



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:55 PM UTC

PDB ID : 1D4D / pdb_00001d4d
Title : CRYSTAL STRUCTURE OF THE SUCCINATE COMPLEXED FORM OF THE FLAVOCYTOCHROME C FUMARATE REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1
Authors : Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.
Deposited on : 1999-10-03
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

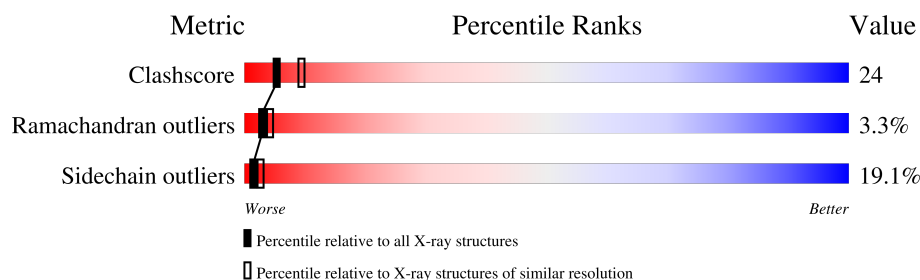
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	572	47% 34% 14% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FAD	A	600	X	-	-	-
4	SIN	A	700	-	X	X	-

2 Entry composition [i](#)

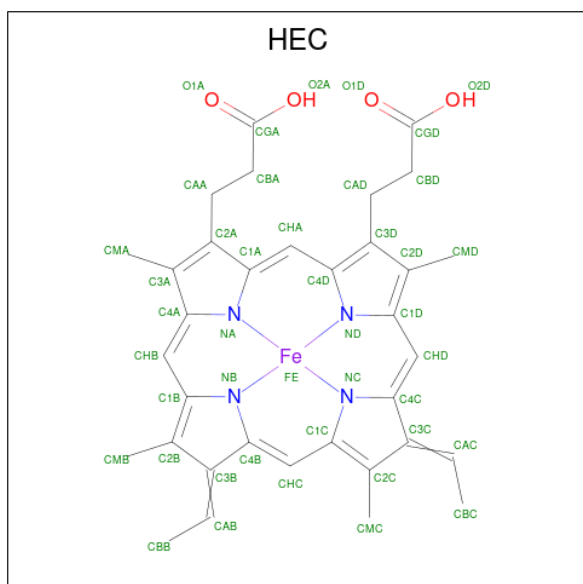
There are 5 unique types of molecules in this entry. The entry contains 4254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVOCYTOCHROME C FUMARATE REDUCTASE.

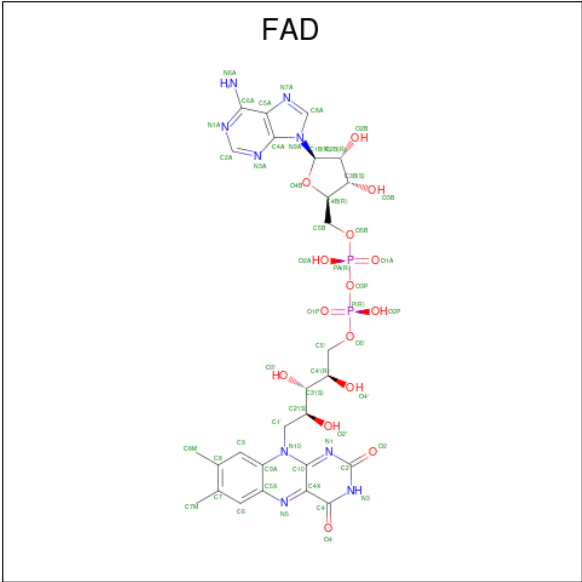
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			3965	2462	710	774	19			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



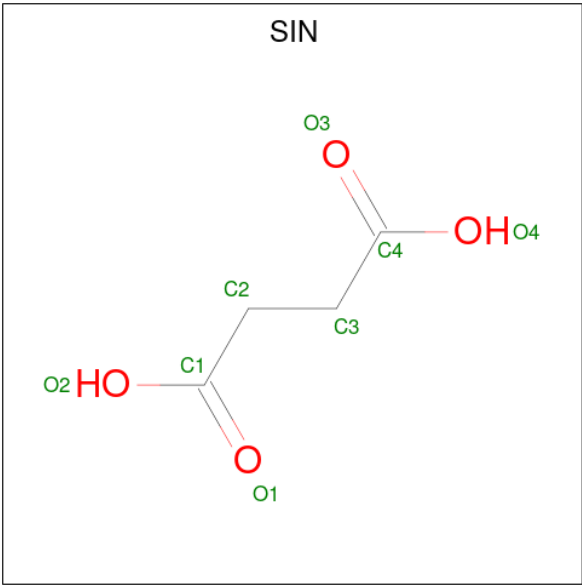
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is water.

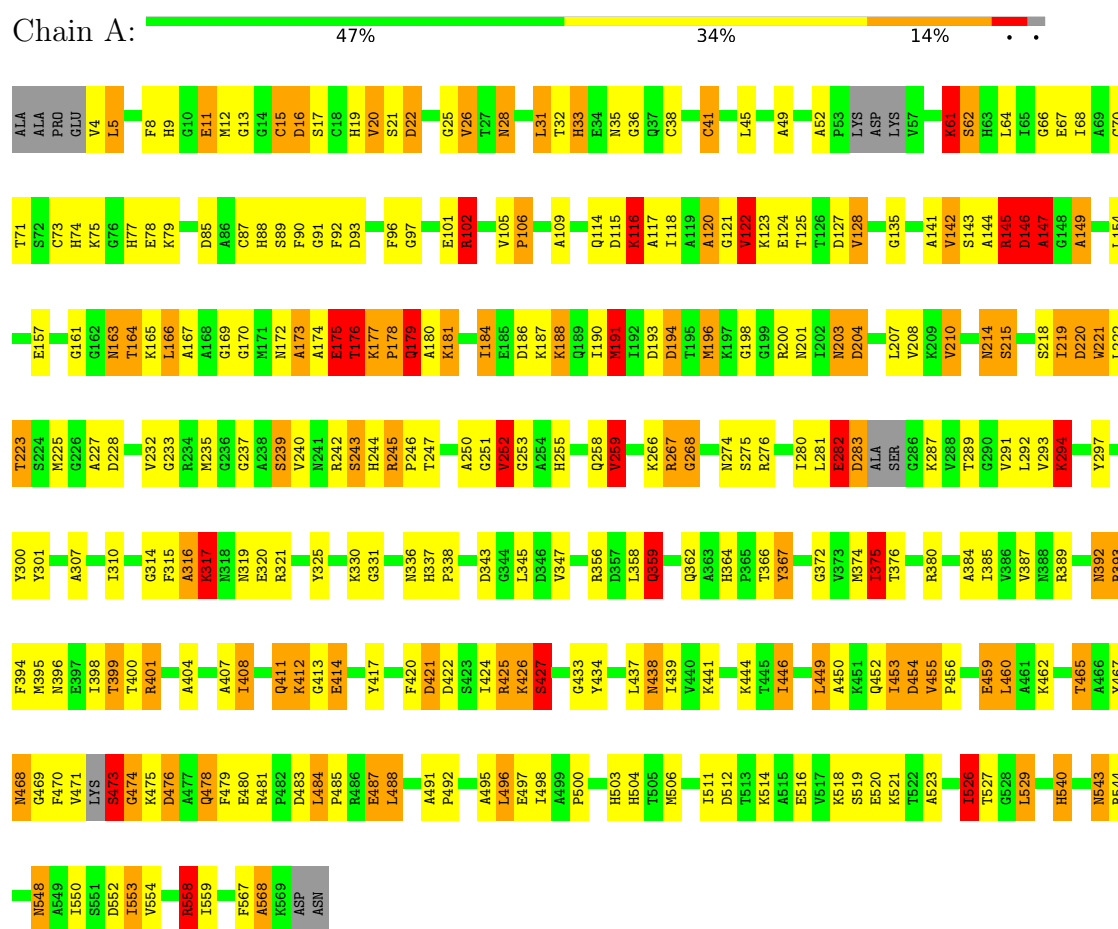
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		

