



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:12 pm BST

PDB ID : 6C71
Title : Nicotine Oxidoreductase in Complex with S-nicotine
Authors : Tararina, M.A.; Allen, K.N.
Deposited on : 2018-01-19
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

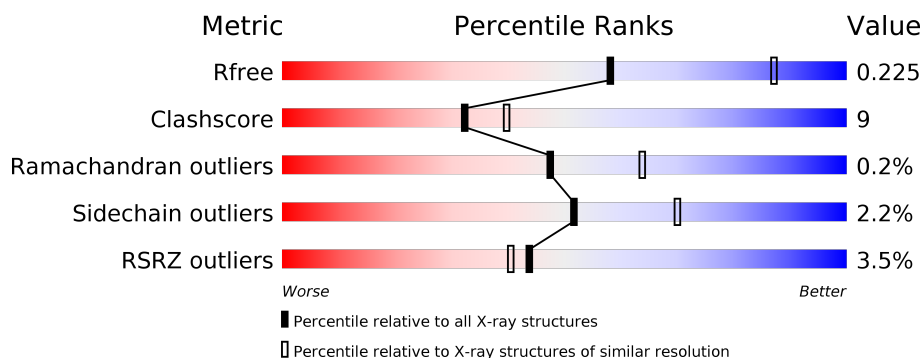
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 on 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	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	490	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	490	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	490	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>22%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14002 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 Amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3354	2126	583	633	12			
1	B	440	Total	C	N	O	S	0	0	0
			3431	2173	603	643	12			
1	C	440	Total	C	N	O	S	0	0	0
			3425	2169	601	643	12			
1	D	439	Total	C	N	O	S	0	0	0
			3427	2171	602	642	12			

There are 32 discrepancies between the modelled and reference sequences:

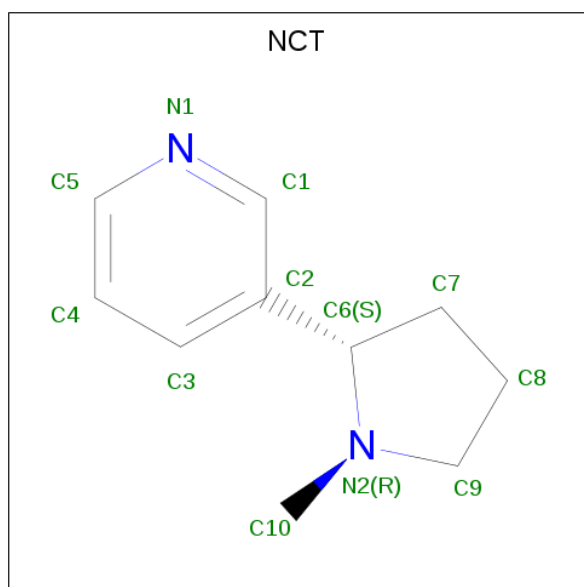
Chain	Residue	Modelled	Actual	Comment	Reference
A	483	LEU	-	expression tag	UNP F8G0P2
A	484	GLU	-	expression tag	UNP F8G0P2
A	485	HIS	-	expression tag	UNP F8G0P2
A	486	HIS	-	expression tag	UNP F8G0P2
A	487	HIS	-	expression tag	UNP F8G0P2
A	488	HIS	-	expression tag	UNP F8G0P2
A	489	HIS	-	expression tag	UNP F8G0P2
A	490	HIS	-	expression tag	UNP F8G0P2
B	483	LEU	-	expression tag	UNP F8G0P2
B	484	GLU	-	expression tag	UNP F8G0P2
B	485	HIS	-	expression tag	UNP F8G0P2
B	486	HIS	-	expression tag	UNP F8G0P2
B	487	HIS	-	expression tag	UNP F8G0P2
B	488	HIS	-	expression tag	UNP F8G0P2
B	489	HIS	-	expression tag	UNP F8G0P2
B	490	HIS	-	expression tag	UNP F8G0P2
C	483	LEU	-	expression tag	UNP F8G0P2
C	484	GLU	-	expression tag	UNP F8G0P2
C	485	HIS	-	expression tag	UNP F8G0P2
C	486	HIS	-	expression tag	UNP F8G0P2
C	487	HIS	-	expression tag	UNP F8G0P2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	488	HIS	-	expression tag	UNP F8G0P2
C	489	HIS	-	expression tag	UNP F8G0P2
C	490	HIS	-	expression tag	UNP F8G0P2
D	483	LEU	-	expression tag	UNP F8G0P2
D	484	GLU	-	expression tag	UNP F8G0P2
D	485	HIS	-	expression tag	UNP F8G0P2
D	486	HIS	-	expression tag	UNP F8G0P2
D	487	HIS	-	expression tag	UNP F8G0P2
D	488	HIS	-	expression tag	UNP F8G0P2
D	489	HIS	-	expression tag	UNP F8G0P2
D	490	HIS	-	expression tag	UNP F8G0P2

- Molecule 2 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: C₁₀H₁₄N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			12	10	2		
2	B	1	Total	C	N	0	0
			12	10	2		
2	C	1	Total	C	N	0	0
			12	10	2		
2	D	1	Total	C	N	0	0
			12	10	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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		

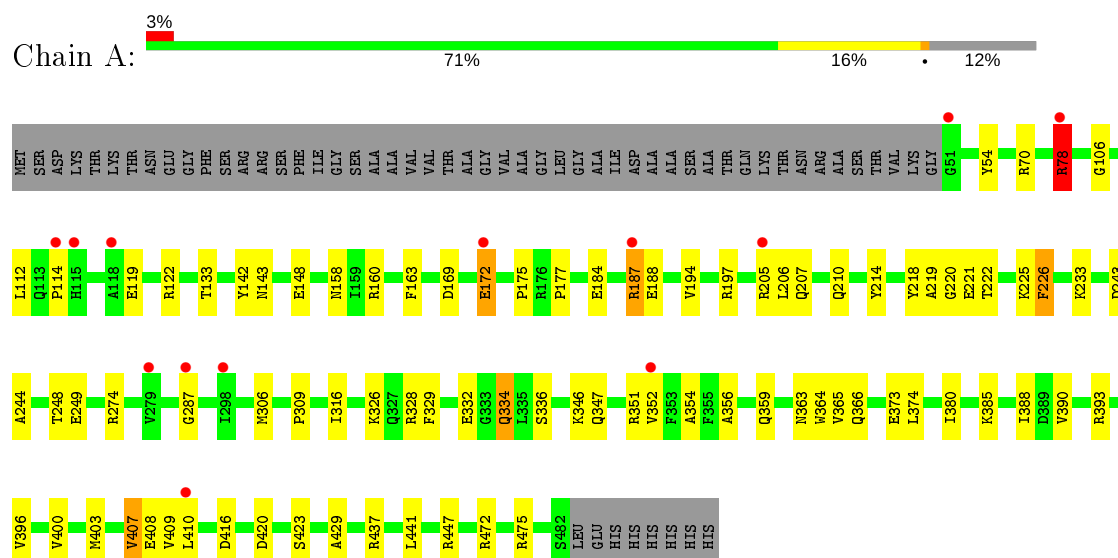
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	24	Total	O	0	0
			24	24		
4	C	38	Total	O	0	0
			38	38		
4	D	15	Total	O	0	0
			15	15		

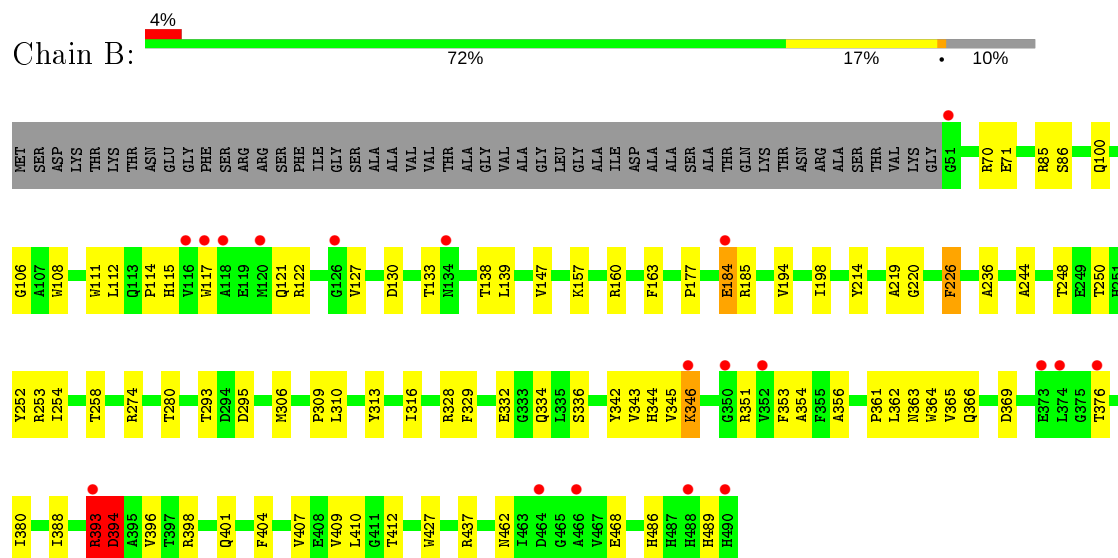
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

