2A
3	A	275	CBD	C14-C1-SA-O3A
3	A	275	CBD	CB2-CB1-SB-O3B
3	A	275	CBD	CB6-CB1-SB-O3B
3	B	275	CBD	C14-C1-SA-O1A
2	B	274	FAD	O2'-C2'-C3'-O3'
2	A	274	FAD	O4B-C4B-C5B-O5B
2	B	274	FAD	O4B-C4B-C5B-O5B
2	B	274	FAD	C3'-C4'-C5'-O5'
2	A	274	FAD	C3B-C4B-C5B-O5B
3	B	275	CBD	C14-C1-SA-O2A
3	B	275	CBD	C14-C1-SA-O3A
2	A	274	FAD	C5B-O5B-PA-O1A
2	B	274	FAD	C2'-C1'-N10-C10
2	B	274	FAD	O2'-C2'-C3'-C4'
2	A	274	FAD	PA-O3P-P-O2P
3	A	275	CBD	CB4-CB5-NB-C13
2	B	274	FAD	C2'-C3'-C4'-O4'
3	A	275	CBD	CB6-CB5-NB-C13
2	A	274	FAD	PA-O3P-P-O1P
2	A	274	FAD	N10-C1'-C2'-C3'

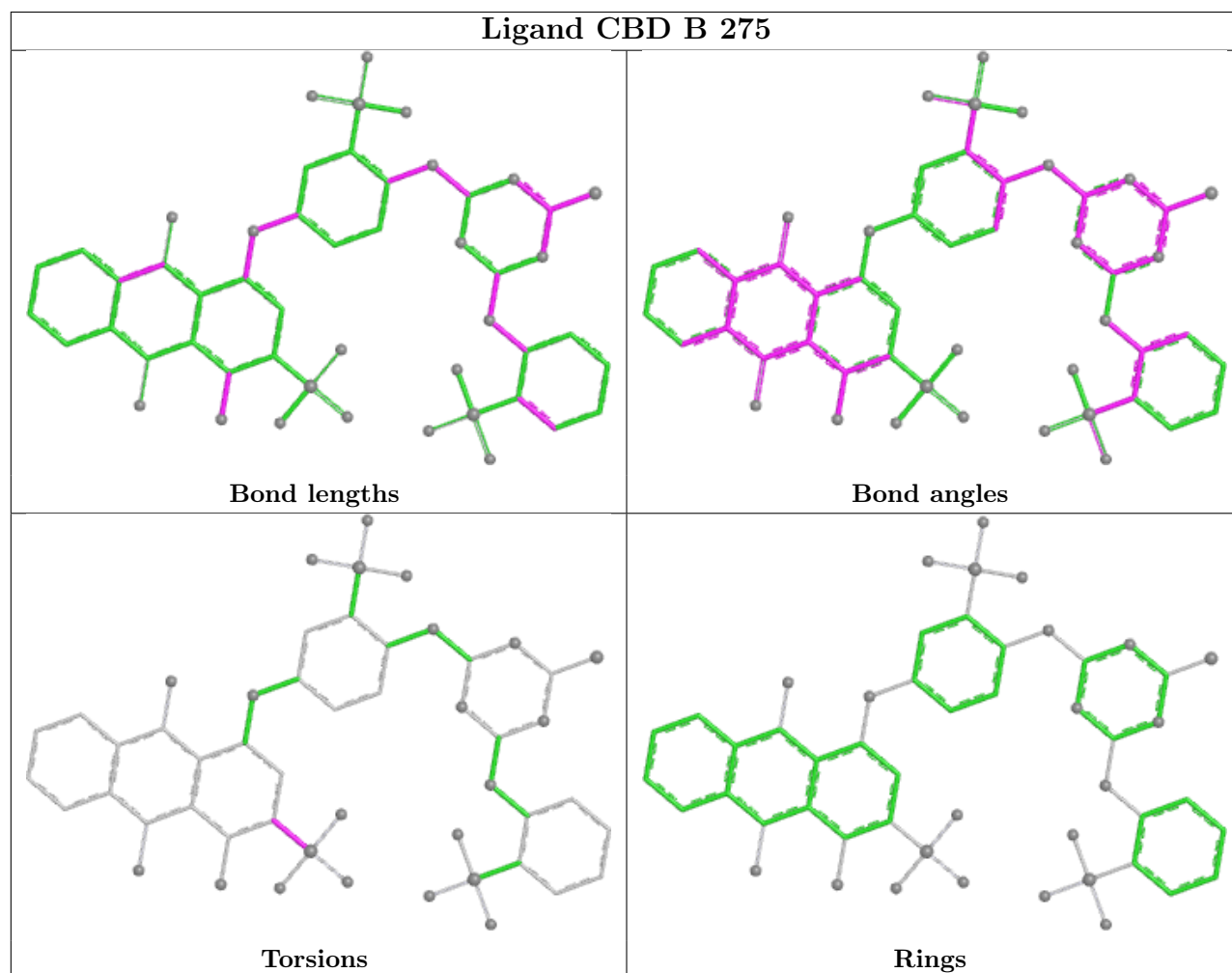
There are no ring outliers.