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: FLAVOCYTOCHROME C FUMARATE REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.86Å 72.86Å 216.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.50 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.50-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4254	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, SIN, 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	0.74	0/4029	2.21	197/5478 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	ASN	CA-CB-CG	17.89	130.49	112.60
1	A	491	ALA	CA-C-O	-15.24	104.11	120.87
1	A	169	GLY	N-CA-C	12.54	128.47	114.67
1	A	468	ASN	CA-CB-CG	-12.29	100.31	112.60
1	A	19	HIS	CA-CB-CG	-11.09	102.71	113.80
1	A	175	GLU	CA-C-N	11.08	142.70	121.54
1	A	175	GLU	C-N-CA	11.08	142.70	121.54
1	A	144	ALA	CA-C-O	10.89	131.92	120.70
1	A	122	VAL	N-CA-CB	10.53	128.61	111.23
1	A	174	ALA	CA-C-O	10.52	132.00	120.32
1	A	491	ALA	O-C-N	10.45	132.68	121.60
1	A	281	LEU	CA-C-O	10.28	131.94	120.43
1	A	178	PRO	CA-C-N	10.05	140.75	121.54
1	A	178	PRO	C-N-CA	10.05	140.75	121.54
1	A	426	LYS	CA-C-O	-9.75	109.81	120.92
1	A	316	ALA	CA-C-O	-9.51	110.72	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	CYS	CA-C-N	9.51	133.40	120.38
1	A	15	CYS	C-N-CA	9.51	133.40	120.38
1	A	15	CYS	CA-C-O	9.39	130.02	119.41
1	A	149	ALA	N-CA-C	9.30	124.28	109.86
1	A	454	ASP	CA-CB-CG	9.24	121.84	112.60
1	A	487	GLU	N-CA-C	9.10	122.38	111.82
1	A	22	ASP	CA-CB-CG	8.93	121.53	112.60
1	A	77	HIS	CA-CB-CG	-8.86	104.94	113.80
1	A	179	GLN	CB-CG-CD	8.71	127.40	112.60
1	A	251	GLY	CA-C-N	8.66	134.50	120.30
1	A	251	GLY	C-N-CA	8.66	134.50	120.30
1	A	385	ILE	CA-C-O	-8.55	111.91	121.92
1	A	147	ALA	CA-C-O	8.55	132.73	120.51
1	A	92	PHE	CA-C-O	-8.46	111.83	121.81
1	A	558	ARG	CD-NE-CZ	8.35	136.09	124.40
1	A	233	GLY	CA-C-O	8.31	129.03	121.47
1	A	421	ASP	N-CA-CB	-8.19	98.15	110.60
1	A	422	ASP	CA-C-O	8.15	129.41	119.31
1	A	527	THR	CA-C-O	8.10	130.23	121.16
1	A	281	LEU	CA-C-N	7.92	134.01	121.66
1	A	281	LEU	C-N-CA	7.92	134.01	121.66
1	A	259	VAL	N-CA-CB	7.91	121.29	110.54
1	A	362	GLN	OE1-CD-NE2	-7.85	114.75	122.60
1	A	184	ILE	N-CA-CB	7.85	121.22	111.41
1	A	356	ARG	NE-CZ-NH1	-7.70	113.80	121.50
1	A	252	VAL	CB-CA-C	-7.68	99.82	112.26
1	A	282	GLU	CB-CG-CD	7.62	125.56	112.60
1	A	142	VAL	N-CA-CB	7.50	118.49	110.62
1	A	11	GLU	CB-CG-CD	7.46	125.29	112.60
1	A	161	GLY	N-CA-C	7.42	125.23	115.36
1	A	310	ILE	N-CA-CB	7.36	119.81	111.21
1	A	421	ASP	N-CA-C	7.27	120.42	109.95
1	A	552	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	455	VAL	N-CA-CB	7.17	121.25	111.21
1	A	452	GLN	CA-C-O	7.17	128.02	120.42
1	A	492	PRO	N-CA-CB	7.16	110.47	102.60
1	A	317	LYS	N-CA-CB	7.15	122.57	110.49
1	A	267	ARG	CA-C-O	-6.99	110.51	120.51
1	A	237	GLY	N-CA-C	6.94	124.59	115.36
1	A	11	GLU	CA-CB-CG	6.90	127.89	114.10
1	A	200	ARG	NE-CZ-NH2	6.83	125.35	119.20
1	A	503	HIS	N-CA-C	6.83	121.46	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	A	178	PRO	CB-CA-C	-6.81	100.33	111.56
1	A	459	GLU	CB-CG-CD	6.78	124.13	112.60
1	A	251	GLY	O-C-N	-6.77	117.58	123.80
1	A	177	LYS	CA-C-N	6.76	128.28	119.84
1	A	177	LYS	C-N-CA	6.76	128.28	119.84
1	A	13	GLY	N-CA-C	6.74	127.14	115.62
1	A	203	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	214	ASN	CB-CG-ND2	6.72	126.49	116.40
1	A	201	ASN	CA-CB-CG	-6.63	105.97	112.60
1	A	526	ILE	N-CA-C	-6.62	100.20	109.21
1	A	543	ASN	CA-CB-CG	-6.58	106.02	112.60
1	A	149	ALA	CA-C-O	6.58	129.73	121.50
1	A	105	VAL	CA-C-O	6.52	123.56	119.51
1	A	247	THR	N-CA-C	6.44	119.96	110.30
1	A	375	ILE	N-CA-CB	6.43	120.01	111.64
1	A	16	ASP	N-CA-CB	-6.40	100.46	110.06
1	A	452	GLN	CA-C-N	6.40	131.29	120.29
1	A	452	GLN	C-N-CA	6.40	131.29	120.29
1	A	223	THR	O-C-N	-6.39	115.34	122.12
1	A	474	GLY	N-CA-C	6.36	128.25	113.18
1	A	422	ASP	CA-CB-CG	-6.32	106.28	112.60
1	A	425	ARG	CD-NE-CZ	6.32	133.25	124.40
1	A	540	HIS	CA-CB-CG	-6.28	107.52	113.80
1	A	519	SER	CA-C-O	-6.27	114.72	121.56
1	A	274	ASN	OD1-CG-ND2	6.25	128.85	122.60
1	A	222	LEU	CB-CA-C	6.23	120.77	110.81
1	A	85	ASP	CA-C-O	-6.22	110.96	119.05
1	A	220	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	220	ASP	N-CA-C	-6.15	103.90	112.45
1	A	268	GLY	CA-C-O	-6.15	109.87	120.57
1	A	425	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	A	208	VAL	CA-C-N	6.11	128.93	120.63
1	A	208	VAL	C-N-CA	6.11	128.93	120.63
1	A	121	GLY	CA-C-N	6.08	132.91	121.97
1	A	121	GLY	C-N-CA	6.08	132.91	121.97
1	A	294	LYS	CA-C-O	-6.08	114.77	121.58
1	A	106	PRO	CA-C-N	6.07	130.72	120.64
1	A	106	PRO	C-N-CA	6.07	130.72	120.64
1	A	87	CYS	N-CA-C	6.05	121.32	113.88
1	A	31	LEU	N-CA-CB	-6.01	103.05	112.13
1	A	128	VAL	N-CA-C	6.01	116.52	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	CYS	CA-C-N	6.01	128.95	120.42
1	A	38	CYS	C-N-CA	6.01	128.95	120.42
1	A	64	LEU	CA-C-O	-6.00	114.55	121.15
1	A	203	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	67	GLU	CA-C-N	-5.99	114.71	123.10
1	A	67	GLU	C-N-CA	-5.99	114.71	123.10
1	A	527	THR	N-CA-C	5.97	119.12	110.28
1	A	462	LYS	CA-CB-CG	5.97	126.03	114.10
1	A	227	ALA	N-CA-C	5.95	118.59	110.55
1	A	32	THR	N-CA-C	5.93	117.74	111.28
1	A	11	GLU	N-CA-C	-5.92	104.16	111.33
1	A	92	PHE	N-CA-C	-5.90	102.59	110.55
1	A	293	VAL	CB-CA-C	-5.88	103.85	110.96
1	A	421	ASP	CA-C-O	-5.87	113.81	121.73
1	A	491	ALA	N-CA-C	5.85	118.63	110.20
1	A	242	ARG	N-CA-C	5.84	121.38	113.21
1	A	247	THR	CA-C-O	5.83	127.09	120.80
1	A	374	MET	CA-C-O	-5.75	115.29	121.56
1	A	117	ALA	N-CA-C	5.74	119.55	112.54
1	A	147	ALA	N-CA-C	-5.71	98.63	110.80
1	A	359	GLN	CA-C-O	-5.71	113.41	119.97
1	A	553	ILE	CA-C-O	-5.70	115.03	120.95
1	A	456	PRO	CA-C-O	5.68	127.51	121.03
1	A	484	LEU	CA-C-N	5.68	125.04	118.85
1	A	484	LEU	C-N-CA	5.68	125.04	118.85
1	A	88	HIS	CA-CB-CG	5.62	119.42	113.80
1	A	559	ILE	N-CA-CB	5.62	117.12	110.55
1	A	172	ASN	O-C-N	5.62	129.78	122.87
1	A	411	GLN	CA-C-O	5.61	128.03	121.46
1	A	116	LYS	N-CA-C	-5.60	104.19	111.02
1	A	143	SER	N-CA-C	5.59	117.37	111.28
1	A	163	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	251	GLY	CA-C-O	5.58	126.00	120.75
1	A	61	LYS	CA-CB-CG	5.58	125.25	114.10
1	A	548	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	36	GLY	N-CA-C	-5.57	106.04	112.73
1	A	210	VAL	O-C-N	-5.57	116.47	121.87
1	A	175	GLU	CA-C-O	5.55	128.45	120.51
1	A	5	LEU	CA-C-O	-5.54	112.59	120.51
1	A	173	ALA	O-C-N	5.54	129.59	123.33
1	A	181	LYS	CA-C-O	-5.54	112.59	120.51
1	A	492	PRO	N-CD-CG	5.53	110.44	103.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	SER	CB-CA-C	-5.52	100.53	111.91
1	A	122	VAL	CA-C-O	5.50	127.66	120.78
1	A	232	VAL	N-CA-C	5.50	116.51	108.53
1	A	376	THR	O-C-N	-5.50	115.79	122.82
1	A	526	ILE	CB-CA-C	5.50	119.14	111.34
1	A	444	LYS	CA-C-O	5.49	126.28	119.97
1	A	201	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	A	144	ALA	CA-C-N	5.47	127.55	120.44
1	A	144	ALA	C-N-CA	5.47	127.55	120.44
1	A	106	PRO	CA-C-O	5.47	127.54	121.36
1	A	204	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	408	ILE	CA-C-O	5.43	126.61	120.85
1	A	314	GLY	N-CA-C	5.42	120.54	112.41
1	A	62	SER	N-CA-C	5.42	115.69	108.38
1	A	93	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	427	SER	N-CA-CB	5.38	119.59	110.49
1	A	164	THR	CA-C-O	5.38	127.31	121.02
1	A	36	GLY	CA-C-O	-5.37	115.22	120.75
1	A	487	GLU	CA-C-O	-5.35	113.82	119.97
1	A	135	GLY	CA-C-O	-5.34	115.25	120.75
1	A	421	ASP	CB-CA-C	-5.31	101.34	111.48
1	A	245	ARG	CA-CB-CG	5.30	124.70	114.10
1	A	251	GLY	N-CA-C	5.26	118.76	110.71
1	A	483	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	492	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	102	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	367	TYR	CA-C-O	-5.22	115.27	121.16
1	A	193	ASP	CA-C-O	-5.20	114.22	120.10
1	A	325	TYR	CB-CA-C	-5.20	100.34	109.07
1	A	145	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	485	PRO	CB-CA-C	-5.17	104.79	112.55
1	A	117	ALA	CA-C-O	-5.17	113.02	119.38
1	A	221	TRP	CB-CA-C	-5.15	102.58	110.81
1	A	146	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	376	THR	CA-C-N	5.14	129.31	120.72
1	A	376	THR	C-N-CA	5.14	129.31	120.72
1	A	201	ASN	CA-C-O	-5.14	114.28	119.78
1	A	376	THR	N-CA-C	5.11	116.88	110.24
1	A	399	THR	N-CA-CB	5.10	117.19	110.25
1	A	120	ALA	N-CA-C	5.10	121.66	110.80
1	A	476	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	473	SER	CA-C-N	5.09	131.38	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	SER	C-N-CA	5.09	131.38	121.41
1	A	32	THR	CA-C-N	5.07	127.34	120.65
1	A	32	THR	C-N-CA	5.07	127.34	120.65
1	A	145	ARG	NH1-CZ-NH2	5.07	125.88	119.30
1	A	191	MET	N-CA-C	-5.06	100.74	110.56
1	A	559	ILE	CA-C-O	-5.06	115.81	121.17
1	A	52	ALA	N-CA-C	5.04	117.60	110.24
1	A	568	ALA	CA-C-O	-5.04	113.30	120.51
1	A	526	ILE	N-CA-CB	5.04	117.17	110.26
1	A	220	ASP	N-CA-CB	5.03	117.75	110.26
1	A	41	CYS	CA-C-N	-5.02	114.34	122.23
1	A	41	CYS	C-N-CA	-5.02	114.34	122.23
1	A	33	HIS	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	VAL	Mainchain