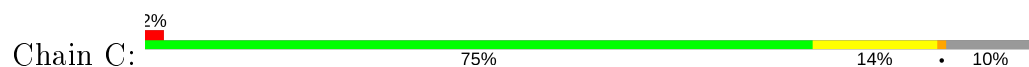
• Molecule 1: Amine oxidase

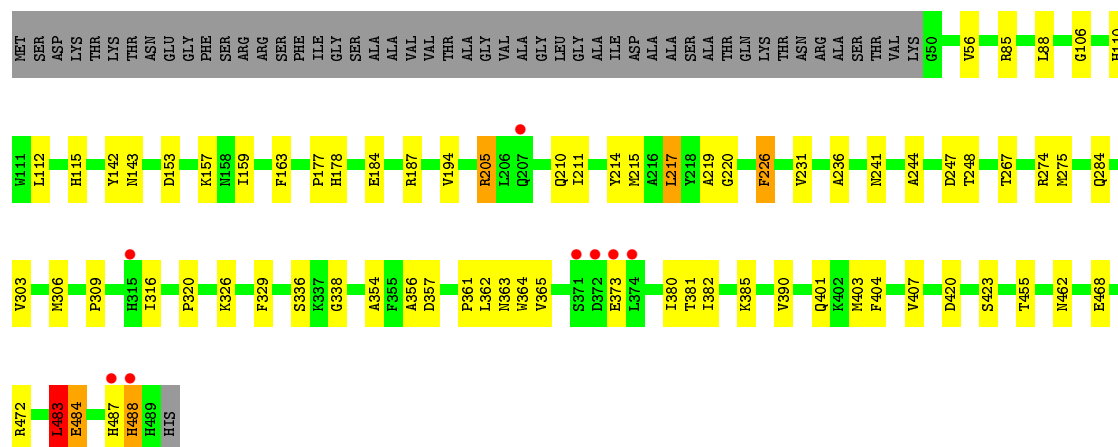


• Molecule 1: Amine oxidase

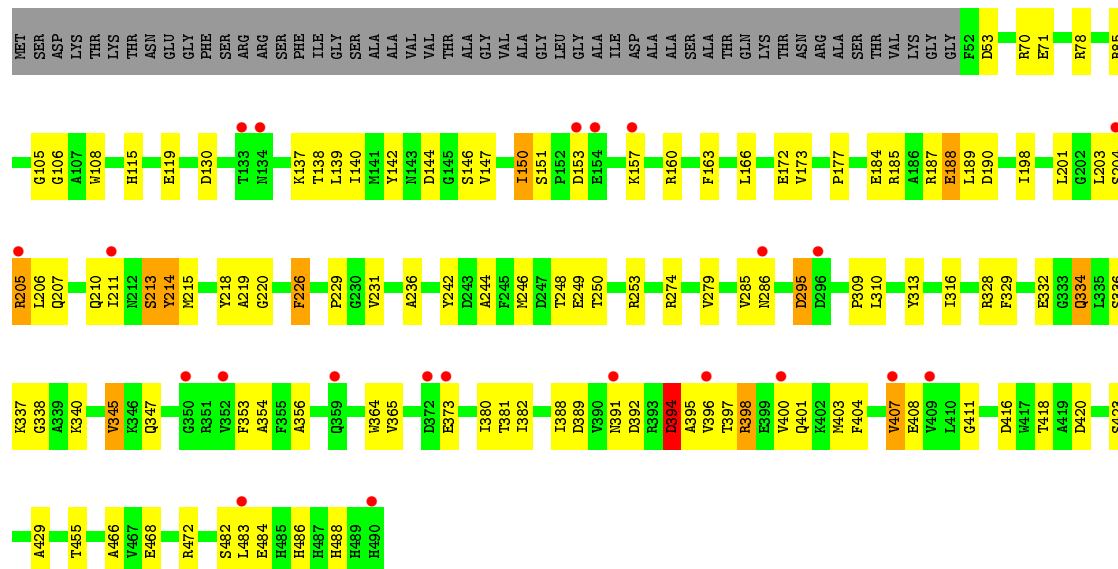


• Molecule 1: Amine oxidase





• Molecule 1: Amine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.76Å 135.10Å 167.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.76 – 2.65 43.38 – 2.65	Depositor EDS
% Data completeness (in resolution range)	92.7 (37.76-2.65) 91.8 (43.38-2.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.192 , 0.226 0.192 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14002	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: NCT, 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	0.34	0/3425	0.67	13/4639 (0.3%)
1	B	0.40	3/3508 (0.1%)	0.67	6/4752 (0.1%)
1	C	0.29	0/3501	0.52	1/4742 (0.0%)
1	D	0.41	3/3504 (0.1%)	0.76	16/4747 (0.3%)
All	All	0.36	6/13938 (0.0%)	0.66	36/18880 (0.2%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	GLU	CB-CG	7.54	1.66	1.52
1	B	393	ARG	CB-CG	-6.36	1.35	1.52
1	D	398	ARG	CB-CG	-5.28	1.38	1.52
1	D	150	ILE	CB-CG2	5.22	1.69	1.52
1	D	188	GLU	CB-CG	5.10	1.61	1.52
1	B	409	VAL	CB-CG1	5.10	1.63	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ARG	NE-CZ-NH1	-15.79	112.40	120.30
1	D	398	ARG	CG-CD-NE	-10.95	88.82	111.80
1	D	205	ARG	NE-CZ-NH1	10.44	125.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	187	ARG	CD-NE-CZ	9.88	137.43	123.60
1	A	187	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	B	185	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	D	187	ARG	CB-CG-CD	-8.55	89.38	111.60
1	B	185	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	409	VAL	CG1-CB-CG2	7.95	123.61	110.90
1	A	187	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	D	394	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	B	394	ASP	CB-CG-OD1	-7.35	111.68	118.30
1	A	172	GLU	CB-CA-C	-6.74	96.93	110.40
1	A	187	ARG	C-N-CA	-6.63	105.12	121.70
1	D	407	VAL	CG1-CB-CG2	6.40	121.14	110.90
1	D	188	GLU	CB-CA-C	-6.36	97.68	110.40
1	D	205	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	78	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	295	ASP	CB-CG-OD1	6.29	123.97	118.30
1	A	78	ARG	CB-CG-CD	-6.20	95.47	111.60
1	A	188	GLU	CB-CG-CD	-5.97	98.08	114.20
1	A	407	VAL	CG1-CB-CG2	5.95	120.42	110.90
1	B	184	GLU	CB-CA-C	5.90	122.21	110.40
1	D	373	GLU	CB-CA-C	-5.82	98.77	110.40
1	D	188	GLU	N-CA-CB	5.80	121.05	110.60
1	D	398	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	D	345	VAL	CG1-CB-CG2	5.62	119.89	110.90
1	C	483	LEU	CA-CB-CG	5.39	127.69	115.30
1	D	337	LYS	CB-CA-C	5.31	121.03	110.40
1	D	150	ILE	CG1-CB-CG2	5.30	123.06	111.40
1	A	194	VAL	CG1-CB-CG2	5.25	119.30	110.90
1	A	78	ARG	CA-CB-CG	5.21	124.86	113.40
1	A	188	GLU	CA-CB-CG	5.10	124.63	113.40
1	D	187	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	78	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	393	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3354	0	3296	62	0
1	B	3431	0	3355	60	1
1	C	3425	0	3351	48	0
1	D	3427	0	3352	84	1
2	A	12	0	14	0	0
2	B	12	0	14	0	0
2	C	12	0	14	0	0
2	D	12	0	14	1	0
3	A	53	0	31	2	0
3	B	53	0	31	3	0
3	C	53	0	31	3	0
3	D	53	0	31	4	0
4	A	28	0	0	3	0
4	B	24	0	0	1	0
4	C	38	0	0	1	0
4	D	15	0	0	2	0
All	All	14002	0	13534	242	1

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 9.

