



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:23 PM UTC

PDB ID : 1U8V / pdb_00001u8v
Title : Crystal Structure of 4-Hydroxybutyryl-CoA Dehydratase from *Clostridium aminobutyricum*: Radical catalysis involving a [4Fe-4S] cluster and flavin
Authors : Martins, B.M.; Dobbek, H.; Cinkaya, I.; Buckel, W.; Messerschmidt, A.
Deposited on : 2004-08-07
Resolution : 1.60 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

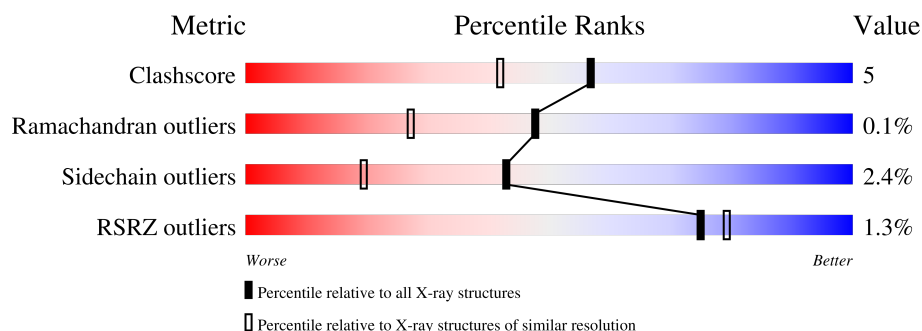
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	490	2% 87% 12% .
1	B	490	% 88% 11% .
1	C	490	% 91% 8% .
1	D	490	% 90% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17824 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.

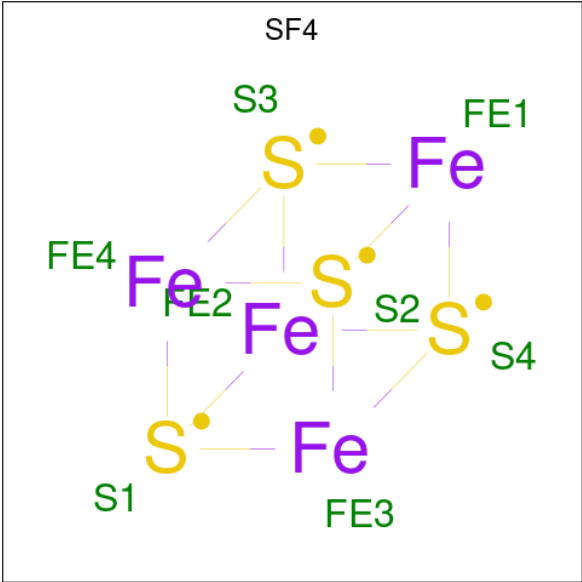
- Molecule 1 is a protein called Gamma-aminobutyrate metabolism dehydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	4	0	0
			3811	2386	663	727	35			
1	B	490	Total	C	N	O	S	6	0	0
			3811	2386	663	727	35			
1	C	490	Total	C	N	O	S	4	0	0
			3811	2386	663	727	35			
1	D	490	Total	C	N	O	S	0	0	0
			3811	2386	663	727	35			

There are 8 discrepancies between the modelled and reference sequences:

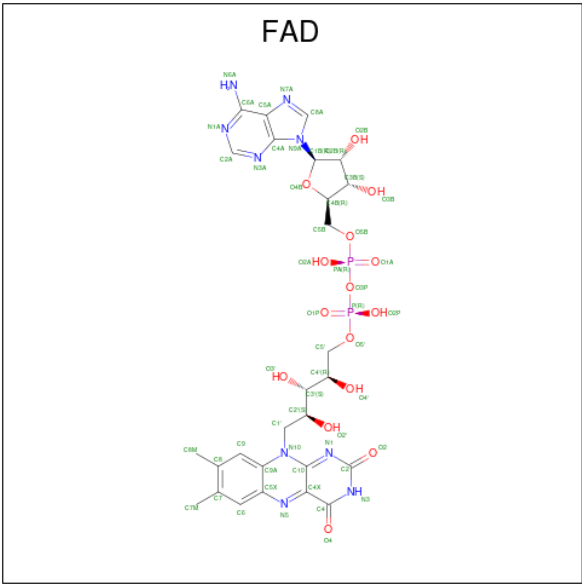
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ASP	GLY	SEE REMARK 999	UNP P55792
A	357	GLY	ASP	SEE REMARK 999	UNP P55792
B	167	ASP	GLY	SEE REMARK 999	UNP P55792
B	357	GLY	ASP	SEE REMARK 999	UNP P55792
C	167	ASP	GLY	SEE REMARK 999	UNP P55792
C	357	GLY	ASP	SEE REMARK 999	UNP P55792
D	167	ASP	GLY	SEE REMARK 999	UNP P55792
D	357	GLY	ASP	SEE REMARK 999	UNP P55792

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

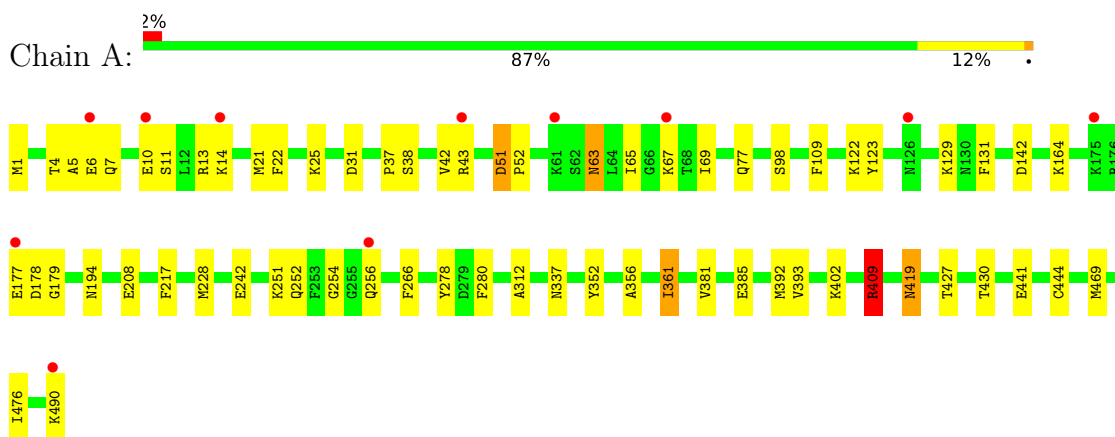
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	519	Total	O	0	0
			519	519		
4	B	573	Total	O	0	0
			573	573		
4	C	636	Total	O	0	0
			636	636		
4	D	608	Total	O	0	0
			608	608		

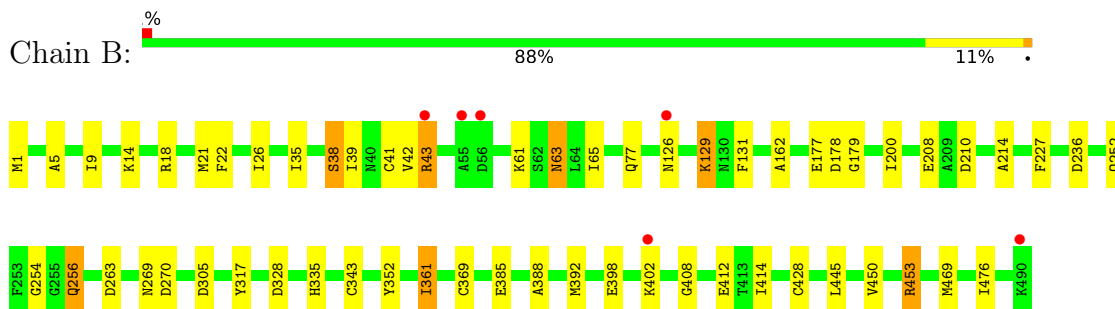
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