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	3965	0	3740	187	0
2	A	172	0	123	17	0
3	A	53	0	31	8	0
4	A	8	0	4	7	0
5	A	56	0	0	1	0
All	All	4254	0	3898	194	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 24.

All (194) 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:15:CYS:SG	2:A:603:HEC:HAB	1.29	1.71
3:A:600:FAD:C1'	3:A:600:FAD:C2'	1.79	1.53
1:A:73:CYS:SG	2:A:602:HEC:HAC	1.50	1.51
1:A:41:CYS:SG	2:A:604:HEC:HAC	1.51	1.50
1:A:15:CYS:SG	2:A:603:HEC:CAB	2.10	1.40
1:A:395:MET:HE2	1:A:407:ALA:HB3	1.41	1.03
1:A:359:GLN:HE21	1:A:359:GLN:H	1.11	0.99
1:A:41:CYS:HG	2:A:604:HEC:HAC	1.32	0.87
1:A:154:LEU:HD23	1:A:275:SER:HB3	1.63	0.80
1:A:426:LYS:O	1:A:427:SER:HB3	1.81	0.79
1:A:558:ARG:HH11	1:A:558:ARG:HG2	1.47	0.79
1:A:446:ILE:HG23	1:A:460:LEU:HD13	1.65	0.77
1:A:453:ILE:HG23	1:A:455:VAL:HG13	1.68	0.76
1:A:412:LYS:HD2	1:A:412:LYS:H	1.53	0.73
1:A:401:ARG:HH12	4:A:700:SIN:H22	1.52	0.72
1:A:449:LEU:HD11	1:A:495:ALA:HB2	1.71	0.72
1:A:567:PHE:O	1:A:568:ALA:HB3	1.89	0.70
1:A:393:ARG:HD3	1:A:478:GLN:HE22	1.57	0.69
1:A:165:LYS:HG3	1:A:166:LEU:HD23	1.76	0.67
1:A:359:GLN:HE21	1:A:359:GLN:N	1.87	0.67
3:A:600:FAD:C1'	3:A:600:FAD:C3'	2.72	0.67
1:A:145:ARG:HD2	1:A:268:GLY:H	1.59	0.66
1:A:141:ALA:O	1:A:145:ARG:HB2	1.95	0.66
1:A:228:ASP:N	1:A:255:HIS:NE2	2.43	0.66
1:A:41:CYS:SG	2:A:604:HEC:C3C	2.84	0.66
1:A:245:ARG:HB2	1:A:246:PRO:HD2	1.78	0.65
1:A:392:ASN:HD22	1:A:393:ARG:H	1.44	0.65
1:A:190:ILE:O	1:A:194:ASP:OD1	2.15	0.65
1:A:394:PHE:HE1	1:A:395:MET:HE3	1.60	0.64
1:A:114:GLN:O	1:A:118:ILE:HG13	1.97	0.64
1:A:394:PHE:CE1	1:A:395:MET:HE3	2.33	0.63
1:A:467:TYR:O	1:A:471:VAL:HG23	1.99	0.63
1:A:142:VAL:HG11	1:A:225:MET:CE	2.29	0.63
1:A:359:GLN:H	1:A:359:GLN:NE2	1.90	0.63
1:A:170:GLY:HA2	1:A:252:VAL:HG21	1.80	0.62
1:A:245:ARG:HB2	1:A:246:PRO:CD	2.29	0.62
1:A:345:LEU:HD11	1:A:358:LEU:HD21	1.82	0.62
1:A:49:ALA:HB1	1:A:61:LYS:HD3	1.81	0.61
3:A:600:FAD:C1'	3:A:600:FAD:O2'	2.48	0.61
1:A:196:MET:HA	1:A:196:MET:HE3	1.82	0.61
1:A:319:ASN:ND2	1:A:331:GLY:H	1.97	0.61
1:A:343:ASP:HB2	5:A:704:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LYS:O	1:A:427:SER:CB	2.46	0.60
1:A:319:ASN:HD21	1:A:330:LYS:HA	1.65	0.60
3:A:600:FAD:C2'	3:A:600:FAD:N10	2.60	0.60
1:A:102:ARG:NH2	1:A:157:GLU:OE1	2.35	0.60
1:A:146:ASP:O	1:A:147:ALA:HB3	2.02	0.60
1:A:316:ALA:O	1:A:317:LYS:CB	2.47	0.59
1:A:73:CYS:SG	2:A:602:HEC:C3C	2.91	0.59
1:A:395:MET:HE1	1:A:404:ALA:O	2.03	0.58
1:A:506:MET:HG3	1:A:540:HIS:HB2	1.86	0.58
1:A:142:VAL:O	1:A:146:ASP:HB2	2.04	0.58
1:A:433:GLY:CA	2:A:601:HEC:HBA2	2.33	0.58
1:A:35:ASN:HD21	1:A:71:THR:H	1.49	0.58
1:A:300:TYR:O	1:A:301:TYR:HB3	2.03	0.57
1:A:8:PHE:O	1:A:11:GLU:HG2	2.05	0.57
1:A:128:VAL:HG22	1:A:307:ALA:HB3	1.86	0.57
1:A:433:GLY:HA3	2:A:601:HEC:HBA2	1.85	0.57
1:A:175:GLU:OE2	1:A:187:LYS:HA	2.05	0.57
1:A:170:GLY:HA3	1:A:243:SER:OG	2.05	0.57
1:A:170:GLY:HA2	1:A:244:HIS:O	2.05	0.57
1:A:364:HIS:O	1:A:500:PRO:HA	2.05	0.56
1:A:319:ASN:HD21	1:A:331:GLY:H	1.52	0.56
1:A:28:ASN:H	1:A:28:ASN:HD22	1.53	0.55
1:A:235:MET:HE2	4:A:700:SIN:H21	1.89	0.55
1:A:401:ARG:HH22	4:A:700:SIN:C1	2.19	0.55
1:A:343:ASP:HB3	3:A:600:FAD:H61A	1.71	0.55
1:A:468:ASN:ND2	1:A:487:GLU:HG2	2.22	0.55
1:A:294:LYS:HG2	1:A:300:TYR:CE2	2.41	0.55
1:A:218:SER:HB2	1:A:554:VAL:HG12	1.90	0.54
1:A:142:VAL:HG11	1:A:225:MET:HE1	1.89	0.54
1:A:246:PRO:HG2	1:A:250:ALA:HB3	1.90	0.54
1:A:45:LEU:HG	2:A:602:HEC:HBB2	1.89	0.54
1:A:550:ILE:HA	1:A:553:ILE:HG12	1.90	0.54
1:A:393:ARG:HH11	1:A:478:GLN:NE2	2.06	0.54
1:A:467:TYR:CZ	1:A:484:LEU:HD23	2.43	0.54
1:A:487:GLU:O	1:A:488:LEU:HB2	2.07	0.54
1:A:389:ARG:HD2	1:A:412:LYS:O	2.09	0.53
1:A:337:HIS:HB2	1:A:338:PRO:HD2	1.89	0.53
1:A:15:CYS:SG	2:A:603:HEC:C3B	2.94	0.52
1:A:66:GLY:H	1:A:258:GLN:HE22	1.56	0.52
1:A:417:TYR:CE2	1:A:497:GLU:HB2	2.44	0.52
1:A:62:SER:HB3	2:A:601:HEC:HBB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:OG1	1:A:400:THR:N	2.43	0.52
1:A:421:ASP:HB2	1:A:424:ILE:HG12	1.92	0.52
1:A:173:ALA:HB3	1:A:244:HIS:CE1	2.44	0.52
1:A:395:MET:CE	1:A:407:ALA:HB3	2.28	0.52
1:A:221:TRP:CH2	1:A:558:ARG:HG3	2.45	0.51
1:A:380:ARG:HA	1:A:384:ALA:HB3	1.93	0.51
1:A:177:LYS:O	1:A:179:GLN:N	2.44	0.51
1:A:550:ILE:HG12	3:A:600:FAD:C2	2.40	0.51
1:A:35:ASN:ND2	1:A:70:CYS:H	2.09	0.51
1:A:421:ASP:CB	1:A:424:ILE:HG12	2.41	0.50