All (242) 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:54:TYR:CD1	1:A:78:ARG:NH2	1.94	1.33
1:A:54:TYR:CE1	1:A:78:ARG:NH2	2.07	1.22
1:D:142:TYR:OH	1:D:205:ARG:NH1	2.02	0.91
1:D:347:GLN:HE22	1:D:408:GLU:H	1.15	0.91
1:D:401:GLN:HG2	1:D:407:VAL:HG22	1.54	0.89
1:D:140:ILE:HD13	1:D:206:LEU:HD12	1.54	0.87
1:A:142:TYR:OH	1:A:205:ARG:NH1	2.11	0.84
1:A:158:ASN:HB3	1:A:210:GLN:HE22	1.48	0.77
1:D:395:ALA:HA	1:D:398:ARG:NH2	1.98	0.77
1:D:70:ARG:NH1	1:D:71:GLU:OE2	2.17	0.77
1:B:70:ARG:NH1	1:B:71:GLU:OE2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:HA	1:A:187:ARG:HD2	1.68	0.76
1:A:205:ARG:NH1	1:A:206:LEU:HB2	2.02	0.75
1:C:110:HIS:HD2	1:C:112:LEU:H	1.35	0.73
1:A:78:ARG:NH1	1:D:295:ASP:OD2	2.22	0.73
1:D:185:ARG:HA	1:D:188:GLU:HB2	1.72	0.72
1:D:279:VAL:O	1:D:316:ILE:HD13	1.91	0.70
1:D:130:ASP:OD1	1:D:253:ARG:NH1	2.26	0.69
1:D:389:ASP:OD1	1:D:391:ASN:HB2	1.91	0.69
1:A:346:LYS:HG3	1:A:410:LEU:HD11	1.76	0.68
1:B:85:ARG:NH2	4:B:602:HOH:O	2.26	0.68
1:D:316:ILE:HD11	3:D:502:FAD:N6A	2.09	0.68
1:A:205:ARG:HG3	1:A:206:LEU:N	2.08	0.67
1:A:274:ARG:HG2	1:D:274:ARG:HG2	1.74	0.67
1:B:274:ARG:HG2	1:C:274:ARG:HG2	1.75	0.67
1:B:130:ASP:OD1	1:B:253:ARG:NH1	2.28	0.67
1:B:342:TYR:O	1:B:412:THR:HA	1.94	0.66
1:D:397:THR:O	1:D:401:GLN:HG3	1.96	0.66
1:D:105:GLY:O	4:D:601:HOH:O	2.13	0.66
1:B:354:ALA:HB3	1:B:365:VAL:HB	1.78	0.65
1:C:455:THR:O	1:C:472:ARG:NH2	2.30	0.65
1:C:241:ASN:ND2	1:C:244:ALA:H	1.95	0.65
1:A:122:ARG:HH22	1:B:122:ARG:HH22	1.43	0.64
1:C:487:HIS:O	1:C:488:HIS:HB2	1.98	0.64
1:D:347:GLN:N	1:D:347:GLN:OE1	2.29	0.64
1:B:394:ASP:HB3	1:B:398:ARG:NH1	2.15	0.62
1:B:486:HIS:CE1	1:D:391:ASN:OD1	2.53	0.62
1:D:53:ASP:O	1:D:78:ARG:NH1	2.33	0.61
1:A:233:LYS:NZ	4:A:602:HOH:O	2.33	0.61
1:A:472:ARG:HG3	1:A:475:ARG:NH2	2.15	0.61
1:B:334:GLN:NE2	1:B:427:TRP:O	2.34	0.61
1:B:127:VAL:HB	1:B:252:TYR:HB3	1.80	0.60
1:B:345:VAL:HG21	1:B:407:VAL:HB	1.83	0.60
1:C:194:VAL:HG11	1:C:215:MET:HE2	1.83	0.60
1:D:396:VAL:O	1:D:400:VAL:HG12	2.01	0.60
1:C:217:LEU:HD13	1:C:364:TRP:HB2	1.86	0.58
1:A:309:PRO:HD3	3:A:502:FAD:H51A	1.86	0.58
1:C:309:PRO:HD3	3:C:502:FAD:H51A	1.85	0.57
1:A:220:GLY:HA3	1:A:336:SER:HA	1.86	0.57
1:C:362:LEU:HD22	1:C:380:ILE:HG21	1.85	0.57
1:A:385:LYS:HE2	1:A:390:VAL:HG22	1.86	0.57
1:D:455:THR:O	1:D:472:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ARG:HG3	1:D:206:LEU:N	2.20	0.57
1:C:88:LEU:HG	1:C:275:MET:HE1	1.87	0.56
1:A:122:ARG:NH2	4:A:605:HOH:O	2.37	0.56
1:A:148:GLU:OE2	1:A:205:ARG:NH2	2.39	0.56
1:C:215:MET:HE3	1:C:231:VAL:HG21	1.86	0.56
1:A:354:ALA:HB3	1:A:365:VAL:HB	1.88	0.55
1:A:207:GLN:HA	1:A:210:GLN:HE21	1.72	0.55
1:B:100:GLN:NE2	1:B:369:ASP:OD2	2.36	0.55
1:C:178:HIS:ND1	4:C:601:HOH:O	2.33	0.55
1:A:326:LYS:NZ	1:A:441:LEU:O	2.39	0.55
1:B:220:GLY:HA3	1:B:336:SER:HA	1.89	0.55
1:D:185:ARG:HG3	1:D:189:LEU:HD13	1.88	0.55
1:D:213:SER:OG	1:D:356:ALA:O	2.23	0.55
1:B:250:THR:OG1	1:B:366:GLN:OE1	2.17	0.54
1:D:138:THR:HA	1:D:353:PHE:O	2.07	0.54
1:D:218:TYR:OH	1:D:249:GLU:OE1	2.24	0.54
1:D:347:GLN:NE2	1:D:408:GLU:H	1.97	0.54
1:D:85:ARG:NH1	1:D:420:ASP:OD2	2.41	0.54
1:D:85:ARG:NH2	4:D:604:HOH:O	2.40	0.54
1:B:133:THR:O	1:B:351:ARG:NH1	2.37	0.54
1:C:354:ALA:HB3	1:C:365:VAL:HB	1.89	0.54
1:A:160:ARG:NH1	1:A:243:ASP:OD2	2.31	0.53
1:A:388:ILE:HD11	1:A:396:VAL:HG12	1.89	0.53
1:A:475:ARG:NH1	1:B:121:GLN:O	2.40	0.53
1:A:143:ASN:HB3	1:A:359:GLN:HE21	1.74	0.53
1:B:393:ARG:HA	1:B:396:VAL:HG22	1.90	0.53
1:D:388:ILE:HD11	1:D:396:VAL:HG12	1.91	0.53
1:D:364:TRP:O	1:D:380:ILE:HA	2.09	0.53
1:C:110:HIS:CD2	1:C:112:LEU:H	2.20	0.53
1:D:347:GLN:HE22	1:D:408:GLU:N	1.95	0.53
1:D:309:PRO:HD3	3:D:502:FAD:H51A	1.91	0.53
1:C:385:LYS:HE2	1:C:390:VAL:HG22	1.90	0.52
1:C:401:GLN:HA	1:C:404:PHE:O	2.10	0.52
1:A:328:ARG:O	1:A:332:GLU:HG3	2.09	0.52
1:D:328:ARG:O	1:D:332:GLU:HG3	2.10	0.52
1:C:211:ILE:O	1:C:215:MET:HG2	2.10	0.52
1:A:106:GLY:HA2	3:A:502:FAD:C4X	2.40	0.51
1:A:205:ARG:CG	1:A:206:LEU:N	2.74	0.51
1:B:293:THR:OG1	1:B:295:ASP:OD1	2.28	0.51
1:B:309:PRO:HD3	3:B:502:FAD:H51A	1.93	0.51
1:B:86:SER:OG	1:C:267:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:VAL:CG2	1:B:407:VAL:HB	2.40	0.51
1:D:70:ARG:NH2	1:D:119:GLU:OE2	2.45	0.50
1:A:206:LEU:HG	1:A:210:GLN:NE2	2.26	0.50
1:A:206:LEU:O	1:A:210:GLN:HG3	2.11	0.50
1:C:244:ALA:O	1:C:248:THR:HG23	2.11	0.50
1:D:220:GLY:HA3	1:D:336:SER:HA	1.93	0.50
1:B:280:THR:O	1:B:316:ILE:HA	2.12	0.49
1:C:483:LEU:HD22	1:C:484:GLU:HB3	1.93	0.49
1:A:169:ASP:OD1	1:A:197:ARG:NH1	2.42	0.49
1:D:184:GLU:CD	1:D:184:GLU:H	2.15	0.49
1:C:184:GLU:OE1	1:C:187:ARG:NH2	2.46	0.49
1:A:112:LEU:HD22	1:B:112:LEU:HD22	1.93	0.49
1:D:215:MET:HE1	1:D:231:VAL:HG21	1.93	0.49
1:B:362:LEU:HD22	1:B:380:ILE:HG21	1.95	0.49
1:D:198:ILE:HA	1:D:201:LEU:HG	1.94	0.48
1:A:221:GLU:HG2	1:A:225:LYS:HD2	1.95	0.48
1:A:347:GLN:HE22	1:A:408:GLU:H	1.60	0.48
1:B:139:LEU:HD23	1:B:147:VAL:HG11	1.95	0.48
1:D:214:TYR:HE2	1:D:246:MET:HE1	1.79	0.48
1:A:221:GLU:HG3	1:A:222:THR:H	1.78	0.48
1:C:215:MET:HE1	1:C:231:VAL:HG11	1.94	0.48
1:D:206:LEU:O	1:D:210:GLN:HG3	2.14	0.48
1:D:173:VAL:HG22	1:D:185:ARG:HG2	1.95	0.48
1:A:244:ALA:O	1:A:248:THR:HG23	2.13	0.48
1:B:244:ALA:O	1:B:248:THR:HG23	2.13	0.48
1:D:166:LEU:HA	1:D:201:LEU:HD21	1.96	0.48
1:A:393:ARG:HH11	1:A:409:VAL:HG12	1.78	0.48
1:B:157:LYS:HD3	1:B:160:ARG:HH21	1.77	0.48
1:A:364:TRP:O	1:A:380:ILE:HA	2.14	0.48
1:A:400:VAL:HG12	1:A:407:VAL:HG21	1.96	0.48
1:B:138:THR:HA	1:B:353:PHE:O	2.14	0.47
1:C:220:GLY:HA3	1:C:336:SER:HA	1.96	0.47
1:D:150:ILE:HG22	1:D:151:SER:N	2.30	0.47
1:D:106:GLY:HA2	3:D:502:FAD:C4X	2.44	0.47
1:D:244:ALA:O	1:D:248:THR:HG23	2.13	0.47
1:D:140:ILE:O	1:D:147:VAL:HA	2.15	0.47
1:D:177:PRO:HG3	1:D:236:ALA:HB1	1.96	0.47
1:A:420:ASP:HB3	1:A:423:SER:OG	2.14	0.47
4:A:605:HOH:O	1:B:122:ARG:NH2	2.42	0.47
1:C:106:GLY:HA2	3:C:502:FAD:C4X	2.44	0.47
1:B:404:PHE:O	1:B:407:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ALA:HB3	1:C:363:ASN:HA	1.96	0.47
1:A:356:ALA:HB3	1:A:363:ASN:HA	1.96	0.47
1:D:285:VAL:CG1	1:D:286:ASN:H	2.28	0.47
1:B:332:GLU:OE1	1:B:437:ARG:NH2	2.48	0.46
1:C:143:ASN:OD1	1:C:357:ASP:HB3	2.15	0.46
1:C:420:ASP:HB3	1:C:423:SER:OG	2.15	0.46
1:B:328:ARG:O	1:B:332:GLU:HG3	2.15	0.46
1:C:85:ARG:HH21	1:C:420:ASP:CG	2.19	0.46
1:A:393:ARG:NH1	1:A:409:VAL:HG12	2.31	0.46
1:B:388:ILE:HD11	1:B:396:VAL:HG12	1.98	0.46
1:D:285:VAL:HG12	1:D:286:ASN:N	2.31	0.46
1:B:254:ILE:HD12	1:B:258:THR:HG22	1.98	0.46
1:A:347:GLN:OE1	1:A:347:GLN:N	2.41	0.46
1:D:211:ILE:O	1:D:215:MET:HG2	2.15	0.46
1:D:420:ASP:HB3	1:D:423:SER:OG	2.16	0.46
1:D:215:MET:HB3	1:D:215:MET:HE3	1.69	0.46
1:B:310:LEU:HA	1:B:313:TYR:HD2	1.81	0.45
1:A:221:GLU:HG3	1:A:222:THR:N	2.31	0.45
1:A:287:GLY:HA2	1:A:447:ARG:NH1	2.32	0.45
1:C:215:MET:CE	1:C:231:VAL:HG21	2.47	0.45
1:D:160:ARG:HG3	1:D:242:TYR:CD2	2.51	0.45
1:B:462:ASN:HA	3:B:502:FAD:N1	2.32	0.45
1:C:153:ASP:O	1:C:157:LYS:HG3	2.16	0.45
1:D:285:VAL:CG1	1:D:286:ASN:N	2.80	0.45
1:A:393:ARG:NH1	1:A:409:VAL:O	2.50	0.45
1:C:284:GLN:HG3	1:C:320:PRO:HD2	1.99	0.45
1:B:106:GLY:HA2	3:B:502:FAD:C4X	2.48	0.44
1:C:142:TYR:CE1	1:C:205:ARG:HD2	2.52	0.44
1:D:203:LEU:N	1:D:203:LEU:HD12	2.32	0.44
1:D:354:ALA:HB3	1:D:365:VAL:HB	1.99	0.44
1:D:115:HIS:CE1	1:D:468:GLU:HB2	2.52	0.44
1:D:218:TYR:CE1	2:D:501:NCT:HC3	2.53	0.44
1:B:344:HIS:O	1:B:410:LEU:N	2.46	0.44
1:D:279:VAL:O	1:D:316:ILE:CD1	2.63	0.44
1:D:482:SER:HB2	1:D:486:HIS:CD2	2.52	0.44
1:A:332:GLU:OE2	1:A:437:ARG:NH2	2.51	0.44
1:B:343:VAL:HG13	1:B:412:THR:HG22	1.99	0.44
1:C:362:LEU:HD12	1:C:403:MET:HE1	1.99	0.44
1:D:392:ASP:OD2	1:D:394:ASP:HB2	2.17	0.44
1:A:219:ALA:HB2	1:A:226:PHE:CG	2.52	0.43
1:A:352:VAL:O	1:A:366:GLN:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ALA:HB2	1:D:226:PHE:CG	2.53	0.43
1:A:385:LYS:HE3	1:A:416:ASP:OD1	2.18	0.43
1:A:334:GLN:CG	1:A:429:ALA:H	2.31	0.43
1:B:219:ALA:HB2	1:B:226:PHE:CG	2.53	0.43
1:D:205:ARG:CG	1:D:206:LEU:N	2.81	0.43
1:D:345:VAL:CG2	1:D:407:VAL:HB	2.48	0.43
1:C:403:MET:HE3	1:C:403:MET:HB2	1.89	0.43
1:B:356:ALA:HB3	1:B:363:ASN:HA	2.01	0.43
1:B:346:LYS:HB2	1:B:410:LEU:HD21	1.99	0.43
1:B:115:HIS:CE1	1:B:468:GLU:HB2	2.54	0.43
1:C:177:PRO:HG3	1:C:236:ALA:HB1	2.00	0.43
1:C:110:HIS:CD2	1:C:248:THR:HG22	2.54	0.43
1:D:364:TRP:HB3	1:D:381:THR:OG1	2.18	0.43
1:D:108:TRP:CG	1:D:250:THR:HA	2.53	0.43
1:B:194:VAL:O	1:B:198:ILE:HG13	2.18	0.43
1:A:172:GLU:O	1:A:175:PRO:HD3	2.18	0.42
1:A:218:TYR:OH	1:A:249:GLU:OE2	2.31	0.42
1:D:215:MET:CE	1:D:231:VAL:HG21	2.49	0.42
1:D:338:GLY:HA2	1:D:382:ILE:O	2.19	0.42
1:B:334:GLN:NE2	1:B:336:SER:H	2.18	0.42
1:C:110:HIS:HE1	1:C:247:ASP:OD2	2.02	0.42
1:C:217:LEU:HD11	1:C:381:THR:HB	2.00	0.42
1:D:190:ASP:HA	1:D:229:PRO:HG2	2.02	0.42
1:D:334:GLN:CG	1:D:429:ALA:H	2.32	0.42
1:A:78:ARG:HB2	1:A:78:ARG:HE	1.32	0.42
1:D:219:ALA:HB2	1:D:226:PHE:CD2	2.55	0.42
1:B:489:HIS:HA	1:D:411:GLY:HA3	2.00	0.42
1:D:416:ASP:OD2	1:D:418:THR:OG1	2.33	0.42
1:D:483:LEU:HA	1:D:483:LEU:HD12	1.73	0.42
1:B:108:TRP:CD1	1:B:253:ARG:HG2	2.55	0.42
1:A:365:VAL:HG21	1:A:403:MET:HE1	2.01	0.42
1:D:144:ASP:OD1	1:D:146:SER:N	2.48	0.42
1:A:70:ARG:HH22	1:A:119:GLU:CD	2.22	0.42
1:B:345:VAL:HG12	1:B:376:THR:HB	2.02	0.41
1:B:306:MET:HE1	1:B:316:ILE:HD13	2.01	0.41
1:C:462:ASN:HA	3:C:502:FAD:N1	2.34	0.41
1:B:111:TRP:HB3	1:B:117:TRP:CE2	2.55	0.41
1:C:219:ALA:HB2	1:C:226:PHE:CG	2.55	0.41
1:C:338:GLY:HA2	1:C:382:ILE:O	2.20	0.41
1:D:137:LYS:HG2	1:D:139:LEU:HD21	2.02	0.41
1:B:364:TRP:O	1:B:380:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:NH1	1:B:71:GLU:OE2	2.53	0.41
1:C:159:ILE:HD13	1:C:210:GLN:HB3	2.00	0.41
1:B:394:ASP:O	1:B:398:ARG:HG3	2.21	0.41
1:C:373:GLU:CD	1:C:373:GLU:H	2.23	0.41
1:A:373:GLU:HG3	1:A:374:LEU:N	2.35	0.41
1:D:310:LEU:HA	1:D:313:TYR:HD1	1.86	0.41
1:B:394:ASP:HB3	1:B:398:ARG:HH12	1.82	0.41
1:A:133:THR:O	1:A:351:ARG:NH1	2.44	0.41
1:B:250:THR:OG1	1:B:250:THR:O	2.38	0.41
1:D:203:LEU:HD23	1:D:207:GLN:HB3	2.03	0.41
1:B:401:GLN:HA	1:B:404:PHE:O	2.21	0.41
1:C:56:VAL:HA	1:C:303:VAL:O	2.21	0.41
1:A:177:PRO:HD2	1:B:111:TRP:CZ2	2.56	0.41
1:C:306:MET:HE1	1:C:316:ILE:HD13	2.03	0.41
1:C:326:LYS:HB2	1:C:326:LYS:HE2	1.93	0.41
1:D:153:ASP:O	1:D:157:LYS:HG3	2.21	0.41
1:A:306:MET:HE1	1:A:316:ILE:HD13	2.03	0.40
1:C:404:PHE:O	1:C:407:VAL:HG22	2.21	0.40
1:C:115:HIS:CE1	1:C:468:GLU:HB2	2.56	0.40
1:D:108:TRP:CD2	1:D:250:THR:HA	2.56	0.40
1:A:114:PRO:HA	1:B:114:PRO:HB3	2.03	0.40
1:B:177:PRO:HG3	1:B:236:ALA:HB1	2.03	0.40
1:D:340:LYS:HD2	1:D:381:THR:HG22	2.04	0.40
1:D:403:MET:HG2	1:D:404:PHE:CE2	2.57	0.40
1:D:466:ALA:HB2	3:D:502:FAD:H5'2	2.03	0.40
1:D:203:LEU:HD12	1:D:203:LEU:H	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ARG:NH2	1:D:488:HIS:CB[2_564]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	430/490 (88%)	425 (99%)	5 (1%)	0	100	100
1	B	438/490 (89%)	431 (98%)	6 (1%)	1 (0%)	47	64
1	C	438/490 (89%)	430 (98%)	6 (1%)	2 (0%)	29	43
1	D	437/490 (89%)	426 (98%)	11 (2%)	0	100	100
All	All	1743/1960 (89%)	1712 (98%)	28 (2%)	3 (0%)	47	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	488	HIS
1	C	361	PRO
1	B	361	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/390 (89%)	341 (98%)	6 (2%)	60	76
1	B	355/390 (91%)	348 (98%)	7 (2%)	55	72
1	C	354/390 (91%)	346 (98%)	8 (2%)	50	68
1	D	355/390 (91%)	345 (97%)	10 (3%)	43	61
All	All	1411/1560 (90%)	1380 (98%)	31 (2%)	52	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	163	PHE
1	A	214	TYR
1	A	226	PHE
1	A	329	PHE