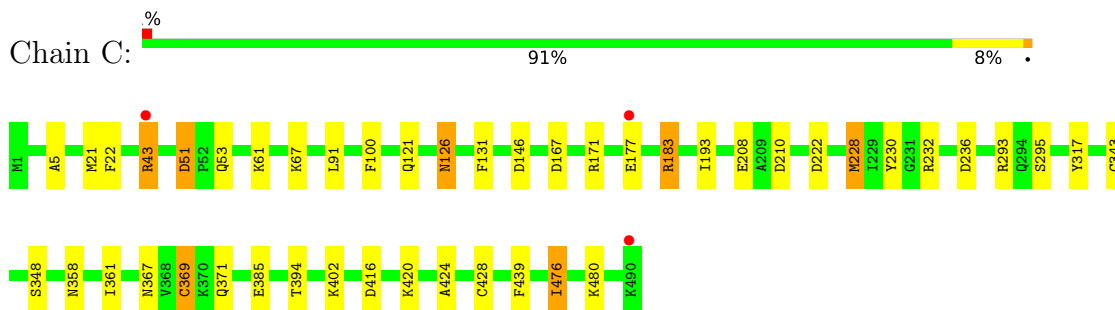
- Molecule 1: Gamma-aminobutyrate metabolism dehydratase/isomerase



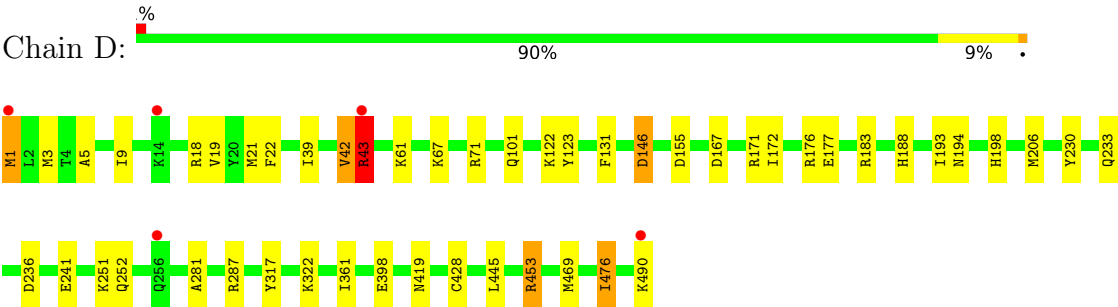
- Molecule 1: Gamma-aminobutyrate metabolism dehydratase/isomerase



- Molecule 1: Gamma-aminobutyrate metabolism dehydratase/isomerase



- Molecule 1: Gamma-aminobutyrate metabolism dehydratase/isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.30Å 130.20Å 175.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 1.60 58.00 – 1.62	Depositor EDS
% Data completeness (in resolution range)	(Not available) (58.00-1.60) 99.7 (58.00-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.62Å)	Xtriage
Refinement program	CNS, SHELX	Depositor
R, R_{free}	0.163 , 0.212 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17824	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0.57	0/3877	1.36	15/5224 (0.3%)
1	B	0.63	0/3877	1.42	27/5224 (0.5%)
1	C	0.76	0/3877	1.49	26/5224 (0.5%)
1	D	0.66	0/3877	1.40	14/5224 (0.3%)
All	All	0.66	0/15508	1.42	82/20896 (0.4%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	ARG	CD-NE-CZ	9.15	137.21	124.40
1	C	126	ASN	CA-CB-CG	8.67	121.27	112.60
1	B	270	ASP	CA-CB-CG	8.14	120.74	112.60
1	C	146	ASP	CA-CB-CG	-7.66	104.94	112.60
1	D	236	ASP	CA-CB-CG	7.54	120.14	112.60
1	C	183	ARG	CD-NE-CZ	7.30	134.62	124.40
1	D	131	PHE	CA-CB-CG	-6.96	106.84	113.80
1	A	51	ASP	CA-C-O	6.90	125.32	119.66
1	C	293	ARG	CA-C-N	6.88	129.38	120.44
1	C	293	ARG	C-N-CA	6.88	129.38	120.44
1	C	131	PHE	CA-CB-CG	-6.88	106.92	113.80
1	C	183	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	D	281	ALA	CA-C-N	6.12	126.78	119.98
1	D	281	ALA	C-N-CA	6.12	126.78	119.98
1	B	254	GLY	O-C-N	-6.11	116.69	123.66
1	C	43	ARG	CD-NE-CZ	6.05	132.87	124.40
1	B	41	CYS	O-C-N	-6.03	115.58	122.09
1	B	131	PHE	CA-CB-CG	-6.00	107.81	113.80
1	A	356	ALA	CA-C-N	-5.98	116.96	123.30
1	A	356	ALA	C-N-CA	-5.98	116.96	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ILE	CA-C-N	5.96	126.60	119.98
1	B	414	ILE	C-N-CA	5.96	126.60	119.98
1	C	210	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	109	PHE	CA-CB-CG	5.90	119.70	113.80
1	C	236	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	65	ILE	CB-CA-C	-5.87	104.49	111.65
1	A	142	ASP	CA-CB-CG	5.80	118.41	112.60
1	B	18	ARG	CA-C-N	5.78	130.79	123.10
1	B	18	ARG	C-N-CA	5.78	130.79	123.10
1	B	227	PHE	CA-CB-CG	5.72	119.52	113.80
1	B	178	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	232	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	D	241	GLU	CA-C-O	5.66	127.50	121.05
1	D	18	ARG	CD-NE-CZ	5.66	132.32	124.40
1	A	63	ASN	CA-C-N	5.64	130.13	120.71
1	A	63	ASN	C-N-CA	5.64	130.13	120.71
1	A	217	PHE	CA-C-O	-5.60	115.29	121.28
1	A	131	PHE	CA-CB-CG	-5.58	108.22	113.80
1	C	367	ASN	O-C-N	5.57	128.50	122.15
1	B	214	ALA	O-C-N	5.56	128.83	122.55
1	D	19	VAL	CA-C-O	-5.55	114.56	120.39
1	B	328	ASP	CA-CB-CG	-5.53	107.07	112.60
1	B	352	TYR	N-CA-C	5.51	113.09	108.13
1	D	445	LEU	CB-CA-C	-5.46	102.12	109.16
1	A	419	ASN	CA-CB-CG	-5.45	107.16	112.60
1	B	335	HIS	CA-CB-CG	-5.44	108.36	113.80
1	C	348	SER	O-C-N	-5.43	116.22	122.09
1	C	232	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	D	287	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	D	172	ILE	CA-C-O	-5.41	114.68	120.85
1	D	193	ILE	O-C-N	-5.40	116.41	121.87
1	D	43	ARG	CD-NE-CZ	5.39	131.94	124.40
1	B	162	ALA	CA-C-O	5.37	125.71	119.32
1	C	51	ASP	CA-C-O	5.37	123.29	119.32
1	C	358	ASN	CA-CB-CG	5.34	117.94	112.60
1	B	208	GLU	O-C-N	-5.33	116.47	122.12
1	A	393	VAL	CA-C-O	-5.33	114.75	119.38
1	B	42	VAL	CB-CA-C	-5.29	103.97	112.16
1	B	445	LEU	CB-CA-C	-5.27	102.27	109.28
1	B	263	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	371	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	D	206	MET	CA-CB-CG	5.24	124.59	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	VAL	CA-C-O	5.23	126.39	120.95
1	B	227	PHE	CA-C-O	-5.22	115.87	121.45
1	C	146	ASP	CA-C-N	5.21	125.67	120.98
1	C	146	ASP	C-N-CA	5.21	125.67	120.98
1	C	416	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	337	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	A	280	PHE	CA-C-O	5.13	125.24	119.18
1	C	369	CYS	O-C-N	-5.10	116.63	122.08
1	B	39	ILE	O-C-N	5.09	127.07	121.83
1	B	256	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	210	ASP	CA-CB-CG	5.08	117.69	112.60
1	C	439	PHE	N-CA-C	-5.08	105.63	111.07
1	C	91	LEU	O-C-N	-5.07	116.81	122.09
1	B	305	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	222	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	236	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	155	ASP	CA-C-O	-5.02	114.64	120.62
1	C	100	PHE	CA-C-N	5.01	131.12	121.54
1	C	100	PHE	C-N-CA	5.01	131.12	121.54
1	A	352	TYR	N-CA-C	5.01	112.73	108.22

There are no chirality outliers.