1:A:20:VAL:HG23	1:A:33:HIS:CD2	2.47	0.50
1:A:127:ASP:CB	1:A:149:ALA:HB1	2.42	0.50
1:A:280:ILE:HD12	1:A:347:VAL:HG12	1.93	0.49
1:A:163:ASN:HD21	1:A:336:ASN:ND2	2.10	0.49
1:A:142:VAL:HG11	1:A:225:MET:HE2	1.94	0.49
1:A:469:GLY:O	1:A:470:PHE:C	2.55	0.49
1:A:512:ASP:OD1	1:A:514:LYS:HB2	2.13	0.49
1:A:395:MET:HE2	1:A:407:ALA:CB	2.28	0.49
1:A:392:ASN:ND2	1:A:393:ARG:H	2.10	0.48
1:A:163:ASN:O	1:A:164:THR:C	2.56	0.48
1:A:25:GLY:H	2:A:603:HEC:CHB	2.26	0.48
1:A:167:ALA:HB3	1:A:253:GLY:CA	2.44	0.48
1:A:471:VAL:HG11	1:A:487:GLU:HG3	1.94	0.48
1:A:214:ASN:O	1:A:215:SER:C	2.56	0.48
1:A:469:GLY:O	1:A:473:SER:HB2	2.13	0.48
1:A:245:ARG:CB	1:A:246:PRO:CD	2.91	0.47
1:A:453:ILE:HG22	1:A:455:VAL:H	1.79	0.47
1:A:8:PHE:HE2	2:A:604:HEC:HHA	1.78	0.47
1:A:115:ASP:O	1:A:116:LYS:C	2.57	0.47
1:A:173:ALA:HB2	1:A:219:ILE:HD12	1.96	0.47
1:A:283:ASP:HB3	1:A:287:LYS:O	2.13	0.47
1:A:26:VAL:HG21	1:A:297:TYR:HB2	1.96	0.47
1:A:170:GLY:CA	1:A:252:VAL:HG21	2.44	0.47
1:A:219:ILE:HD13	1:A:244:HIS:CD2	2.50	0.47
1:A:407:ALA:O	1:A:411:GLN:HG2	2.15	0.47
1:A:434:TYR:HB3	1:A:439:ILE:HD11	1.97	0.47
1:A:5:LEU:HG	1:A:96:PHE:CD1	2.50	0.46
1:A:420:PHE:HE1	1:A:496:LEU:HD11	1.79	0.46
1:A:567:PHE:O	1:A:568:ALA:CB	2.53	0.46
1:A:395:MET:HE3	1:A:408:ILE:HG13	1.97	0.46
1:A:413:GLY:O	1:A:414:GLU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PHE:HB3	1:A:476:ASP:HA	1.97	0.46
1:A:450:ALA:HB1	1:A:455:VAL:O	2.15	0.46
1:A:375:ILE:HD12	1:A:434:TYR:CE2	2.51	0.46
1:A:235:MET:CE	4:A:700:SIN:H21	2.46	0.46
1:A:526:ILE:HG13	1:A:529:LEU:HB2	1.97	0.46
1:A:514:LYS:HD3	1:A:516:GLU:OE2	2.17	0.45
1:A:167:ALA:HB3	1:A:253:GLY:HA3	1.96	0.45
3:A:600:FAD:C1'	3:A:600:FAD:O3'	2.64	0.45
1:A:316:ALA:O	1:A:317:LYS:HB3	2.17	0.45
1:A:367:TYR:OH	1:A:372:GLY:HA2	2.17	0.45
1:A:453:ILE:CG2	1:A:455:VAL:HG13	2.41	0.45
1:A:179:GLN:O	1:A:180:ALA:C	2.59	0.45
1:A:465:THR:O	1:A:468:ASN:HB2	2.17	0.45
1:A:394:PHE:HA	1:A:479:PHE:CZ	2.52	0.45
1:A:453:ILE:HD11	1:A:495:ALA:HB1	1.99	0.44
1:A:511:ILE:HA	1:A:516:GLU:O	2.16	0.44
1:A:66:GLY:H	1:A:258:GLN:NE2	2.16	0.44
1:A:319:ASN:HD21	1:A:331:GLY:N	2.15	0.44
1:A:219:ILE:HD13	1:A:244:HIS:CG	2.53	0.44
1:A:221:TRP:CZ2	1:A:558:ARG:HG3	2.53	0.44
1:A:127:ASP:HB2	1:A:149:ALA:HB1	1.99	0.44
1:A:146:ASP:CG	1:A:267:ARG:HH11	2.26	0.44
1:A:255:HIS:O	1:A:259:VAL:HG13	2.17	0.44
1:A:420:PHE:HE1	1:A:496:LEU:CD1	2.30	0.44
1:A:145:ARG:HH11	1:A:268:GLY:H	1.65	0.44
1:A:437:LEU:O	1:A:438:ASN:HB2	2.16	0.44
1:A:20:VAL:HG23	1:A:33:HIS:CG	2.53	0.44
1:A:504:HIS:CD2	1:A:544:ARG:HE	2.36	0.44
1:A:5:LEU:HD22	1:A:9:HIS:CE1	2.52	0.43
1:A:188:LYS:O	1:A:191:MET:HB3	2.18	0.43
1:A:20:VAL:HG23	1:A:33:HIS:CE1	2.52	0.43
1:A:315:PHE:O	1:A:316:ALA:C	2.60	0.43
1:A:283:ASP:CB	1:A:289:THR:HG23	2.48	0.43
1:A:4:VAL:O	1:A:5:LEU:C	2.61	0.43
1:A:146:ASP:O	1:A:147:ALA:CB	2.63	0.43
1:A:433:GLY:HA2	2:A:601:HEC:HBA2	1.99	0.43
1:A:204:ASP:HB3	1:A:207:LEU:HD12	2.01	0.42
1:A:401:ARG:HH22	4:A:700:SIN:H22	1.83	0.42
1:A:437:LEU:O	1:A:438:ASN:CB	2.66	0.42
2:A:604:HEC:HHA	2:A:604:HEC:HAA1	1.96	0.42
1:A:106:PRO:HG2	1:A:109:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ARG:NH1	4:A:700:SIN:H22	2.26	0.42
1:A:453:ILE:HG21	1:A:455:VAL:HG22	1.99	0.42
1:A:220:ASP:O	1:A:223:THR:HB	2.19	0.42
1:A:74:HIS:HB3	2:A:604:HEC:HMB2	2.01	0.42
1:A:245:ARG:CB	1:A:246:PRO:HD2	2.48	0.42
1:A:198:GLY:O	1:A:543:ASN:HB3	2.19	0.42
1:A:480:GLU:O	1:A:481:ARG:C	2.62	0.42
1:A:487:GLU:O	1:A:488:LEU:CB	2.68	0.42
1:A:412:LYS:H	1:A:412:LYS:CD	2.27	0.42
1:A:421:ASP:HB3	1:A:424:ILE:H	1.83	0.42
1:A:276:ARG:NH2	1:A:343:ASP:OD1	2.52	0.42
1:A:366:THR:HA	1:A:498:ILE:HB	2.00	0.42
1:A:393:ARG:HD3	1:A:478:GLN:NE2	2.30	0.42
1:A:175:GLU:HB3	1:A:176:THR:H	1.48	0.41
1:A:558:ARG:HG2	1:A:558:ARG:NH1	2.22	0.41
1:A:90:PHE:O	1:A:91:GLY:C	2.62	0.41
1:A:282:GLU:H	1:A:282:GLU:HG3	1.35	0.41
1:A:145:ARG:HD2	1:A:268:GLY:N	2.30	0.41
1:A:35:ASN:ND2	1:A:70:CYS:N	2.68	0.41
1:A:283:ASP:N	1:A:287:LYS:O	2.45	0.41
1:A:239:SER:O	1:A:240:VAL:C	2.62	0.41
1:A:401:ARG:HH22	4:A:700:SIN:C2	2.34	0.41
1:A:498:ILE:HD12	1:A:498:ILE:O	2.21	0.41
3:A:600:FAD:H8A	3:A:600:FAD:H2B	1.95	0.40
1:A:283:ASP:HB2	1:A:289:THR:HG23	2.03	0.40
1:A:266:LYS:C	1:A:267:ARG:O	2.63	0.40
1:A:543:ASN:ND2	1:A:543:ASN:C	2.79	0.40
1:A:186:ASP:OD1	1:A:187:LYS:N	2.55	0.40
1:A:392:ASN:HD22	1:A:393:ARG:N	2.17	0.40