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Mol	Chain	Res	Type
1	A	334	GLN
1	B	163	PHE
1	B	184	GLU
1	B	214	TYR
1	B	226	PHE
1	B	329	PHE
1	B	346	LYS
1	B	394	ASP
1	C	163	PHE
1	C	205	ARG
1	C	214	TYR
1	C	217	LEU
1	C	226	PHE
1	C	329	PHE
1	C	483	LEU
1	C	484	GLU
1	D	163	PHE
1	D	172	GLU
1	D	204	SER
1	D	213	SER
1	D	214	TYR
1	D	226	PHE
1	D	329	PHE
1	D	334	GLN
1	D	394	ASP
1	D	484	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	359	GLN
1	B	334	GLN
1	B	490	HIS
1	C	110	HIS
1	C	241	ASN
1	D	401	GLN
1	D	488	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
3	FAD	C	502	-	51,58,58	1.44	5 (9%)	60,89,89	2.05	14 (23%)
3	FAD	A	502	-	51,58,58	1.43	5 (9%)	60,89,89	2.07	15 (25%)
2	NCT	A	501	-	13,13,13	5.43	5 (38%)	17,17,17	1.38	3 (17%)
2	NCT	D	501	-	13,13,13	5.42	5 (38%)	17,17,17	1.30	3 (17%)
2	NCT	B	501	-	13,13,13	5.42	5 (38%)	17,17,17	1.33	3 (17%)
2	NCT	C	501	-	13,13,13	5.42	5 (38%)	17,17,17	1.32	3 (17%)
3	FAD	D	502	-	51,58,58	1.43	5 (9%)	60,89,89	2.06	17 (28%)
3	FAD	B	502	-	51,58,58	1.42	5 (9%)	60,89,89	2.07	16 (26%)