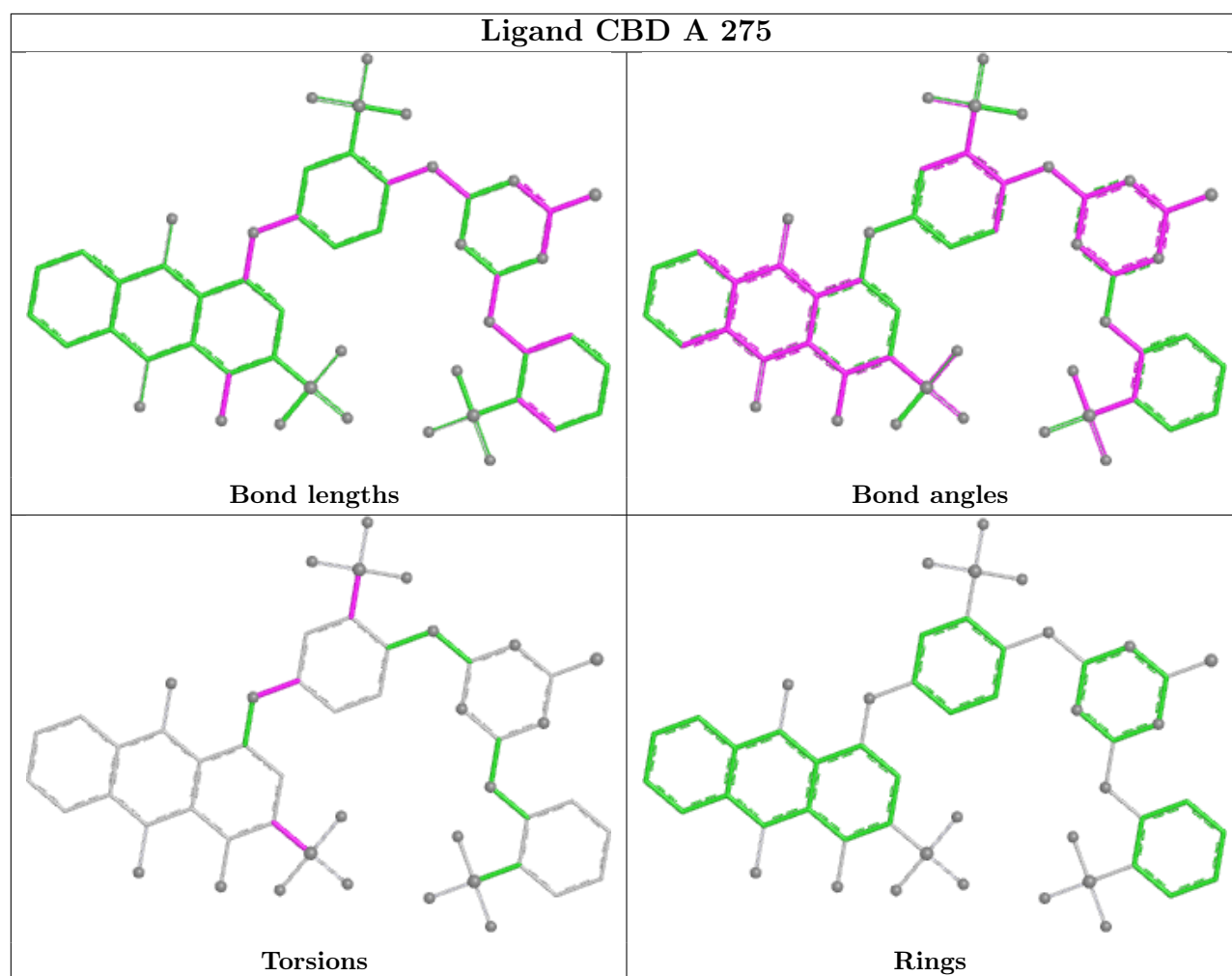
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	275	CBD	3	0
3	A	275	CBD	3	0
4	A	276	DQN	4	0
4	B	276	DQN	4	0