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	552/572 (96%)	492 (89%)	42 (8%)	18 (3%)	3 4

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	474	GLY
1	A	120	ALA
1	A	175	GLU
1	A	176	THR
1	A	178	PRO
1	A	317	LYS
1	A	427	SER
1	A	521	LYS
1	A	147	ALA
1	A	181	LYS
1	A	215	SER
1	A	523	ALA
1	A	412	LYS
1	A	488	LEU
1	A	97	GLY
1	A	179	GLN
1	A	122	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	377/429 (88%)	305 (81%)	72 (19%)	1 3

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	SER
1	A	20	VAL

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Mol	Chain	Res	Type
1	A	21	SER
1	A	22	ASP
1	A	26	VAL
1	A	28	ASN
1	A	31	LEU
1	A	61	LYS
1	A	68	ILE
1	A	75	LYS
1	A	78	GLU
1	A	79	LYS
1	A	89	SER
1	A	101	GLU
1	A	102	ARG
1	A	116	LYS
1	A	122	VAL
1	A	123	LYS
1	A	124	GLU
1	A	125	THR
1	A	145	ARG
1	A	146	ASP
1	A	166	LEU
1	A	175	GLU
1	A	176	THR
1	A	184	ILE
1	A	188	LYS
1	A	191	MET
1	A	194	ASP
1	A	196	MET
1	A	203	ASN
1	A	219	ILE
1	A	239	SER
1	A	243	SER
1	A	252	VAL
1	A	259	VAL
1	A	282	GLU
1	A	283	ASP
1	A	291	VAL
1	A	292	LEU
1	A	294	LYS
1	A	320	GLU
1	A	321	ARG
1	A	359	GLN

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Mol	Chain	Res	Type
1	A	375	ILE
1	A	387	VAL
1	A	392	ASN
1	A	396	ASN
1	A	398	ILE
1	A	401	ARG
1	A	414	GLU
1	A	425	ARG
1	A	427	SER
1	A	441	LYS
1	A	446	ILE
1	A	449	LEU
1	A	453	ILE
1	A	454	ASP
1	A	459	GLU
1	A	460	LEU
1	A	465	THR
1	A	473	SER
1	A	475	LYS
1	A	478	GLN
1	A	496	LEU
1	A	518	LYS
1	A	520	GLU
1	A	526	ILE
1	A	529	LEU
1	A	548	ASN
1	A	558	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	35	ASN
1	A	114	GLN
1	A	213	ASN
1	A	258	GLN
1	A	319	ASN
1	A	336	ASN
1	A	359	GLN
1	A	392	ASN
1	A	411	GLN
1	A	452	GLN

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Mol	Chain	Res	Type
1	A	468	ASN
1	A	478	GLN
1	A	543	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	$\# Z > 2$
4	SIN	A	700	-	7,7,7	1.40	1 (14%)	8,8,8	2.43	4 (50%)
3	FAD	A	600	-	58,58,58	3.01	8 (13%)	85,89,89	2.69	30 (35%)
2	HEC	A	602	1	46,50,50	1.91	7 (15%)	58,82,82	1.69	6 (10%)
2	HEC	A	603	1	46,50,50	1.89	7 (15%)	58,82,82	1.48	7 (12%)
2	HEC	A	601	1	46,50,50	2.00	11 (23%)	58,82,82	1.89	7 (12%)
2	HEC	A	604	1	46,50,50	1.91	9 (19%)	58,82,82	2.21	13 (22%)

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
4	SIN	A	700	-	-	4/5/5/5	-
3	FAD	A	600	-	2/2/9/9	12/34/50/50	0/6/6/6
2	HEC	A	602	1	-	7/14/54/54	-
2	HEC	A	603	1	-	9/14/54/54	-
2	HEC	A	601	1	-	7/14/54/54	-
2	HEC	A	604	1	-	8/14/54/54	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	C1'-C2'	19.38	1.79	1.52
2	A	601	HEC	CAC-C3C	7.12	1.58	1.35
3	A	600	FAD	C5B-C4B	7.06	1.72	1.51
2	A	602	HEC	CAB-C3B	7.03	1.57	1.35
2	A	601	HEC	CAB-C3B	6.87	1.57	1.35
2	A	602	HEC	CAC-C3C	6.84	1.57	1.35
2	A	603	HEC	CAB-C3B	6.80	1.57	1.35
2	A	604	HEC	CAB-C3B	6.64	1.56	1.35
2	A	603	HEC	CAC-C3C	6.58	1.56	1.35
2	A	604	HEC	CAC-C3C	6.44	1.55	1.35
3	A	600	FAD	P-O3P	-4.34	1.54	1.59
2	A	603	HEC	CBB-CAB	-3.76	1.35	1.49
2	A	601	HEC	CBC-CAC	-3.66	1.35	1.49
2	A	604	HEC	CBC-CAC	-3.61	1.36	1.49
2	A	602	HEC	CBB-CAB	-3.60	1.36	1.49
2	A	603	HEC	CBC-CAC	-3.57	1.36	1.49
3	A	600	FAD	C5X-N5	-3.56	1.32	1.39
2	A	601	HEC	CBB-CAB	-3.36	1.37	1.49
2	A	604	HEC	CBB-CAB	-3.29	1.37	1.49
2	A	602	HEC	CBC-CAC	-3.14	1.37	1.49
3	A	600	FAD	C5'-C4'	-2.53	1.48	1.51
2	A	601	HEC	CMB-C2B	2.46	1.55	1.50
2	A	601	HEC	C3C-C2C	-2.44	1.32	1.41
2	A	604	HEC	CMD-C2D	2.43	1.55	1.50
4	A	700	SIN	O3-C4	2.39	1.29	1.22
2	A	602	HEC	CMA-C3A	2.38	1.55	1.50
2	A	601	HEC	CMA-C3A	2.36	1.55	1.50
2	A	601	HEC	CMC-C2C	2.30	1.55	1.50
3	A	600	FAD	C6-C7	2.29	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	HEC	C3C-C2C	-2.25	1.33	1.41
2	A	601	HEC	CMD-C2D	2.24	1.55	1.50
2	A	602	HEC	C3B-C2B	-2.21	1.33	1.41
2	A	602	HEC	CAA-C2A	2.20	1.57	1.51
2	A	604	HEC	CMC-C2C	2.20	1.55	1.50
2	A	604	HEC	C3C-C2C	-2.19	1.33	1.41
2	A	604	HEC	C3B-C2B	-2.15	1.33	1.41
3	A	600	FAD	P-O1P	-2.12	1.43	1.50
3	A	600	FAD	C8-C7	2.10	1.46	1.40
2	A	601	HEC	C3D-C2D	-2.07	1.33	1.38
2	A	601	HEC	C3B-C2B	-2.05	1.34	1.41
2	A	604	HEC	CMB-C2B	2.03	1.54	1.50
2	A	603	HEC	CMC-C2C	2.03	1.54	1.50
2	A	603	HEC	CMA-C3A	2.03	1.54	1.50