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	FAD	C	502	-	-	6/30/50/50	0/6/6/6
3	FAD	A	502	-	-	6/30/50/50	0/6/6/6
2	NCT	A	501	-	-	0/4/14/14	0/2/2/2
2	NCT	D	501	-	-	0/4/14/14	0/2/2/2
2	NCT	B	501	-	-	0/4/14/14	0/2/2/2
2	NCT	C	501	-	-	0/4/14/14	0/2/2/2
3	FAD	D	502	-	-	6/30/50/50	0/6/6/6
3	FAD	B	502	-	-	5/30/50/50	0/6/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NCT	C10-N2	-15.65	1.14	1.46
2	D	501	NCT	C10-N2	-15.63	1.14	1.46
2	B	501	NCT	C10-N2	-15.61	1.14	1.46
2	C	501	NCT	C10-N2	-15.60	1.14	1.46
2	C	501	NCT	C7-C6	-7.84	1.33	1.54
2	A	501	NCT	C7-C6	-7.83	1.33	1.54
2	B	501	NCT	C7-C6	-7.80	1.33	1.54
2	D	501	NCT	C7-C6	-7.77	1.33	1.54
2	D	501	NCT	C9-N2	-6.96	1.27	1.46
2	C	501	NCT	C9-N2	-6.95	1.27	1.46
2	A	501	NCT	C9-N2	-6.92	1.27	1.46
2	B	501	NCT	C9-N2	-6.90	1.27	1.46
3	A	502	FAD	C10-N1	4.58	1.39	1.33
3	C	502	FAD	C10-N1	4.57	1.39	1.33
3	D	502	FAD	C10-N1	4.54	1.39	1.33
3	B	502	FAD	C10-N1	4.46	1.39	1.33
3	C	502	FAD	C4X-N5	4.33	1.39	1.33
3	D	502	FAD	C4X-N5	4.30	1.39	1.33
3	A	502	FAD	C4X-N5	4.29	1.39	1.33
3	B	502	FAD	C4X-N5	4.28	1.39	1.33
2	C	501	NCT	C6-N2	3.83	1.59	1.46
2	B	501	NCT	C6-N2	3.83	1.59	1.46
2	A	501	NCT	C6-N2	3.80	1.59	1.46
2	D	501	NCT	C6-N2	3.78	1.59	1.46
3	C	502	FAD	C2A-N3A	3.61	1.37	1.32
3	B	502	FAD	C2A-N3A	3.51	1.37	1.32
3	D	502	FAD	C2A-N3A	3.50	1.37	1.32
3	A	502	FAD	C2A-N3A	3.48	1.37	1.32
3	C	502	FAD	C4-N3	3.37	1.38	1.33
3	A	502	FAD	C4-N3	3.30	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	FAD	C4-N3	3.30	1.38	1.33
3	B	502	FAD	C4-N3	3.28	1.38	1.33
3	D	502	FAD	C2A-N1A	2.48	1.38	1.33
3	C	502	FAD	C2A-N1A	2.46	1.38	1.33
3	B	502	FAD	C2A-N1A	2.44	1.38	1.33
3	A	502	FAD	C2A-N1A	2.42	1.38	1.33
2	B	501	NCT	C2-C6	2.09	1.55	1.51
2	A	501	NCT	C2-C6	2.05	1.55	1.51
2	C	501	NCT	C2-C6	2.05	1.55	1.51
2	D	501	NCT	C2-C6	2.02	1.54	1.51

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	FAD	N3A-C2A-N1A	-6.49	118.53	128.68
3	B	502	FAD	N3A-C2A-N1A	-6.46	118.57	128.68
3	A	502	FAD	N3A-C2A-N1A	-6.45	118.60	128.68
3	C	502	FAD	N3A-C2A-N1A	-6.42	118.65	128.68
3	B	502	FAD	C4X-N5-C5X	5.19	121.95	116.77
3	A	502	FAD	C4X-N5-C5X	5.02	121.79	116.77
3	D	502	FAD	O2'-C2'-C3'	4.91	121.05	109.10
3	C	502	FAD	O2'-C2'-C3'	4.89	121.00	109.10
3	C	502	FAD	C4X-N5-C5X	4.89	121.66	116.77
3	B	502	FAD	O2'-C2'-C3'	4.88	120.97	109.10
3	A	502	FAD	O2'-C2'-C3'	4.87	120.93	109.10
3	D	502	FAD	C4X-N5-C5X	4.85	121.62	116.77
3	D	502	FAD	C4-N3-C2	4.76	119.16	115.14
3	A	502	FAD	C4-N3-C2	4.71	119.12	115.14
3	C	502	FAD	C4-N3-C2	4.70	119.11	115.14
3	B	502	FAD	C4-N3-C2	4.59	119.02	115.14
3	A	502	FAD	C9A-C5X-N5	-4.30	115.63	122.36
3	C	502	FAD	O2'-C2'-C1'	4.03	119.28	109.59
3	C	502	FAD	C5'-C4'-C3'	-3.96	104.56	112.20
3	B	502	FAD	C5'-C4'-C3'	-3.95	104.58	112.20
3	D	502	FAD	C5'-C4'-C3'	-3.94	104.58	112.20
3	D	502	FAD	O2'-C2'-C1'	3.91	119.00	109.59
3	B	502	FAD	C9A-C5X-N5	-3.82	116.39	122.36
3	B	502	FAD	O2'-C2'-C1'	3.80	118.75	109.59
3	A	502	FAD	O2'-C2'-C1'	3.77	118.66	109.59
3	C	502	FAD	C9A-C5X-N5	-3.57	116.78	122.36
3	A	502	FAD	C5'-C4'-C3'	-3.54	105.37	112.20
3	D	502	FAD	C9A-C5X-N5	-3.34	117.13	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	FAD	C4X-C10-N10	-2.90	117.32	120.30
3	C	502	FAD	O4B-C1B-C2B	-2.79	102.84	106.93
3	D	502	FAD	O3'-C3'-C4'	-2.78	102.09	108.81
2	B	501	NCT	C5-N1-C1	2.78	121.65	116.85
2	D	501	NCT	C5-N1-C1	2.76	121.63	116.85
2	C	501	NCT	C5-N1-C1	2.76	121.62	116.85
3	C	502	FAD	C4X-C10-N10	-2.76	117.47	120.30
2	A	501	NCT	C5-N1-C1	2.74	121.59	116.85
3	A	502	FAD	C2A-N1A-C6A	2.73	123.43	118.75
3	D	502	FAD	C2A-N1A-C6A	2.72	123.40	118.75
3	B	502	FAD	C2A-N1A-C6A	2.71	123.39	118.75
3	B	502	FAD	C4X-C10-N10	-2.71	117.52	120.30
3	D	502	FAD	C4X-C4-N3	-2.68	119.76	123.43
3	A	502	FAD	O3'-C3'-C4'	-2.68	102.33	108.81
3	A	502	FAD	C9A-N10-C10	-2.68	118.40	121.91
3	B	502	FAD	O3'-C3'-C4'	-2.67	102.37	108.81
3	C	502	FAD	O3'-C3'-C4'	-2.66	102.38	108.81
3	C	502	FAD	C2A-N1A-C6A	2.64	123.27	118.75
3	D	502	FAD	C4X-C10-N10	-2.61	117.62	120.30
3	A	502	FAD	C4X-C4-N3	-2.58	119.90	123.43
3	C	502	FAD	C4X-C4-N3	-2.58	119.91	123.43
3	A	502	FAD	C1'-C2'-C3'	2.56	116.95	109.79
2	A	501	NCT	C3-C2-C1	2.54	119.58	116.88
3	B	502	FAD	C4X-C4-N3	-2.52	119.98	123.43
3	B	502	FAD	C1'-C2'-C3'	2.50	116.76	109.79
2	A	501	NCT	C2-C1-N1	-2.44	120.31	124.14
2	C	501	NCT	C3-C2-C1	2.43	119.47	116.88
2	D	501	NCT	C2-C1-N1	-2.42	120.34	124.14
2	C	501	NCT	C2-C1-N1	-2.41	120.36	124.14
2	D	501	NCT	C3-C2-C1	2.41	119.44	116.88
2	B	501	NCT	C2-C1-N1	-2.38	120.40	124.14
3	D	502	FAD	C1'-C2'-C3'	2.37	116.41	109.79
2	B	501	NCT	C3-C2-C1	2.37	119.40	116.88
3	C	502	FAD	C9A-N10-C10	-2.35	118.83	121.91
3	B	502	FAD	O4B-C1B-C2B	-2.30	103.57	106.93
3	B	502	FAD	C9A-N10-C10	-2.29	118.91	121.91
3	A	502	FAD	O4B-C1B-C2B	-2.27	103.60	106.93
3	C	502	FAD	C1'-C2'-C3'	2.27	116.14	109.79
3	B	502	FAD	C1B-N9A-C4A	-2.19	122.78	126.64
3	D	502	FAD	C9A-N10-C10	-2.17	119.07	121.91
3	B	502	FAD	C1'-N10-C9A	2.13	119.97	118.29
3	A	502	FAD	C1'-N10-C9A	2.09	119.93	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	FAD	C1'-N10-C9A	2.08	119.93	118.29
3	D	502	FAD	C5X-C9A-N10	2.07	119.22	117.72
3	D	502	FAD	O4B-C1B-C2B	-2.03	103.95	106.93
3	D	502	FAD	C1B-N9A-C4A	-2.02	123.09	126.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	FAD	N10-C1'-C2'-O2'
3	A	502	FAD	N10-C1'-C2'-O2'
3	D	502	FAD	N10-C1'-C2'-O2'
3	D	502	FAD	O4'-C4'-C5'-O5'
3	B	502	FAD	N10-C1'-C2'-O2'
3	A	502	FAD	O2'-C2'-C3'-O3'
3	B	502	FAD	O2'-C2'-C3'-O3'
3	C	502	FAD	O2'-C2'-C3'-O3'
3	A	502	FAD	O2'-C2'-C3'-C4'
3	C	502	FAD	PA-O3P-P-O5'
3	A	502	FAD	PA-O3P-P-O5'
3	B	502	FAD	O2'-C2'-C3'-C4'
3	D	502	FAD	O2'-C2'-C3'-O3'
3	C	502	FAD	O4B-C4B-C5B-O5B
3	C	502	FAD	O4'-C4'-C5'-O5'
3	A	502	FAD	O4'-C4'-C5'-O5'
3	A	502	FAD	O4B-C4B-C5B-O5B
3	D	502	FAD	C5B-O5B-PA-O3P
3	B	502	FAD	C5B-O5B-PA-O3P
3	B	502	FAD	O4B-C4B-C5B-O5B
3	D	502	FAD	C3'-C4'-C5'-O5'
3	D	502	FAD	O4B-C4B-C5B-O5B
3	C	502	FAD	O2'-C2'-C3'-C4'