There are no planarity outliers.

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	3811	0	3753	50	0
1	B	3811	0	3753	31	0
1	C	3811	0	3753	26	0
1	D	3811	0	3753	37	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	1	0
2	D	8	0	0	0	0
3	A	53	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	30	0	0
3	C	53	0	31	0	0
3	D	53	0	29	1	0
4	A	519	0	0	19	0
4	B	573	0	0	11	0
4	C	636	0	0	10	0
4	D	608	0	0	21	0
All	All	17824	0	15132	140	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 (140) 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:D:1:MET:HE1	1:D:3:MET:HG3	1.59	0.84
1:B:5:ALA:HB1	1:B:43:ARG:HG3	1.62	0.80
1:D:398:GLU:HG3	4:D:8522:HOH:O	1.83	0.79
1:A:476:ILE:HB	4:C:7423:HOH:O	1.83	0.78
1:B:61:LYS:HB2	4:B:7747:HOH:O	1.83	0.77
1:C:67:LYS:HE3	4:C:7967:HOH:O	1.84	0.77
1:D:67:LYS:HD3	4:D:8137:HOH:O	1.84	0.77
3:D:492:FAD:H5'1	4:D:7196:HOH:O	1.84	0.77
1:D:167:ASP:HA	4:D:8119:HOH:O	1.85	0.76
1:A:77:GLN:HG3	4:A:8064:HOH:O	1.86	0.75
1:B:129:LYS:HE3	4:B:8329:HOH:O	1.85	0.75
1:A:4:THR:H	1:A:7:GLN:HE21	1.36	0.74
1:B:252:GLN:HG3	4:B:8358:HOH:O	1.89	0.73
1:B:398:GLU:HG3	4:B:7512:HOH:O	1.88	0.72
1:A:5:ALA:HB1	1:A:43:ARG:HG3	1.72	0.72
1:A:312:ALA:HB1	1:C:476:ILE:HD11	1.72	0.72
1:B:63:ASN:HB3	4:B:7342:HOH:O	1.89	0.72
1:D:419:ASN:HB3	4:D:8760:HOH:O	1.93	0.69
1:B:385:GLU:HA	1:B:392:MET:HE1	1.74	0.69
1:C:171:ARG:HG2	4:C:8468:HOH:O	1.92	0.69
1:A:6:GLU:HG3	4:A:7863:HOH:O	1.93	0.69
1:D:322:LYS:HD2	4:D:8410:HOH:O	1.92	0.68
1:D:469:MET:HE2	4:D:7051:HOH:O	1.96	0.65
1:A:11:SER:HA	1:A:14:LYS:HE3	1.78	0.64
1:B:77:GLN:HG3	4:B:7342:HOH:O	1.96	0.64
1:B:21:MET:HG2	1:B:22:PHE:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ARG:HD3	4:C:8393:HOH:O	1.97	0.62
1:D:171:ARG:HG2	4:D:8119:HOH:O	1.99	0.62
1:A:10:GLU:HG2	4:A:8332:HOH:O	1.98	0.62
1:A:10:GLU:HG3	4:A:8279:HOH:O	2.00	0.62
1:A:10:GLU:O	1:A:14:LYS:HE3	2.00	0.62
1:C:402:LYS:HE2	4:C:7482:HOH:O	2.00	0.61
1:A:361:ILE:H	1:A:361:ILE:HD13	1.67	0.60
1:B:388:ALA:HB3	1:B:392:MET:HE2	1.84	0.60
1:C:193:ILE:HA	1:C:228:MET:HE2	1.84	0.59
1:C:5:ALA:HB1	1:C:43:ARG:HG3	1.83	0.59
1:A:208:GLU:HG3	1:A:278:TYR:CE1	2.37	0.59
1:C:476:ILE:HD13	1:C:480:LYS:HE3	1.85	0.58
1:C:5:ALA:HB1	1:C:43:ARG:CD	2.33	0.58
1:C:21:MET:HG2	1:C:22:PHE:CD2	2.39	0.57
1:A:38:SER:HB3	1:A:256:GLN:NE2	2.20	0.57
1:A:25:LYS:HE3	4:A:8240:HOH:O	2.04	0.56
1:A:21:MET:HG2	1:A:22:PHE:CD2	2.40	0.56
1:B:402:LYS:O	1:B:402:LYS:HG2	2.03	0.56
1:D:5:ALA:HB1	1:D:43:ARG:HD2	1.86	0.56
1:A:312:ALA:CB	1:C:476:ILE:HD11	2.35	0.56
1:A:252:GLN:HG2	4:A:8134:HOH:O	2.05	0.56
1:D:43:ARG:HD3	4:D:8072:HOH:O	2.05	0.56
1:A:409:ARG:HD3	4:A:7387:HOH:O	2.05	0.56
1:D:21:MET:HG2	1:D:22:PHE:CD2	2.41	0.56
1:D:5:ALA:HB1	1:D:43:ARG:CD	2.36	0.55
1:A:427:THR:HB	4:A:7412:HOH:O	2.06	0.55
1:D:1:MET:HE1	1:D:3:MET:CG	2.35	0.55
1:B:21:MET:HE3	1:B:26:ILE:HG13	1.90	0.54
1:B:21:MET:HG2	1:B:22:PHE:HD2	1.71	0.54
1:C:394:THR:OG1	1:D:188:HIS:HD2	1.91	0.54
1:D:122:LYS:HE2	1:D:123:TYR:CZ	2.44	0.52
1:B:408:GLY:HA3	1:B:412:GLU:OE1	2.09	0.52
1:A:469:MET:HE2	4:A:6888:HOH:O	2.10	0.52
1:D:61:LYS:HD3	4:D:7445:HOH:O	2.10	0.52
1:A:11:SER:HA	1:A:14:LYS:CE	2.40	0.51
1:C:51:ASP:OD1	1:C:53:GLN:HG2	2.09	0.51
1:D:233:GLN:HG2	4:D:7572:HOH:O	2.09	0.51
1:D:251:LYS:HE3	4:D:7938:HOH:O	2.10	0.51
1:A:252:GLN:HG3	4:A:6246:HOH:O	2.11	0.50
1:B:43:ARG:HD3	4:B:6871:HOH:O	2.10	0.50
1:C:476:ILE:CD1	1:C:480:LYS:HE3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ARG:HG2	4:D:7311:HOH:O	2.11	0.50
1:A:5:ALA:HB1	1:A:43:ARG:HE	1.76	0.50
1:A:37:PRO:HD2	4:A:7729:HOH:O	2.12	0.50
1:A:10:GLU:C	1:A:14:LYS:HE3	2.37	0.49
1:D:188:HIS:HE1	4:D:6171:HOH:O	1.94	0.49
1:D:42:VAL:HG13	1:D:101:GLN:HB2	1.94	0.49
1:B:469:MET:HE1	4:B:7543:HOH:O	2.13	0.49
1:D:9:ILE:HD11	1:D:43:ARG:HD3	1.94	0.49
1:D:317:TYR:CD1	1:D:428:CYS:HB3	2.48	0.48
1:D:42:VAL:HG21	1:D:194:ASN:ND2	2.29	0.48
1:A:381:VAL:HG13	1:A:444:CYS:SG	2.54	0.48
1:C:5:ALA:HB1	1:C:43:ARG:CG	2.44	0.48
1:A:65:ILE:HG13	1:A:67:LYS:HG2	1.95	0.48
1:B:179:GLY:HA2	1:B:269:ASN:ND2	2.28	0.48
1:C:167:ASP:HA	4:C:8468:HOH:O	2.14	0.48
1:A:67:LYS:HE3	1:A:69:ILE:HG22	1.95	0.48
1:D:43:ARG:HG3	4:D:8170:HOH:O	2.13	0.47
1:A:392:MET:HE3	1:A:441:GLU:HA	1.95	0.47
1:B:256:GLN:HB2	4:B:8029:HOH:O	2.14	0.47
1:C:295:SER:HB3	2:C:491:SF4:S3	2.55	0.47
1:A:5:ALA:CB	1:A:43:ARG:HG3	2.42	0.47
1:A:256:GLN:NE2	4:A:7729:HOH:O	2.48	0.47
1:B:63:ASN:HD22	1:B:63:ASN:H	1.61	0.47
1:B:14:LYS:O	1:B:14:LYS:HG2	2.14	0.47
1:B:388:ALA:CB	1:B:392:MET:HE2	2.45	0.46
1:C:183:ARG:HD3	4:C:7601:HOH:O	2.15	0.46
1:A:51:ASP:OD1	1:A:52:PRO:HD2	2.16	0.46
1:B:361:ILE:H	1:B:361:ILE:HD13	1.81	0.46
1:B:317:TYR:CD1	1:B:428:CYS:HB3	2.51	0.45
1:C:121:GLN:NE2	4:C:7234:HOH:O	2.49	0.45
1:A:37:PRO:HB2	4:A:7729:HOH:O	2.15	0.45
1:A:13:ARG:NH2	1:A:31:ASP:OD1	2.50	0.45
1:C:385:GLU:OE2	1:D:453:ARG:NH2	2.50	0.45
1:A:385:GLU:OE2	1:B:453:ARG:NH2	2.50	0.45
1:D:146:ASP:OD1	1:D:198:HIS:ND1	2.49	0.45
1:C:43:ARG:NH1	4:C:7867:HOH:O	2.50	0.45
1:C:343:CYS:HB3	1:C:369:CYS:HB2	1.99	0.44
1:A:13:ARG:HH21	1:A:31:ASP:CG	2.25	0.44
1:B:43:ARG:HG2	4:B:8306:HOH:O	2.17	0.44
1:C:5:ALA:HB1	1:C:43:ARG:NE	2.31	0.44
1:D:183:ARG:NH1	4:D:7719:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:NH2	4:D:6680:HOH:O	2.50	0.44
1:A:4:THR:OG1	1:A:7:GLN:HG3	2.17	0.44
1:C:420:LYS:NZ	4:C:8295:HOH:O	2.50	0.44
1:A:419:ASN:HA	1:A:430:THR:HG21	2.00	0.44
1:A:43:ARG:NH2	4:A:7450:HOH:O	2.50	0.44
1:B:9:ILE:HD11	1:B:43:ARG:HD2	2.00	0.44
1:A:251:LYS:NZ	4:A:8796:HOH:O	2.50	0.44
1:D:176:ARG:NH2	4:D:7481:HOH:O	2.49	0.44
1:A:13:ARG:NH1	4:A:8279:HOH:O	2.50	0.43
1:C:21:MET:HG3	1:C:230:TYR:CD2	2.53	0.43
1:A:51:ASP:HA	1:A:52:PRO:HD3	1.87	0.43
1:A:164:LYS:HE2	4:A:8200:HOH:O	2.18	0.43
1:A:65:ILE:HD11	1:A:67:LYS:HE3	2.01	0.43
1:A:361:ILE:H	1:A:361:ILE:CD1	2.30	0.43
1:D:252:GLN:NE2	4:D:8690:HOH:O	2.49	0.42
1:B:469:MET:HE2	4:B:7033:HOH:O	2.19	0.42
1:D:71:ARG:HD3	4:D:6710:HOH:O	2.20	0.42
1:A:67:LYS:NZ	4:A:7722:HOH:O	2.49	0.41
1:A:178:ASP:OD1	1:A:178:ASP:N	2.49	0.41
1:A:254:GLY:HA2	4:A:7779:HOH:O	2.18	0.41
1:B:5:ALA:CB	1:B:43:ARG:HG3	2.41	0.41
1:A:179:GLY:HA3	1:A:266:PHE:CE1	2.56	0.41
1:C:317:TYR:CD1	1:C:428:CYS:HB3	2.56	0.41
1:D:476:ILE:O	1:D:476:ILE:HD12	2.20	0.41
1:D:122:LYS:HE2	1:D:123:TYR:CE2	2.55	0.41
1:B:1:MET:HE3	1:B:1:MET:HB3	1.87	0.41
1:B:35:ILE:O	1:B:38:SER:HB2	2.21	0.41
1:D:21:MET:HG3	1:D:230:TYR:CD2	2.55	0.41
1:B:343:CYS:HB3	1:B:369:CYS:HB2	2.03	0.41
1:A:122:LYS:HD3	1:A:123:TYR:CE2	2.56	0.40
1:D:469:MET:HE1	4:D:8063:HOH:O	2.21	0.40
1:D:39:ILE:O	1:D:43:ARG:HB3	2.21	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	488/490 (100%)	474 (97%)	14 (3%)	0	100	100
1	B	488/490 (100%)	474 (97%)	14 (3%)	0	100	100
1	C	488/490 (100%)	475 (97%)	12 (2%)	1 (0%)	43	24
1	D	488/490 (100%)	474 (97%)	14 (3%)	0	100	100
All	All	1952/1960 (100%)	1897 (97%)	54 (3%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	424	ALA