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	C5B-C4B-C3B	-11.31	74.49	115.21
3	A	600	FAD	O5B-C5B-C4B	8.74	138.74	108.99
2	A	604	HEC	CBD-CAD-C3D	8.44	135.88	112.53
2	A	604	HEC	CBA-CAA-C2A	7.82	134.16	112.53
2	A	601	HEC	CBB-CAB-C3B	-7.77	111.91	127.43
2	A	601	HEC	CBC-CAC-C3C	-7.50	112.44	127.43
3	A	600	FAD	O4B-C4B-C5B	7.38	132.96	109.33
2	A	604	HEC	CBB-CAB-C3B	-6.95	113.55	127.43
3	A	600	FAD	O4B-C1B-N9A	-6.45	95.70	108.09
2	A	602	HEC	CBB-CAB-C3B	-6.23	114.97	127.43
2	A	602	HEC	CBC-CAC-C3C	-5.81	115.82	127.43
2	A	603	HEC	CBC-CAC-C3C	-5.62	116.19	127.43
4	A	700	SIN	C2-C3-C4	4.70	126.12	113.67
2	A	603	HEC	CBB-CAB-C3B	-4.46	118.52	127.43
3	A	600	FAD	C6-C5X-C9A	4.09	124.67	119.05
3	A	600	FAD	O4'-C4'-C3'	-4.08	99.71	109.25
3	A	600	FAD	O4B-C1B-C2B	-3.77	98.56	106.62
3	A	600	FAD	C4B-O4B-C1B	-3.66	101.38	109.47
3	A	600	FAD	O2-C2-N1	-3.56	115.88	121.80
2	A	602	HEC	CBD-CAD-C3D	3.55	122.36	112.53
3	A	600	FAD	C9A-C5X-N5	-3.51	118.73	122.45
3	A	600	FAD	C4A-N9A-C8A	3.48	109.39	105.74
3	A	600	FAD	C2B-C1B-N9A	-3.46	104.70	113.30
3	A	600	FAD	C7M-C7-C6	3.27	125.34	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	O2A-PA-O3P	3.26	116.09	107.27
3	A	600	FAD	C4'-C3'-C2'	-3.21	108.22	113.57
2	A	604	HEC	O1A-CGA-CBA	-3.18	113.01	123.09
3	A	600	FAD	C4-N3-C2	-3.17	120.02	125.64
3	A	600	FAD	C6-C7-C8	-2.94	115.38	119.69
2	A	602	HEC	O1D-CGD-CBD	-2.92	113.83	123.09
2	A	604	HEC	CAA-CBA-CGA	-2.82	106.17	113.67
4	A	700	SIN	C3-C2-C1	2.82	121.14	113.67
2	A	604	HEC	CBC-CAC-C3C	-2.80	121.84	127.43
3	A	600	FAD	C9-C9A-N10	2.76	125.56	121.85
3	A	600	FAD	O4-C4-C4X	-2.75	119.26	126.53
2	A	601	HEC	CHA-C1A-C2A	2.75	129.20	124.86
2	A	604	HEC	CAA-C2A-C1A	-2.74	119.28	124.85
2	A	604	HEC	C2A-C1A-NA	-2.73	107.69	110.32
2	A	603	HEC	CHB-C4A-NA	2.68	127.38	124.45
2	A	603	HEC	CMA-C3A-C4A	-2.67	120.02	124.73
2	A	603	HEC	CHA-C1A-NA	-2.66	121.55	124.45
3	A	600	FAD	N6A-C6A-N1A	2.65	124.28	118.38
3	A	600	FAD	C9-C8-C7	2.58	123.48	119.69
2	A	603	HEC	CHA-C1A-C2A	2.51	128.83	124.86
2	A	602	HEC	CHA-C1A-C2A	2.48	128.79	124.86
3	A	600	FAD	C4A-N9A-C1B	-2.47	120.85	126.63
4	A	700	SIN	O1-C1-C2	-2.47	115.25	123.09
2	A	604	HEC	CAA-C2A-C3A	2.43	132.41	127.87
3	A	600	FAD	O5'-C5'-C4'	2.40	115.77	109.36
3	A	600	FAD	O2'-C2'-C1'	-2.34	100.56	110.20
2	A	602	HEC	CHA-C1A-NA	-2.34	121.90	124.45
2	A	601	HEC	C3D-C4D-ND	-2.33	107.57	110.15
2	A	601	HEC	CHA-C1A-NA	-2.33	121.92	124.45
3	A	600	FAD	C5X-N5-C4X	2.33	121.85	118.09
3	A	600	FAD	O2'-C2'-C3'	-2.29	103.88	109.25
3	A	600	FAD	C10-N1-C2	2.28	121.79	116.85
4	A	700	SIN	O3-C4-C3	-2.24	115.97	123.09
2	A	603	HEC	CMA-C3A-C2A	2.24	132.20	126.15
3	A	600	FAD	O4-C4-N3	2.22	124.28	120.11
2	A	604	HEC	CHA-C1A-NA	2.20	126.85	124.45
2	A	604	HEC	CHC-C4B-C3B	2.15	128.83	125.21
3	A	600	FAD	C9-C9A-C5X	-2.11	116.30	120.03
2	A	601	HEC	O2D-CGD-O1D	2.11	128.75	123.33
3	A	600	FAD	C1'-N10-C9A	2.10	124.72	120.63
2	A	601	HEC	O1A-CGA-CBA	-2.07	116.52	123.09
2	A	604	HEC	CHC-C4B-NB	-2.03	122.24	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	HEC	O2A-CGA-O1A	2.01	128.50	123.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	FAD	C4'
3	A	600	FAD	C3'

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C2C-C3C-CAC-CBC
2	A	601	HEC	C4C-C3C-CAC-CBC
2	A	602	HEC	C2C-C3C-CAC-CBC
2	A	602	HEC	C4C-C3C-CAC-CBC
2	A	602	HEC	C2D-C3D-CAD-CBD
2	A	602	HEC	C4D-C3D-CAD-CBD
2	A	603	HEC	C2C-C3C-CAC-CBC
2	A	603	HEC	C4C-C3C-CAC-CBC
2	A	604	HEC	C2C-C3C-CAC-CBC
2	A	604	HEC	C4C-C3C-CAC-CBC
3	A	600	FAD	C1'-C2'-C3'-O3'
3	A	600	FAD	C1'-C2'-C3'-C4'
3	A	600	FAD	C3'-C4'-C5'-O5'
3	A	600	FAD	O4'-C4'-C5'-O5'
3	A	600	FAD	C3B-C4B-C5B-O5B
2	A	603	HEC	C2A-CAA-CBA-CGA
2	A	603	HEC	C3D-CAD-CBD-CGD
3	A	600	FAD	O4B-C4B-C5B-O5B
2	A	604	HEC	C1A-C2A-CAA-CBA
3	A	600	FAD	PA-O3P-P-O5'
3	A	600	FAD	O2'-C2'-C3'-C4'
2	A	601	HEC	C4B-C3B-CAB-CBB
2	A	602	HEC	C4B-C3B-CAB-CBB
2	A	603	HEC	C4B-C3B-CAB-CBB
2	A	604	HEC	C4B-C3B-CAB-CBB
3	A	600	FAD	O2'-C2'-C3'-O3'
2	A	601	HEC	C2B-C3B-CAB-CBB
2	A	602	HEC	C2B-C3B-CAB-CBB
2	A	604	HEC	C2B-C3B-CAB-CBB
3	A	600	FAD	C5'-O5'-P-O1P
2	A	604	HEC	C3A-C2A-CAA-CBA