There are no ring outliers.

5 monomers are involved in 13 short contacts:

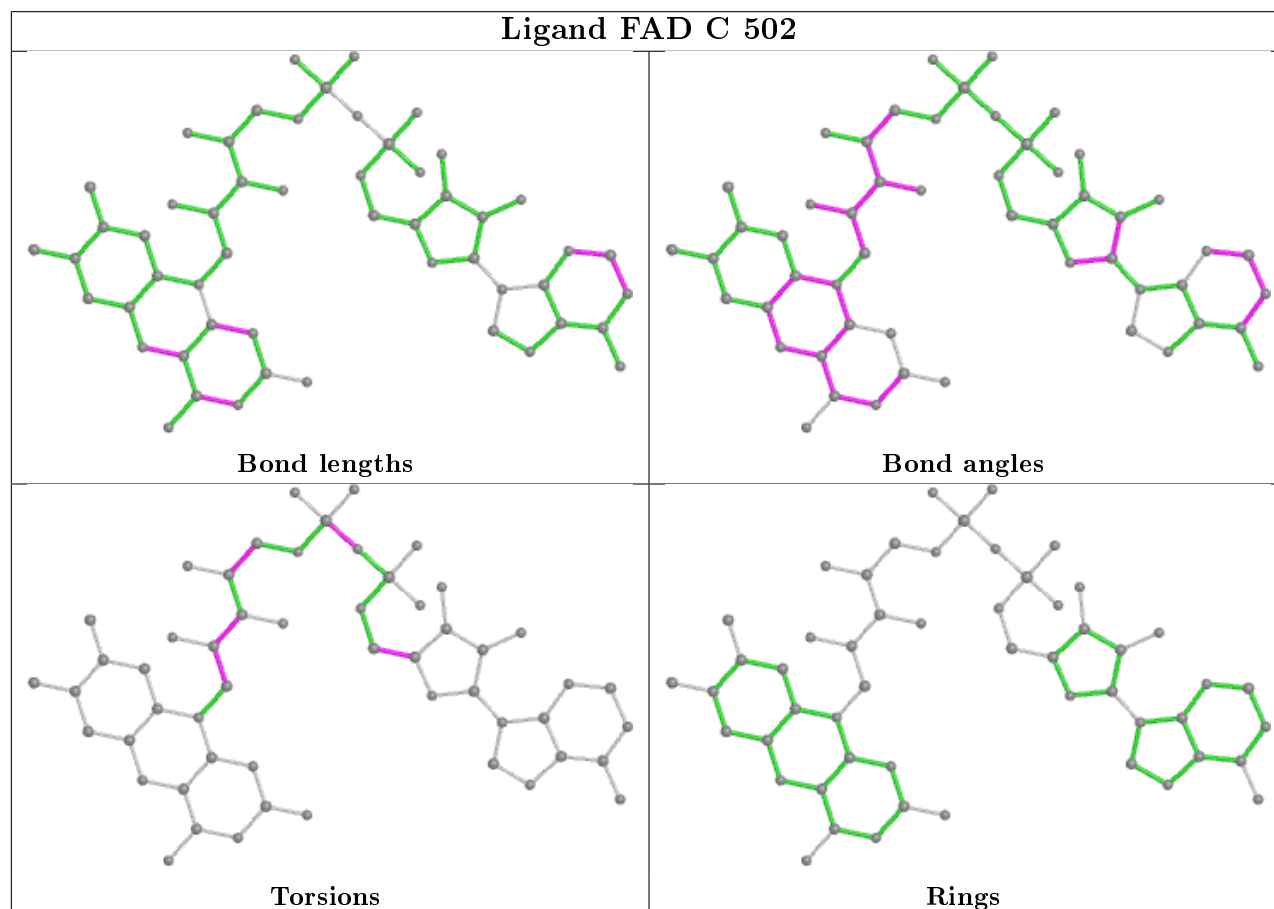
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	FAD	3	0
3	A	502	FAD	2	0
2	D	501	NCT	1	0
3	D	502	FAD	4	0