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	403/403 (100%)	390 (97%)	13 (3%)	34	12
1	B	403/403 (100%)	393 (98%)	10 (2%)	42	18
1	C	403/403 (100%)	396 (98%)	7 (2%)	53	30
1	D	403/403 (100%)	394 (98%)	9 (2%)	45	22
All	All	1612/1612 (100%)	1573 (98%)	39 (2%)	43	19

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	42	VAL
1	A	63	ASN
1	A	98	SER
1	A	129	LYS

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Mol	Chain	Res	Type
1	A	177	GLU
1	A	194	ASN
1	A	228	MET
1	A	242	GLU
1	A	361	ILE
1	A	402	LYS
1	A	409	ARG
1	A	490	LYS
1	B	38	SER
1	B	43	ARG
1	B	63	ASN
1	B	126	ASN
1	B	129	LYS
1	B	177	GLU
1	B	200	ILE
1	B	361	ILE
1	B	453	ARG
1	B	476	ILE
1	C	61	LYS
1	C	126	ASN
1	C	177	GLU
1	C	208	GLU
1	C	228	MET
1	C	361	ILE
1	C	476	ILE
1	D	1	MET
1	D	42	VAL
1	D	43	ARG
1	D	146	ASP
1	D	177	GLU
1	D	361	ILE
1	D	453	ARG
1	D	476	ILE
1	D	490	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	28	ASN
1	A	74	ASN
1	A	77	GLN

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Mol	Chain	Res	Type
1	A	139	GLN
1	A	194	ASN
1	A	233	GLN
1	A	252	GLN
1	A	256	GLN
1	A	335	HIS
1	B	53	GLN
1	B	63	ASN
1	B	74	ASN
1	B	77	GLN
1	B	94	GLN
1	B	141	ASN
1	B	194	ASN
1	B	198	HIS
1	B	269	ASN
1	B	335	HIS
1	B	464	GLN
1	C	74	ASN
1	C	94	GLN
1	C	139	GLN
1	C	141	ASN
1	C	269	ASN
1	C	360	GLN
1	D	53	GLN
1	D	94	GLN
1	D	139	GLN
1	D	141	ASN
1	D	188	HIS
1	D	189	GLN
1	D	233	GLN
1	D	252	GLN
1	D	256	GLN
1	D	269	ASN
1	D	335	HIS
1	D	360	GLN
1	D	419	ASN

5.3.3 RNA ⓘ

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](#)