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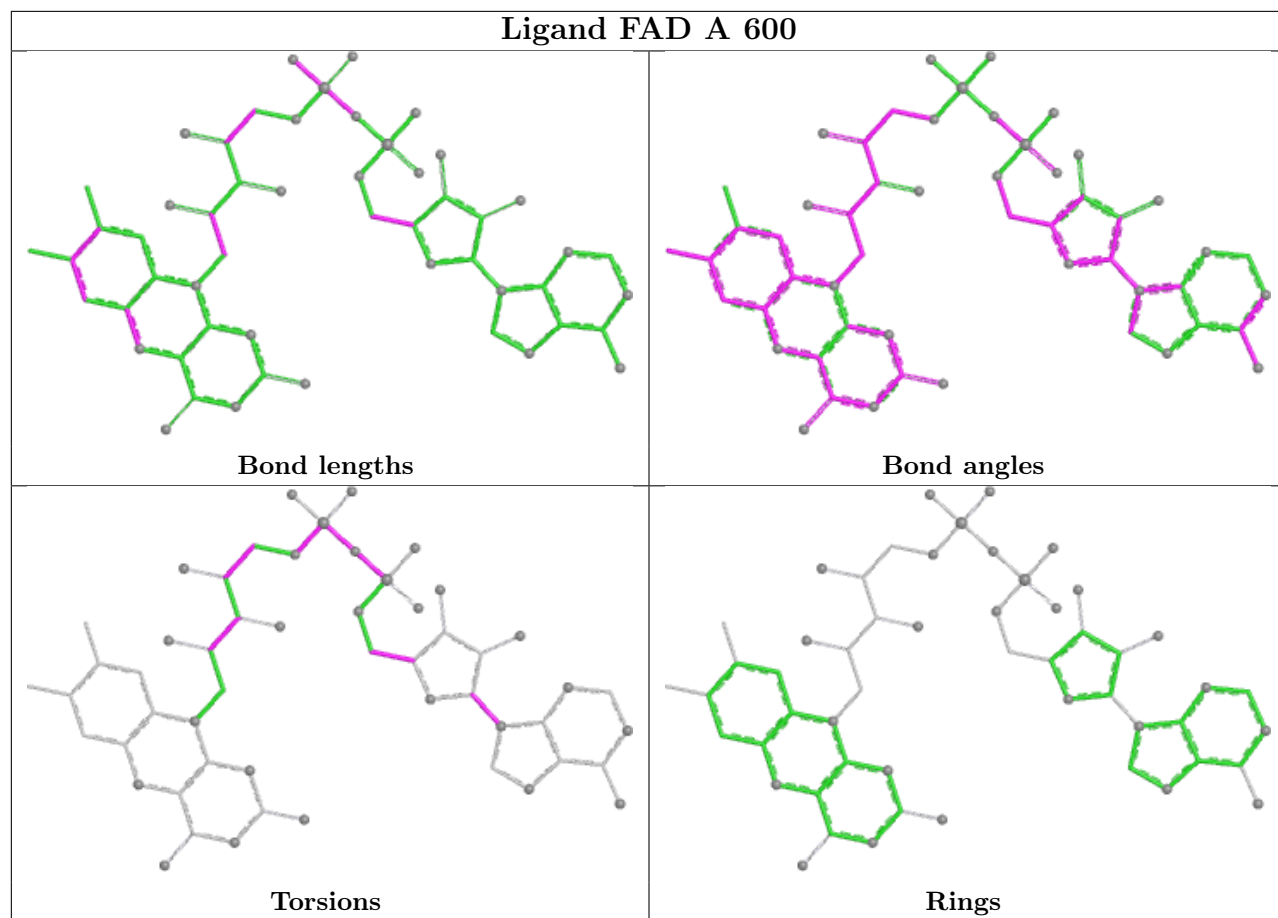
Mol	Chain	Res	Type	Atoms
3	A	600	FAD	P-O3P-PA-O2A
2	A	604	HEC	CAA-CBA-CGA-O2A
4	A	700	SIN	C2-C3-C4-O3
2	A	603	HEC	CAA-CBA-CGA-O2A
4	A	700	SIN	C2-C3-C4-O4
2	A	603	HEC	CAA-CBA-CGA-O1A
4	A	700	SIN	O1-C1-C2-C3
2	A	603	HEC	CAD-CBD-CGD-O1D
2	A	603	HEC	CAD-CBD-CGD-O2D
4	A	700	SIN	O2-C1-C2-C3
2	A	604	HEC	CAA-CBA-CGA-O1A
2	A	601	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAD-CBD-CGD-O1D
3	A	600	FAD	C2B-C1B-N9A-C8A
2	A	602	HEC	CAA-CBA-CGA-O2A
2	A	601	HEC	CAA-CBA-CGA-O2A

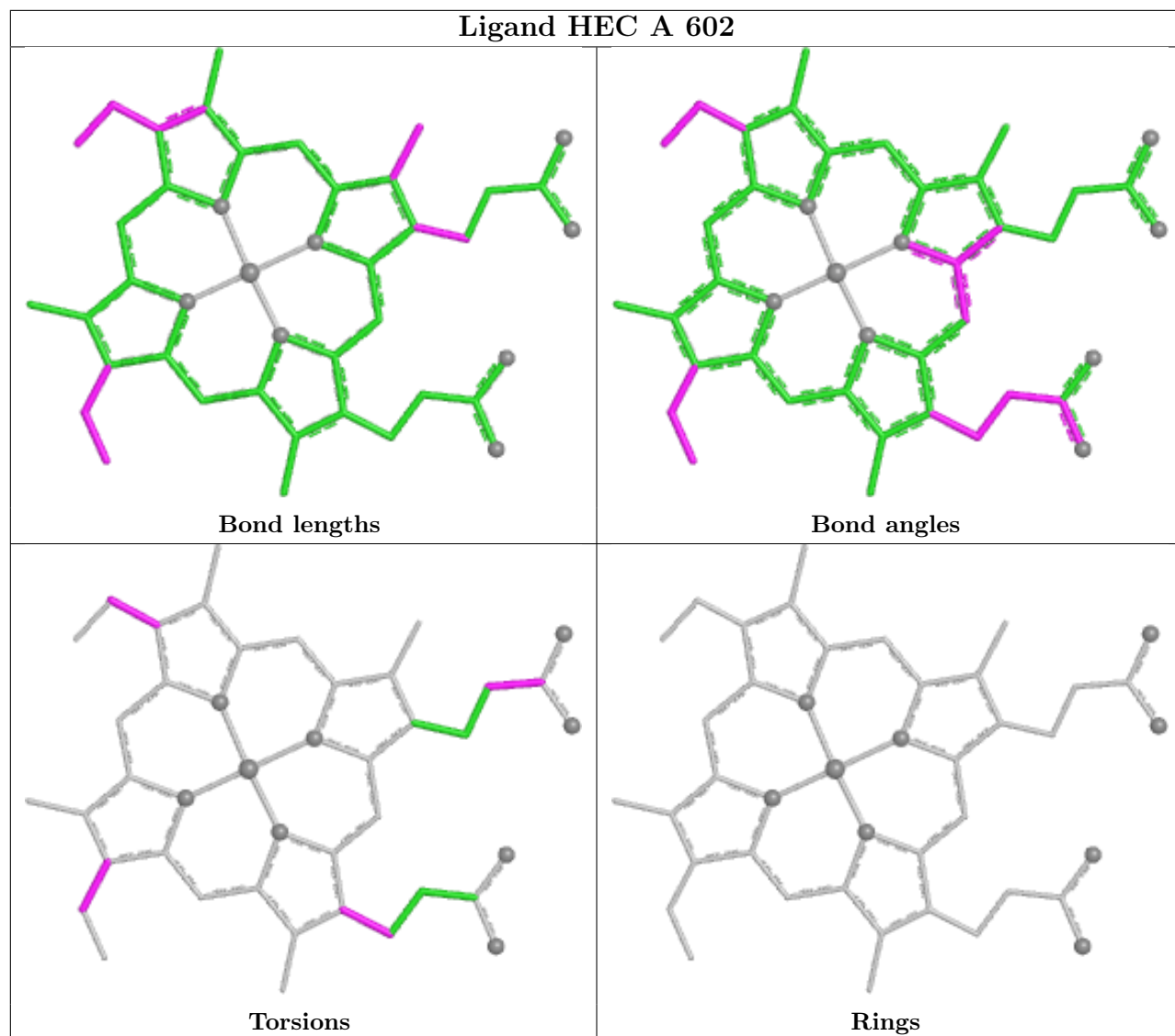
There are no ring outliers.

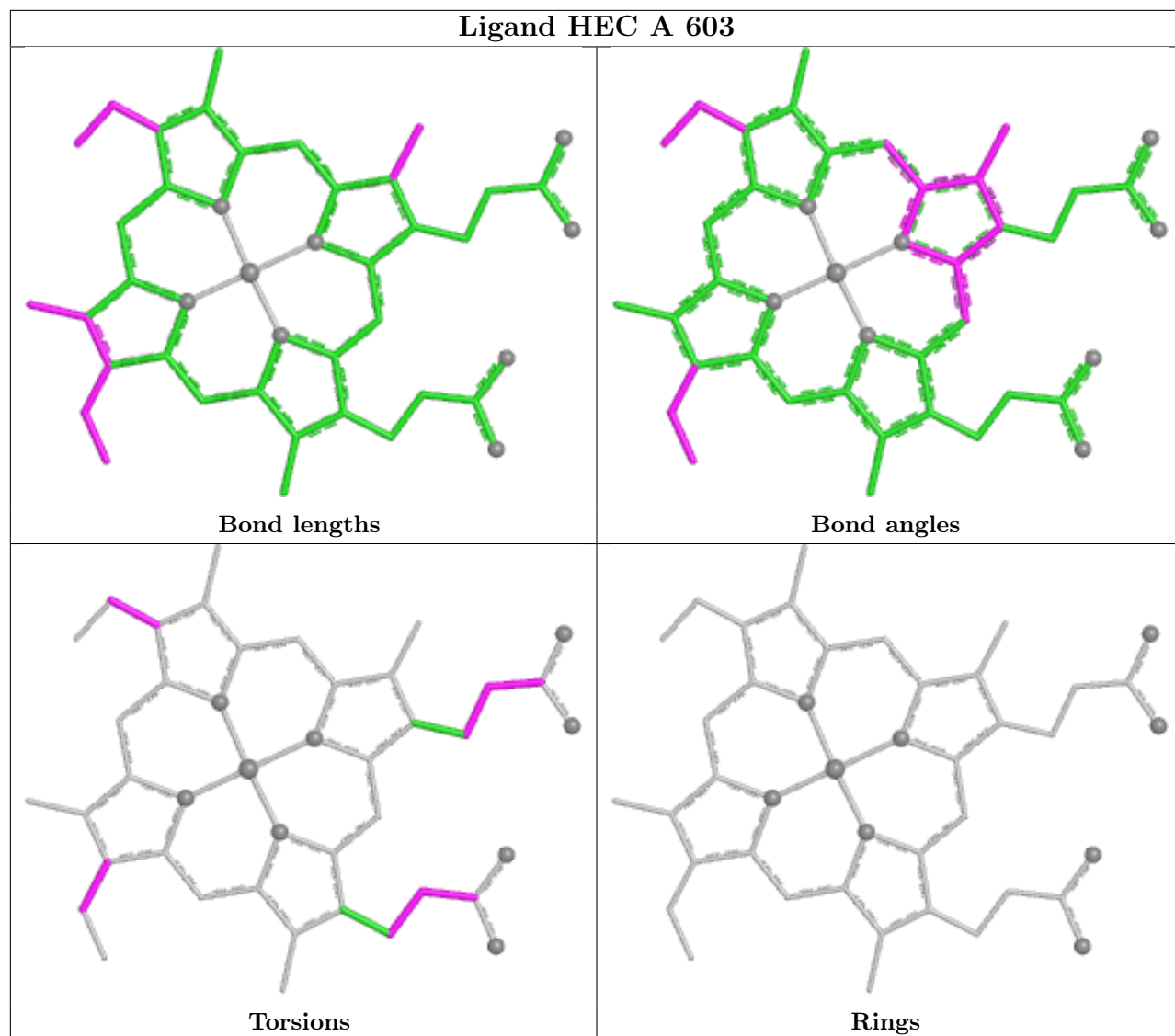
6 monomers are involved in 32 short contacts:

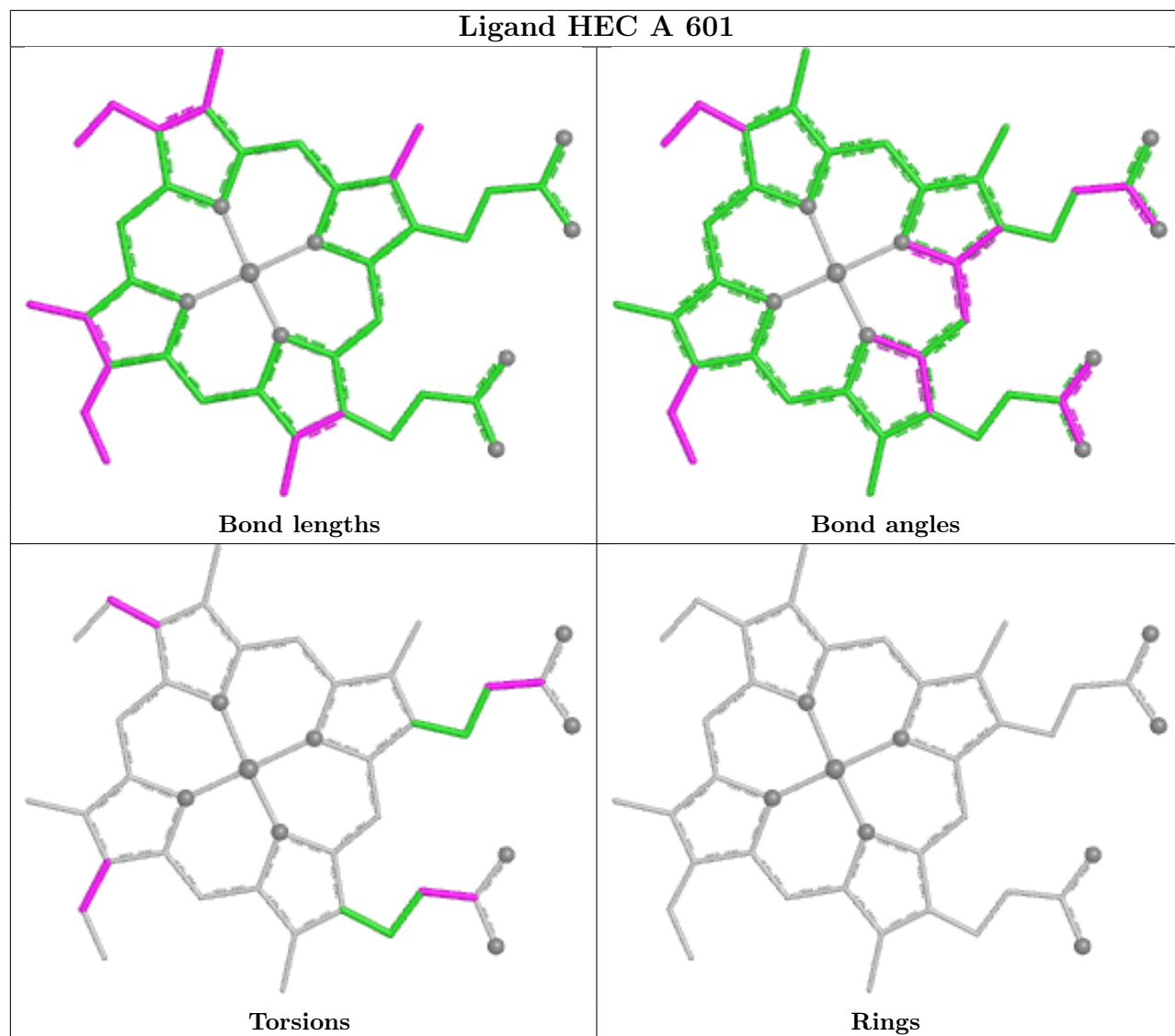
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	SIN	7	0
3	A	600	FAD	8	0
2	A	602	HEC	3	0
2	A	603	HEC	4	0
2	A	601	HEC	4	0
2	A	604	HEC	6	0

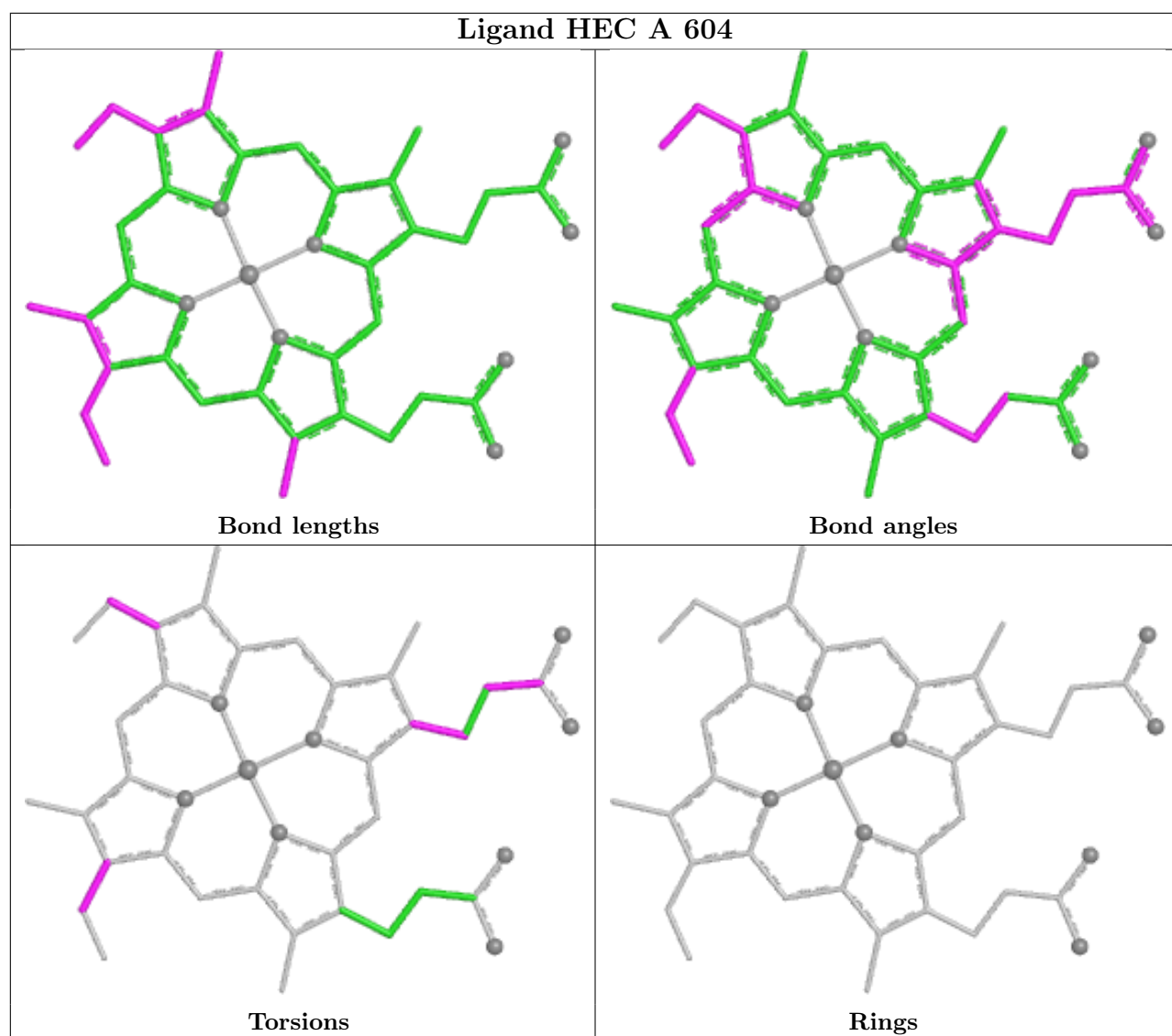
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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