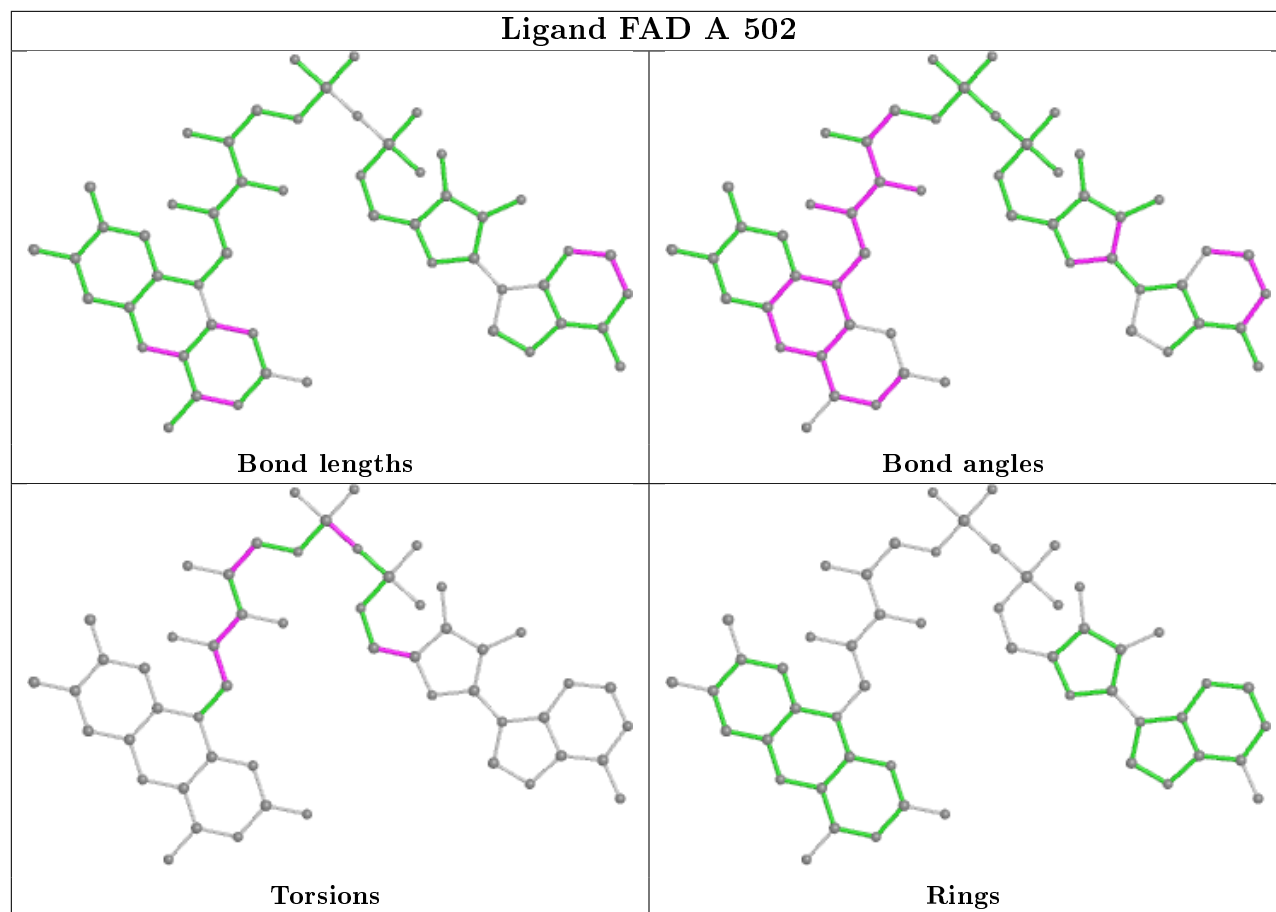
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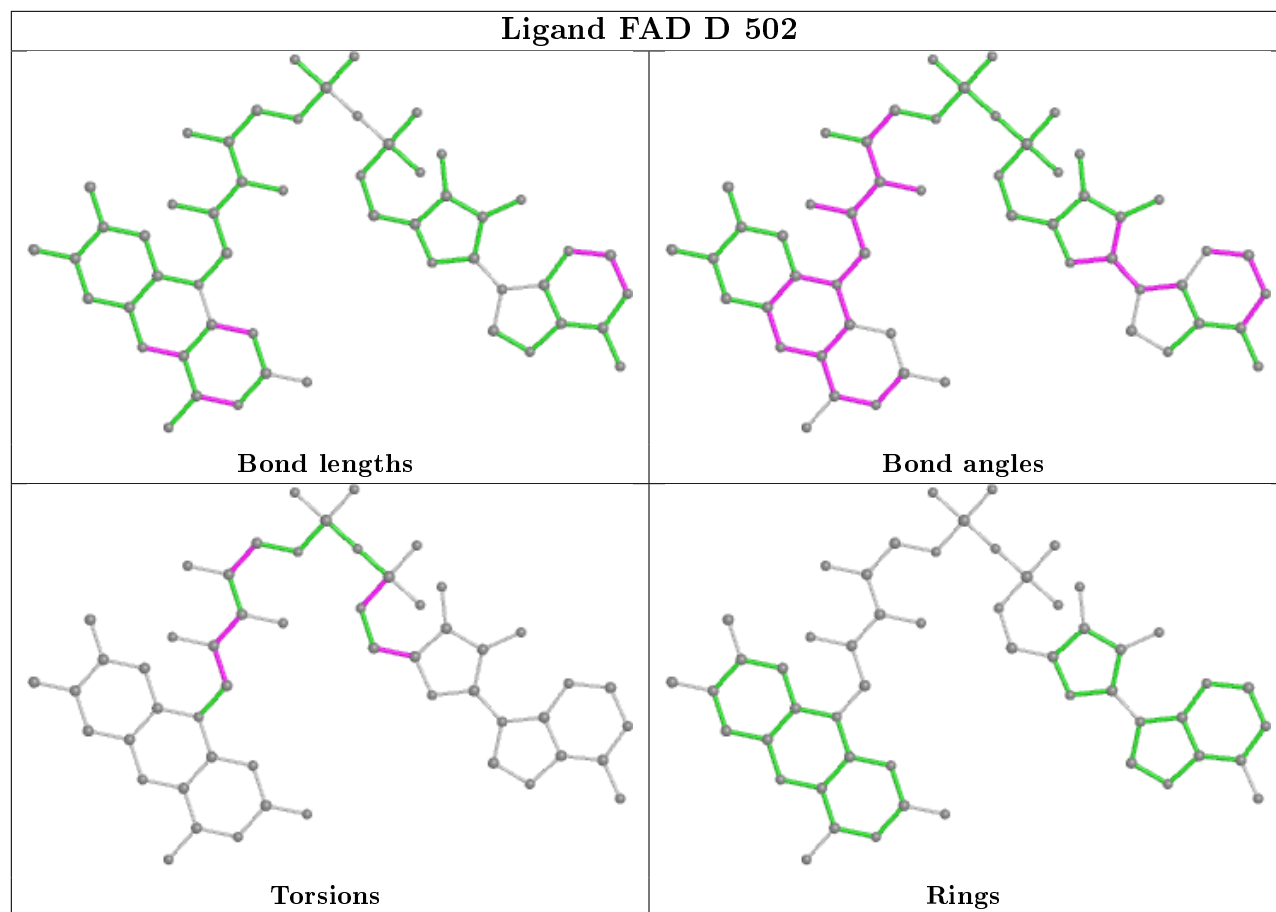
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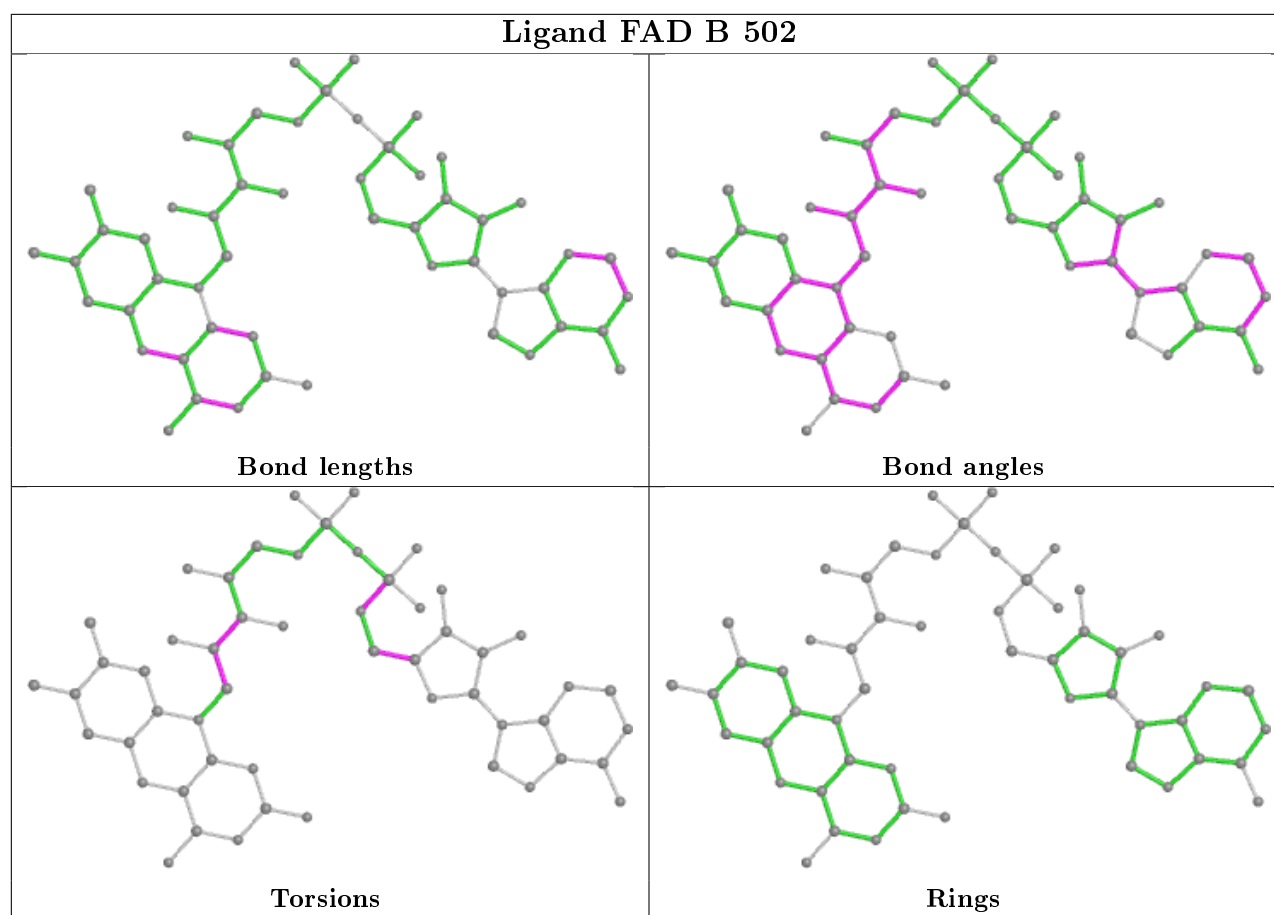
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	FAD	3	0