8 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$
2	SF4	D	491	1	0,12,12	-	-	-		
3	FAD	D	492	-	58,58,58	1.36	6 (10%)	85,89,89	2.05	18 (21%)
3	FAD	A	492	-	58,58,58	1.16	3 (5%)	85,89,89	1.52	14 (16%)
2	SF4	B	491	1,4	0,12,12	-	-	-		
3	FAD	B	492	-	58,58,58	1.31	4 (6%)	85,89,89	1.53	15 (17%)
3	FAD	C	492	-	58,58,58	1.34	5 (8%)	85,89,89	1.62	16 (18%)
2	SF4	A	491	1	0,12,12	-	-	-		
2	SF4	C	491	1	0,12,12	-	-	-		

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
2	SF4	D	491	1	-	-	0/6/5/5
3	FAD	D	492	-	-	10/34/50/50	0/6/6/6
3	FAD	A	492	-	-	1/34/50/50	0/6/6/6
2	SF4	B	491	1,4	-	-	0/6/5/5
3	FAD	B	492	-	-	2/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	492	-	-	2/34/50/50	0/5/6/6
2	SF4	A	491	1	-	-	0/6/5/5
2	SF4	C	491	1	-	-	0/6/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	492	FAD	P-O3P	4.57	1.64	1.59
3	C	492	FAD	C4X-N5	4.19	1.39	1.30
3	D	492	FAD	C4X-N5	3.91	1.39	1.30
3	C	492	FAD	P-O3P	3.83	1.63	1.59
3	D	492	FAD	C5'-C4'	3.83	1.57	1.51
3	A	492	FAD	C4X-N5	3.51	1.38	1.30
3	C	492	FAD	PA-O3P	3.04	1.62	1.59
3	D	492	FAD	C2'-C3'	-3.02	1.48	1.53
3	C	492	FAD	C10-N1	2.81	1.38	1.33
3	B	492	FAD	C4X-N5	2.69	1.36	1.30
3	B	492	FAD	O4B-C4B	-2.67	1.39	1.45
3	D	492	FAD	C2A-N1A	2.58	1.38	1.33
3	D	492	FAD	C4'-C3'	-2.51	1.49	1.53
3	A	492	FAD	C5A-N7A	-2.43	1.34	1.39
3	D	492	FAD	C5A-N7A	-2.33	1.34	1.39
3	C	492	FAD	PA-O2A	-2.29	1.44	1.55
3	B	492	FAD	PA-O3P	2.17	1.61	1.59
3	A	492	FAD	C2A-N1A	2.02	1.37	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	492	FAD	O4'-C4'-C5'	-8.62	90.97	109.99
3	D	492	FAD	C4'-C3'-C2'	8.18	127.18	113.57
3	C	492	FAD	N3A-C2A-N1A	-5.69	119.97	128.58
3	D	492	FAD	C5'-C4'-C3'	-4.91	102.95	112.22
3	D	492	FAD	N3A-C2A-N1A	-4.83	121.27	128.58
3	D	492	FAD	O4'-C4'-C3'	4.74	120.35	109.25
3	C	492	FAD	C4X-C10-N10	4.25	122.57	116.48
3	C	492	FAD	C9A-N10-C10	-3.56	115.32	120.75
3	B	492	FAD	C4X-C10-N10	3.52	121.53	116.48
3	A	492	FAD	N3A-C2A-N1A	-3.48	123.31	128.58
3	B	492	FAD	N9A-C8A-N7A	-3.37	109.16	113.94
3	A	492	FAD	C4'-C3'-C2'	3.32	119.09	113.57
3	A	492	FAD	C3B-C2B-C1B	-3.27	95.27	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	492	FAD	O4'-C4'-C3'	3.22	116.78	109.25
3	D	492	FAD	C4X-C10-N10	3.15	121.00	116.48
3	A	492	FAD	O3B-C3B-C4B	3.14	120.09	111.08
3	D	492	FAD	N9A-C8A-N7A	-3.13	109.49	113.94
3	B	492	FAD	N3A-C2A-N1A	-3.13	123.85	128.58
3	B	492	FAD	O3B-C3B-C4B	3.09	119.95	111.08
3	B	492	FAD	C5B-C4B-C3B	3.01	126.03	115.21
3	C	492	FAD	N9A-C8A-N7A	-3.00	109.67	113.94
3	A	492	FAD	N9A-C8A-N7A	-2.98	109.71	113.94
3	A	492	FAD	C10-C4X-N5	-2.89	118.92	124.81
3	A	492	FAD	C5A-N7A-C8A	2.88	107.98	103.45
3	C	492	FAD	C3B-C2B-C1B	-2.88	96.01	101.46
3	B	492	FAD	O2A-PA-O1A	2.88	125.83	112.44
3	A	492	FAD	C4X-C10-N10	2.84	120.55	116.48
3	B	492	FAD	C5A-C4A-N3A	-2.82	122.84	126.72
3	A	492	FAD	C5A-C4A-N3A	-2.81	122.85	126.72
3	D	492	FAD	C5A-N7A-C8A	2.78	107.81	103.45
3	B	492	FAD	C5A-N7A-C8A	2.73	107.75	103.45
3	B	492	FAD	C4A-C5A-N7A	-2.72	107.47	110.58
3	D	492	FAD	C4-N3-C2	-2.65	120.93	125.64
3	C	492	FAD	C5A-N7A-C8A	2.64	107.60	103.45
3	C	492	FAD	O3B-C3B-C4B	2.61	118.59	111.08
3	A	492	FAD	C5B-C4B-C3B	2.60	124.56	115.21
3	C	492	FAD	C2A-N3A-C4A	2.60	118.17	111.83
3	A	492	FAD	C4A-C5A-N7A	-2.59	107.62	110.58
3	C	492	FAD	C10-C4X-N5	-2.57	119.56	124.81
3	D	492	FAD	C10-C4X-N5	-2.53	119.64	124.81
3	C	492	FAD	O2A-PA-O1A	2.48	124.00	112.44
3	A	492	FAD	C4-C4X-N5	2.48	121.63	118.21
3	C	492	FAD	C4-N3-C2	-2.44	121.31	125.64
3	D	492	FAD	O3B-C3B-C4B	2.31	117.72	111.08
3	B	492	FAD	C10-C4X-N5	-2.28	120.15	124.81
3	D	492	FAD	O3'-C3'-C4'	2.27	114.09	108.93
3	D	492	FAD	C2A-N1A-C6A	2.26	122.45	118.73
3	B	492	FAD	C6A-C5A-C4A	2.26	120.26	117.18
3	D	492	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
3	C	492	FAD	C2A-N1A-C6A	2.23	122.39	118.73
3	A	492	FAD	C1'-N10-C9A	-2.22	116.31	120.63
3	C	492	FAD	C5A-C4A-N3A	-2.17	123.72	126.72
3	A	492	FAD	C6A-C5A-C4A	2.16	120.13	117.18
3	D	492	FAD	C3B-C2B-C1B	-2.15	97.39	101.46
3	D	492	FAD	C4X-C10-N1	-2.13	119.36	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	492	FAD	C5B-C4B-C3B	2.13	122.88	115.21
3	C	492	FAD	C4A-C5A-N7A	-2.13	108.15	110.58
3	C	492	FAD	C5B-C4B-C3B	2.05	122.60	115.21
3	C	492	FAD	O4B-C1B-N9A	-2.05	104.16	108.09
3	B	492	FAD	O4-C4-C4X	-2.05	121.13	126.53
3	B	492	FAD	C9A-N10-C10	-2.04	117.64	120.75
3	D	492	FAD	C4X-C4-N3	2.03	118.41	113.25
3	B	492	FAD	C5'-C4'-C3'	2.02	116.03	112.22

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	492	FAD	C2'-C1'-N10-C10
3	B	492	FAD	C2'-C1'-N10-C10
3	C	492	FAD	C5B-O5B-PA-O2A
3	C	492	FAD	C2'-C1'-N10-C10
3	D	492	FAD	C5B-O5B-PA-O2A
3	D	492	FAD	C1'-C2'-C3'-C4'
3	D	492	FAD	O2'-C2'-C3'-C4'
3	D	492	FAD	C3'-C4'-C5'-O5'
3	D	492	FAD	O4'-C4'-C5'-O5'
3	D	492	FAD	C2'-C3'-C4'-O4'
3	D	492	FAD	C2'-C3'-C4'-C5'
3	D	492	FAD	O3'-C3'-C4'-C5'
3	D	492	FAD	C5B-O5B-PA-O3P
3	D	492	FAD	C4'-C5'-O5'-P
3	B	492	FAD	N10-C1'-C2'-O2'