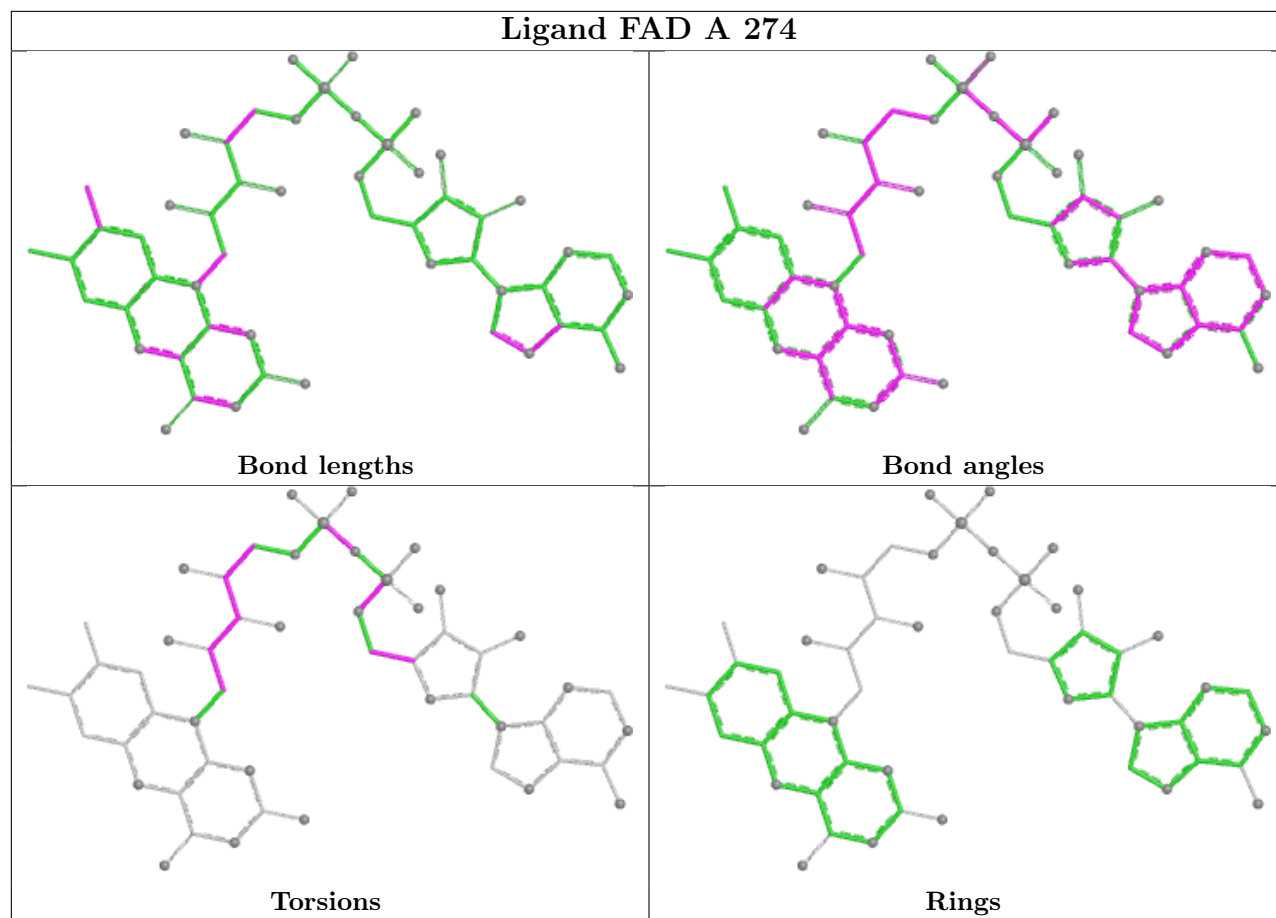
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

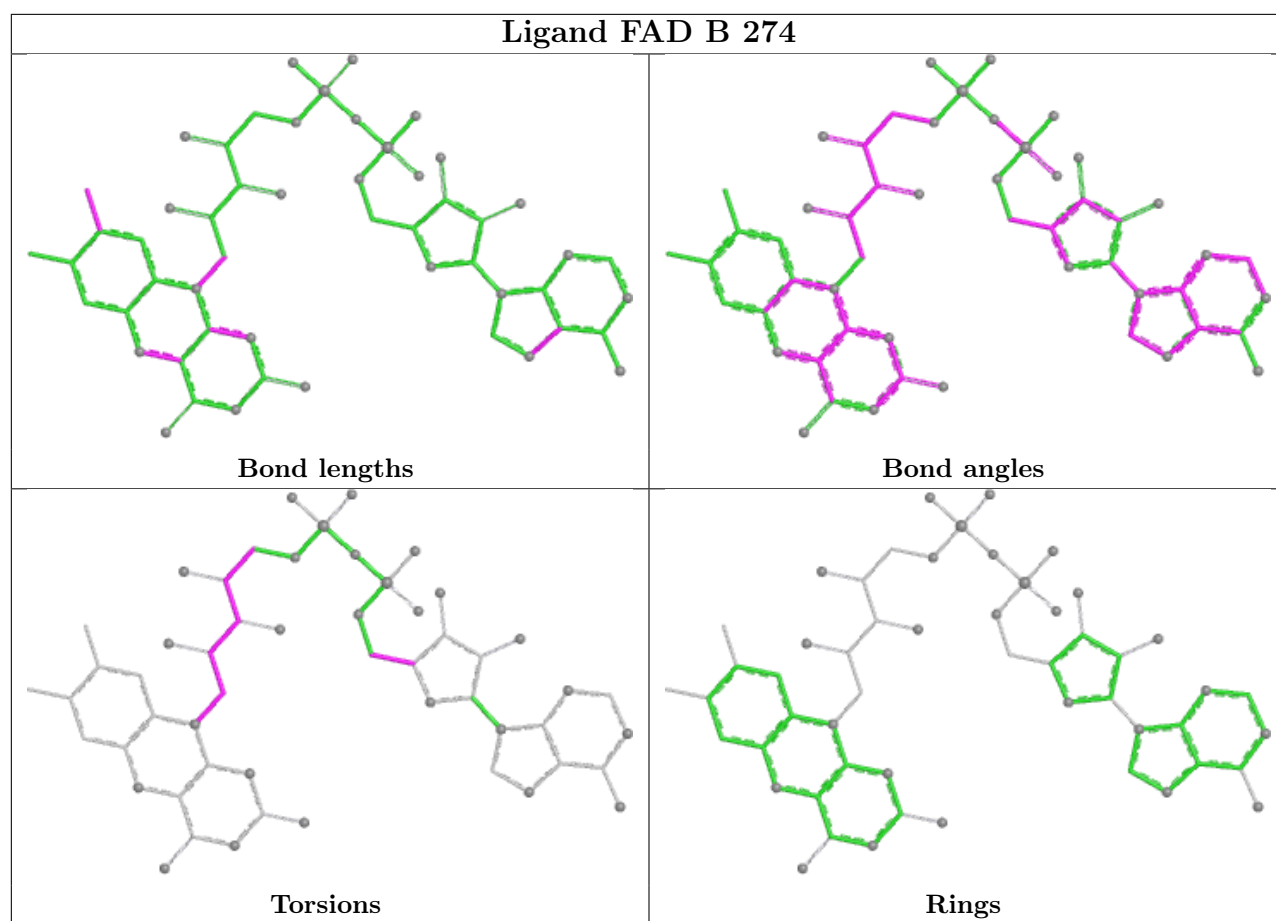
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.





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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.