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	432/490 (88%)	0.05	13 (3%) 50 46	37, 55, 72, 92	0
1	B	440/490 (89%)	0.13	19 (4%) 35 31	37, 53, 73, 105	0
1	C	440/490 (89%)	-0.15	8 (1%) 68 66	37, 53, 72, 94	0
1	D	439/490 (89%)	0.21	22 (5%) 28 25	36, 63, 89, 106	0
All	All	1751/1960 (89%)	0.06	62 (3%) 44 40	36, 55, 81, 106	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	373	GLU	4.9
1	B	490	HIS	3.9
1	D	204	SER	3.9
1	B	488	HIS	3.7
1	A	352	VAL	3.6
1	A	51	GLY	3.6
1	B	374	LEU	3.5
1	D	153	ASP	3.3
1	D	391	ASN	3.3
1	D	211	ILE	3.2
1	D	407	VAL	3.0
1	D	483	LEU	3.0
1	B	350	GLY	3.0
1	D	359	GLN	2.9
1	C	373	GLU	2.8
1	B	126	GLY	2.8
1	B	346	LYS	2.8
1	D	205	ARG	2.7
1	D	352	VAL	2.7
1	B	393	ARG	2.6
1	A	287	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	286	ASN	2.6
1	B	376	THR	2.5
1	C	488	HIS	2.5
1	A	114	PRO	2.5
1	B	464	ASP	2.5
1	B	352	VAL	2.5
1	A	115	HIS	2.4
1	C	374	LEU	2.4
1	D	409	VAL	2.4
1	D	396	VAL	2.4
1	A	205	ARG	2.4
1	A	410	LEU	2.3
1	A	78	ARG	2.3
1	B	373	GLU	2.3
1	A	298	ILE	2.3
1	B	134	ASN	2.3
1	D	350	GLY	2.3
1	B	116	VAL	2.3
1	C	207	GLN	2.3
1	D	154	GLU	2.3
1	A	118	ALA	2.2
1	A	279	VAL	2.2
1	C	371	SER	2.2
1	A	187	ARG	2.2
1	D	157	LYS	2.2
1	B	51	GLY	2.2
1	B	120	MET	2.2
1	C	372	ASP	2.2
1	B	118	ALA	2.1
1	B	117	TRP	2.1
1	A	172	GLU	2.1
1	B	184	GLU	2.1
1	D	134	ASN	2.1
1	D	133	THR	2.1
1	C	487	HIS	2.1
1	D	296	ASP	2.1
1	C	315	HIS	2.0
1	B	466	ALA	2.0
1	D	400	VAL	2.0
1	D	490	HIS	2.0
1	D	372	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

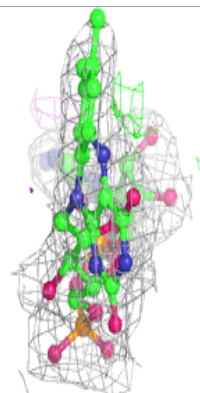
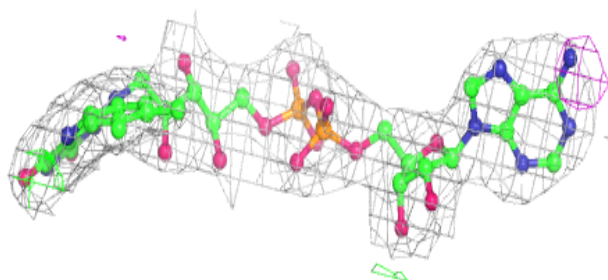
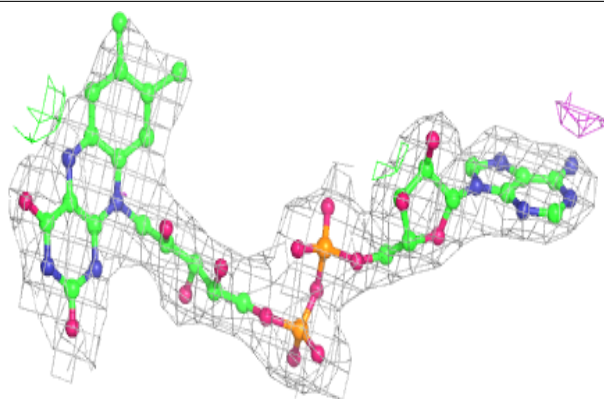
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NCT	C	501	12/12	0.94	0.17	47,51,58,60	0
2	NCT	A	501	12/12	0.95	0.19	49,52,60,62	0
3	FAD	A	502	53/53	0.95	0.15	40,47,53,55	0
3	FAD	D	502	53/53	0.95	0.18	44,51,60,60	0
3	FAD	C	502	53/53	0.96	0.14	36,42,52,56	0
2	NCT	D	501	12/12	0.96	0.17	55,63,67,67	0
3	FAD	B	502	53/53	0.96	0.16	38,42,53,55	0
2	NCT	B	501	12/12	0.97	0.13	50,53,58,62	0

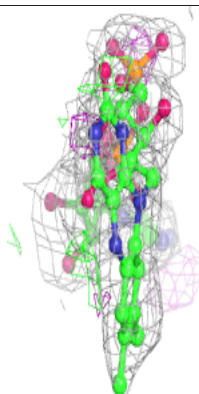
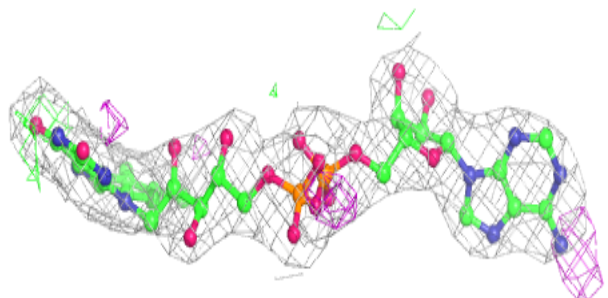
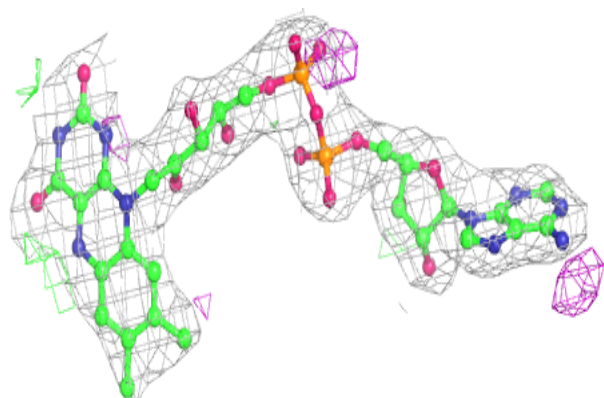
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 502:

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

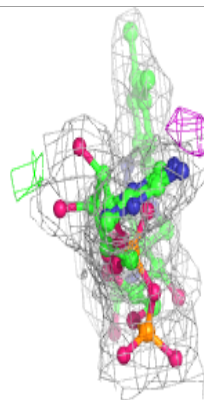
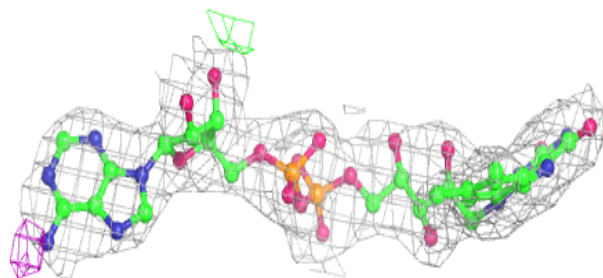
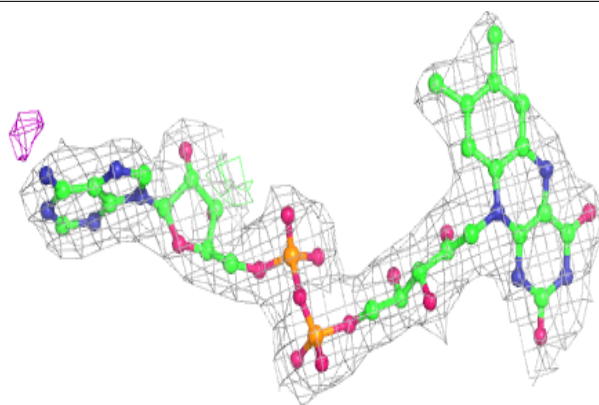
**Electron density around FAD D 502:**

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

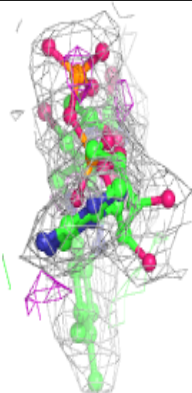
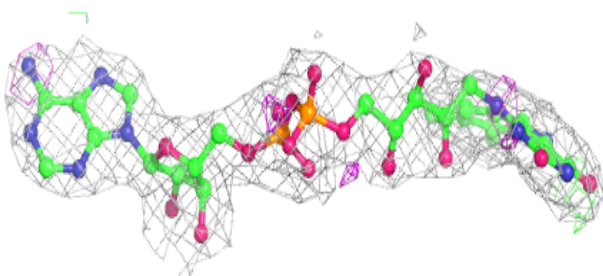
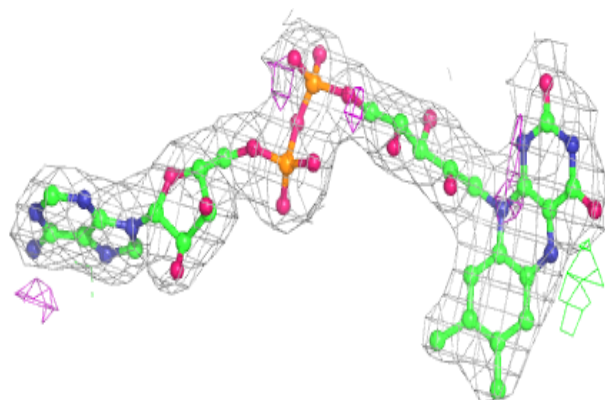


Electron density around FAD C 502:

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

**Electron density around FAD B 502:**

$2mF_o-DF_c$ (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.