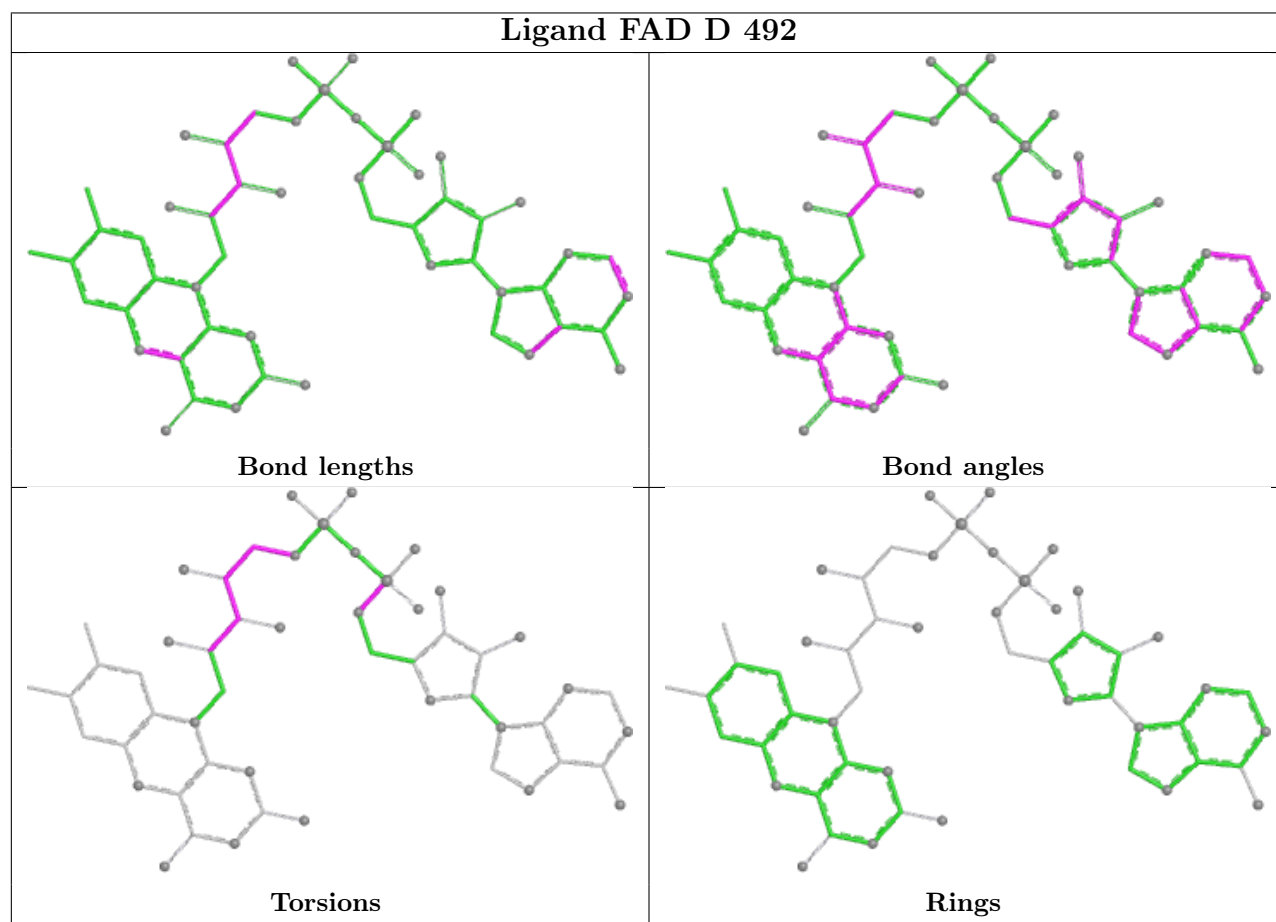
There are no ring outliers.

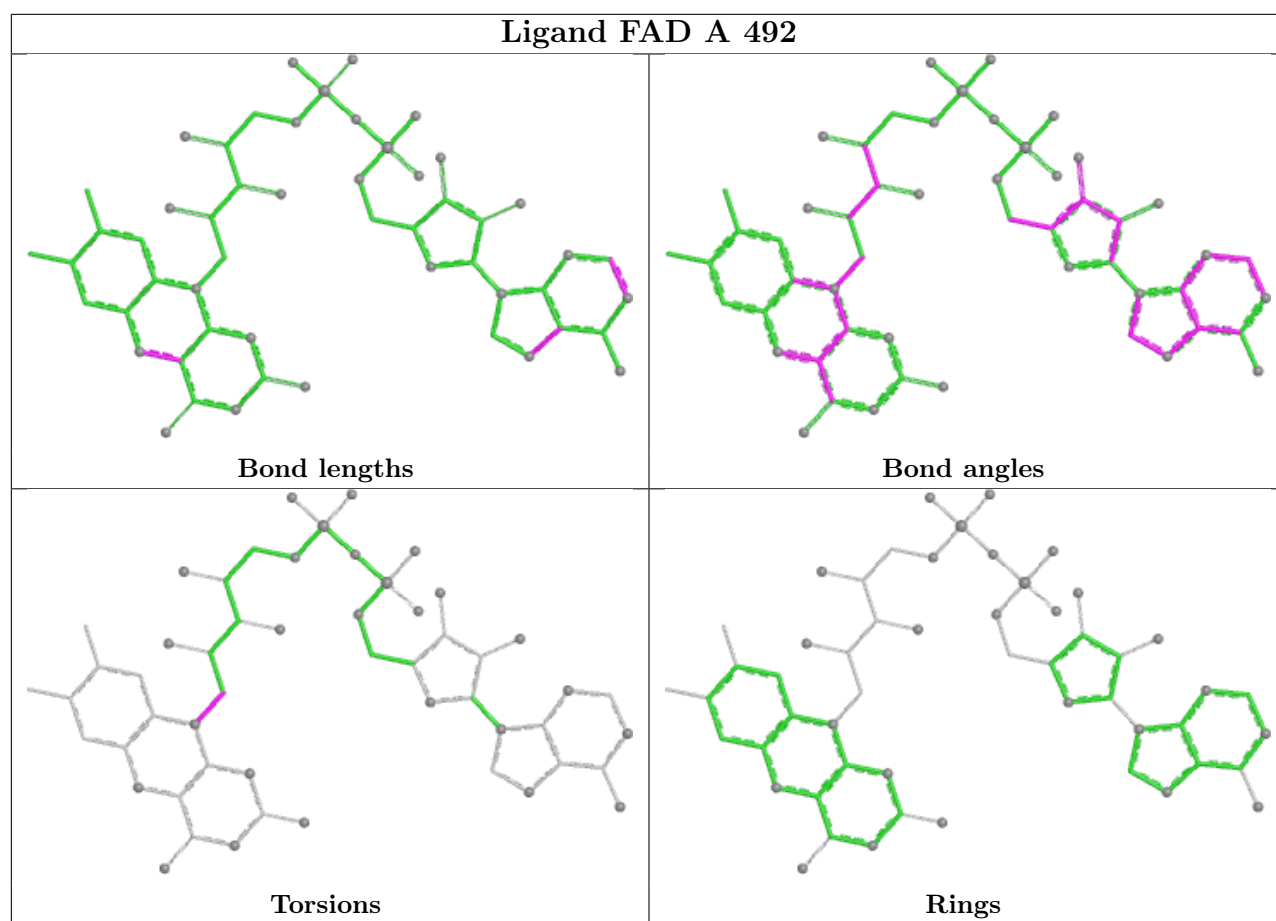
2 monomers are involved in 2 short contacts:

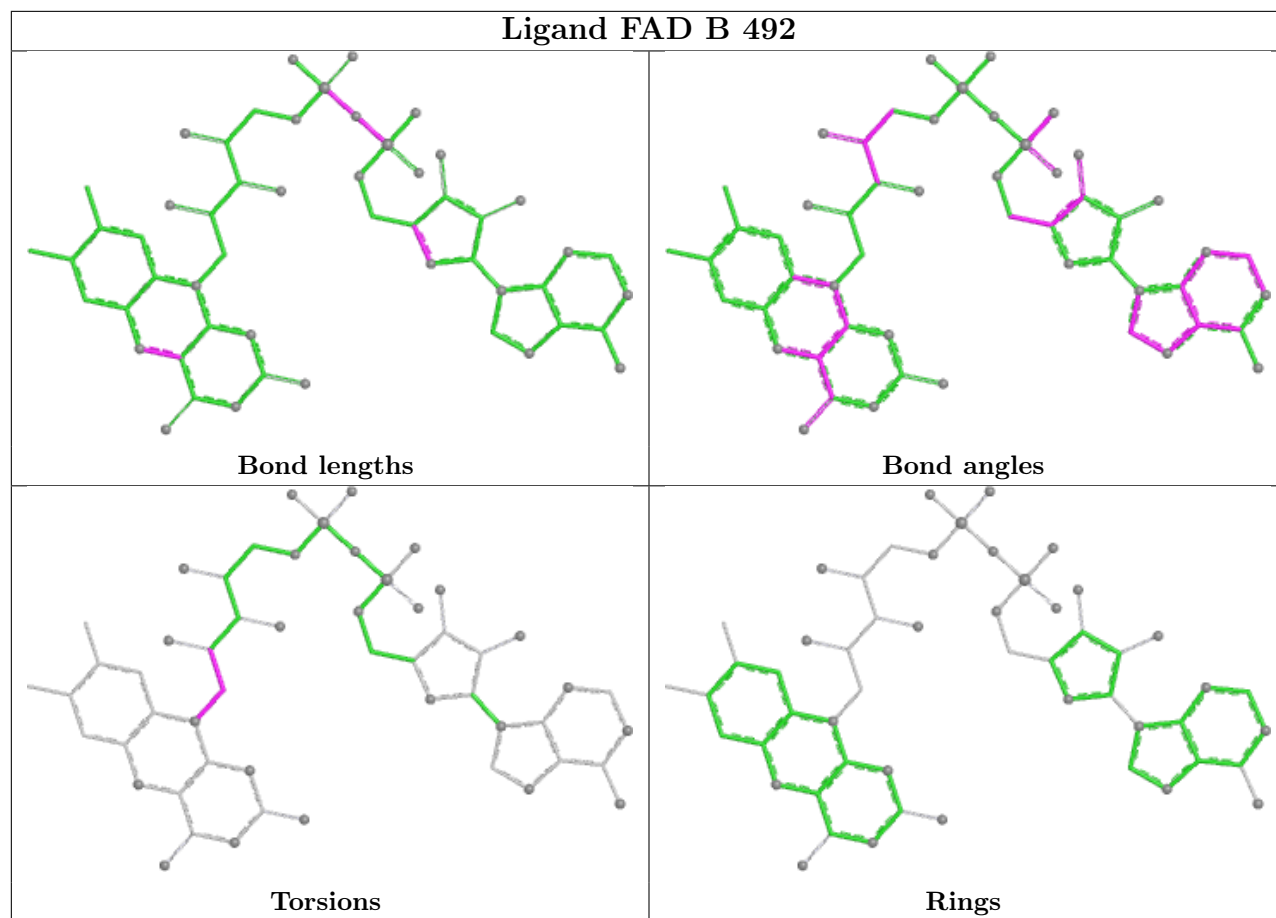
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	492	FAD	1	0
2	C	491	SF4	1	0

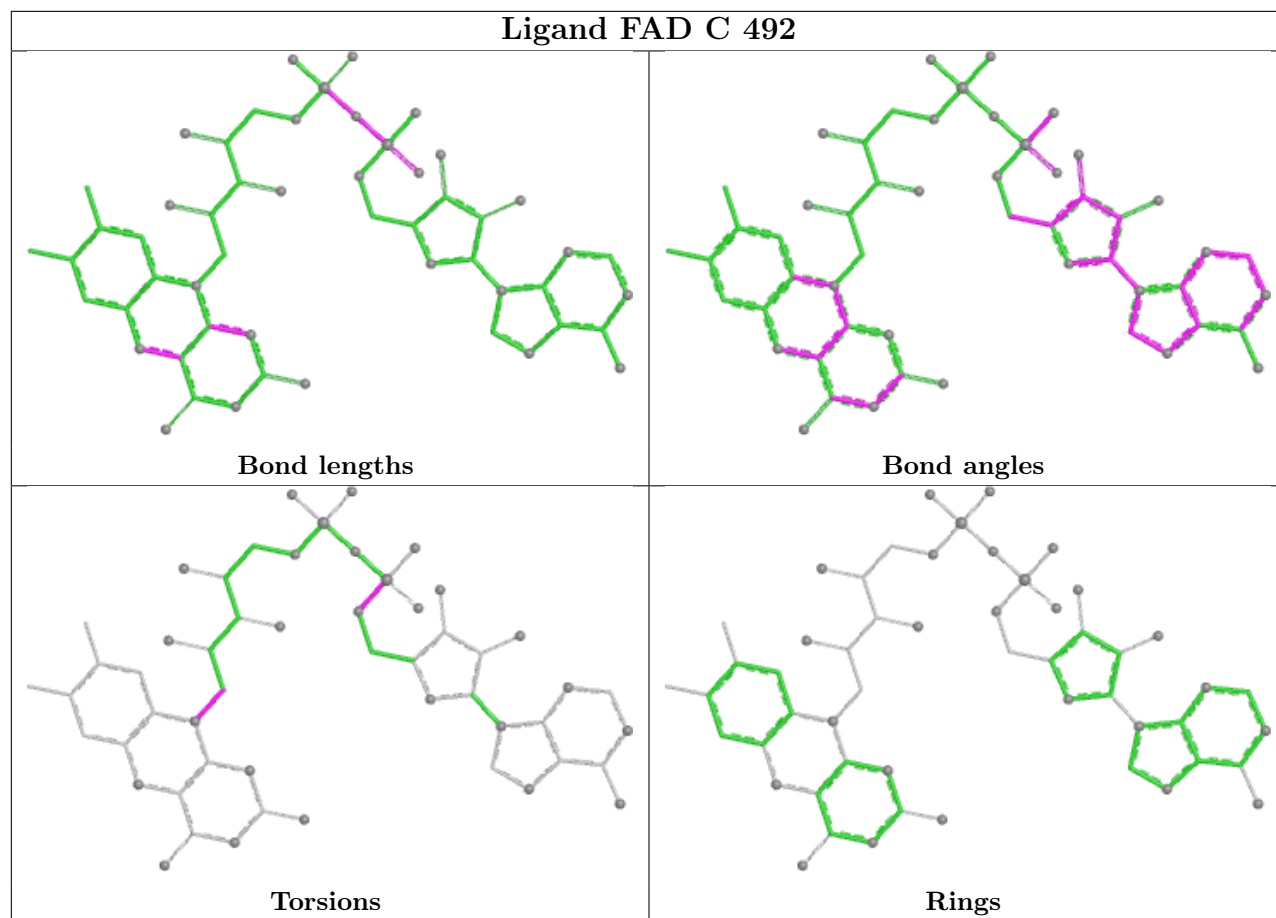
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/490 (100%)	0.08	11 (2%) 62 66	11, 23, 44, 78	1 (0%)
1	B	490/490 (100%)	-0.07	6 (1%) 76 80	8, 20, 37, 69	1 (0%)
1	C	490/490 (100%)	-0.40	3 (0%) 85 88	10, 16, 29, 83	1 (0%)
1	D	490/490 (100%)	-0.28	5 (1%) 79 83	11, 18, 34, 73	0
All	All	1960/1960 (100%)	-0.17	25 (1%) 75 79	8, 19, 37, 83	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	ALA	4.2
1	B	490	LYS	3.7
1	B	43	ARG	3.2
1	A	490	LYS	3.0
1	C	43	ARG	2.9
1	B	402	LYS	2.9
1	D	14	LYS	2.9
1	A	126	ASN	2.8
1	A	175	LYS	2.7
1	C	177	GLU	2.7
1	C	490	LYS	2.6
1	D	1	MET	2.6
1	D	490	LYS	2.5
1	A	43	ARG	2.5
1	A	256	GLN	2.4
1	D	256	GLN	2.4
1	B	56	ASP	2.4
1	D	43	ARG	2.2
1	A	61	LYS	2.2
1	A	10	GLU	2.2
1	B	126	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	14	LYS	2.1
1	A	6	GLU	2.1
1	A	177	GLU	2.0
1	A	67	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

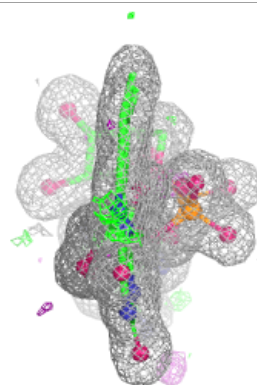
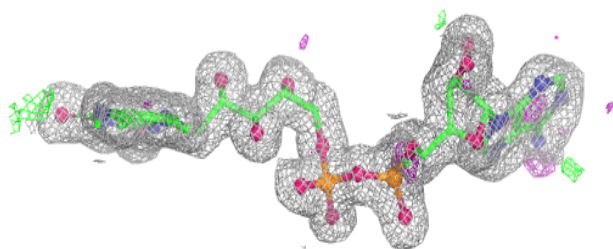
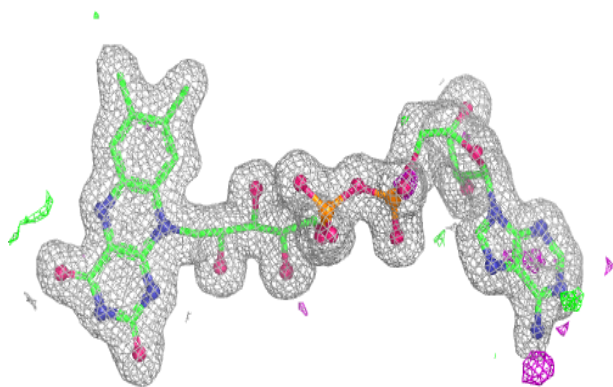
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	A	492	53/53	0.97	0.06	14,19,27,38	0
3	FAD	B	492	53/53	0.98	0.06	10,16,32,37	0
3	FAD	C	492	53/53	0.98	0.06	10,15,28,41	0
3	FAD	D	492	53/53	0.98	0.06	11,16,28,43	0
2	SF4	A	491	8/8	0.99	0.04	21,23,27,27	0
2	SF4	B	491	8/8	0.99	0.04	18,22,24,25	0
2	SF4	C	491	8/8	0.99	0.06	15,19,21,22	0
2	SF4	D	491	8/8	0.99	0.04	18,21,24,25	0

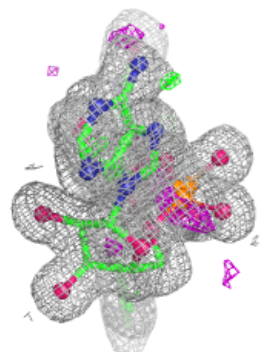
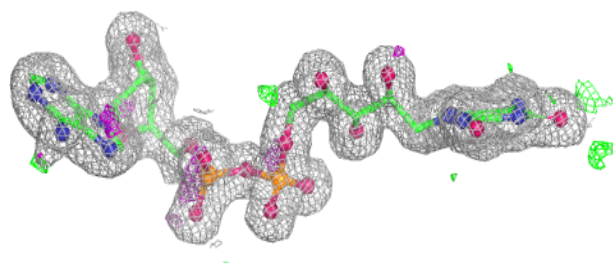
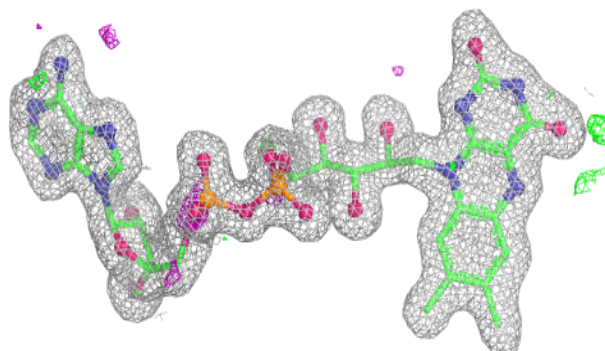
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 492:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

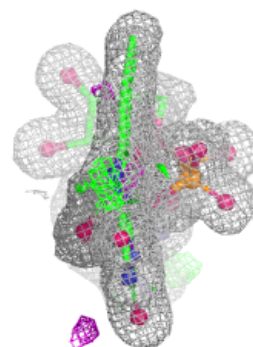
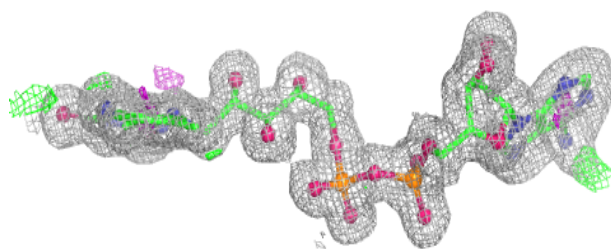
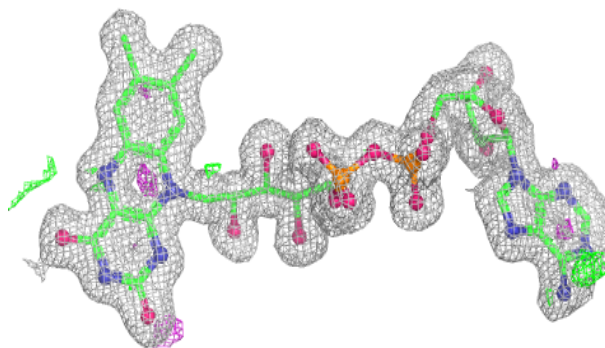
**Electron density around FAD B 492:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

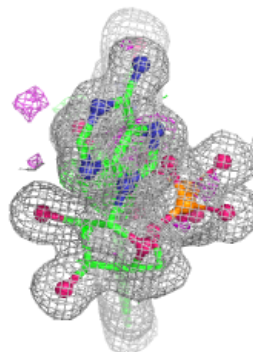
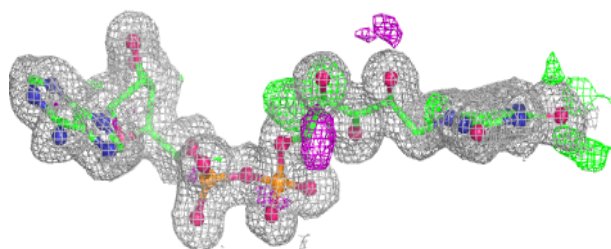
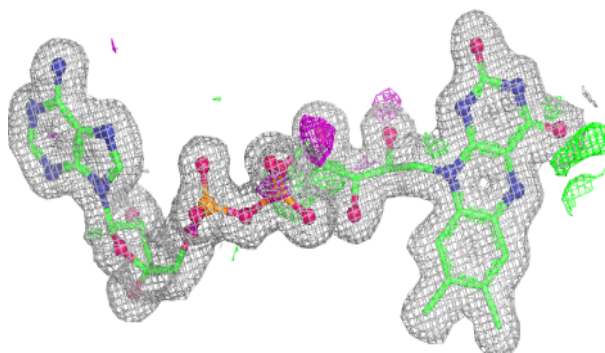


Electron density around FAD C 492:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD D 492:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.