



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:09 PM UTC

PDB ID : 1GET / pdb_00001get
Title : ANATOMY OF AN ENGINEERED NAD-BINDING SITE
Authors : Mittl, P.R.E.; Schulz, G.E.
Deposited on : 1994-01-18
Resolution : 2.00 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

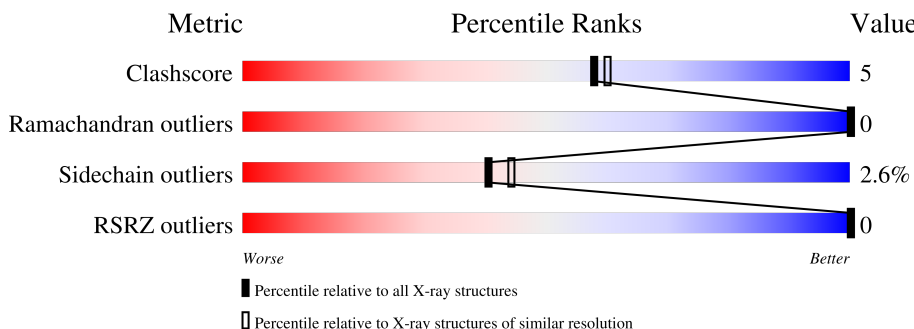
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	450	
1	B	450	

2 Entry composition [i](#)

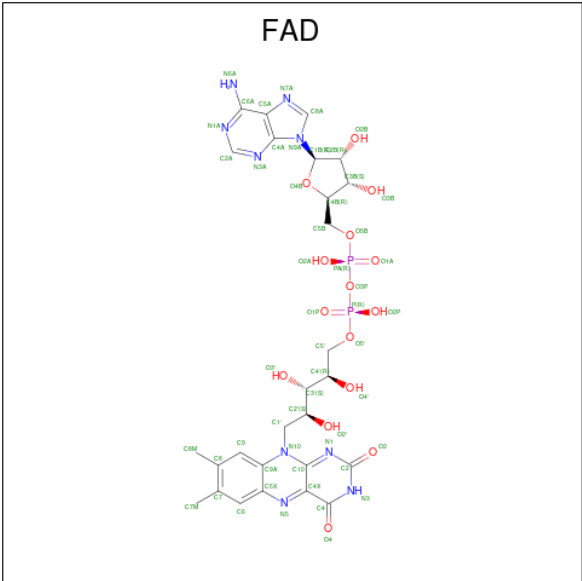
There are 4 unique types of molecules in this entry. The entry contains 7489 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTATHIONE REDUCTASE.

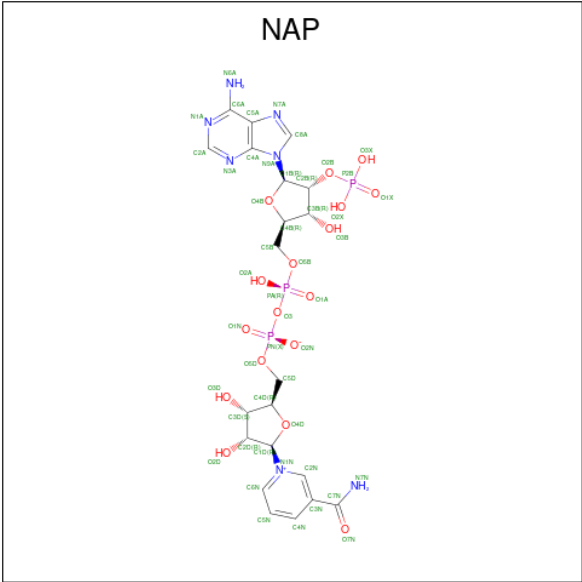
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	1	0
			3415	2156	589	652	18			
1	B	449	Total	C	N	O	S	0	1	0
			3422	2160	590	654	18			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

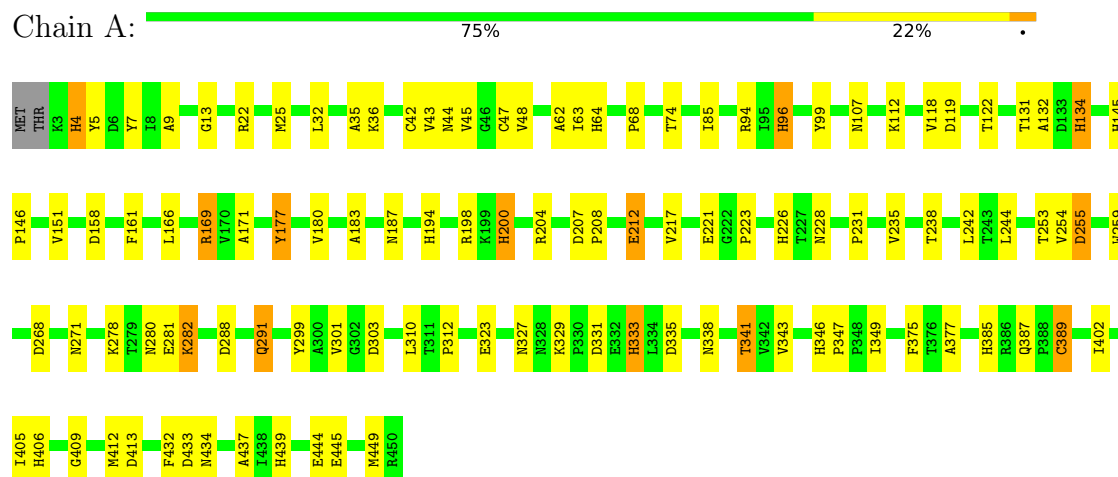
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	B	236	Total	O	0	0
			236	236		

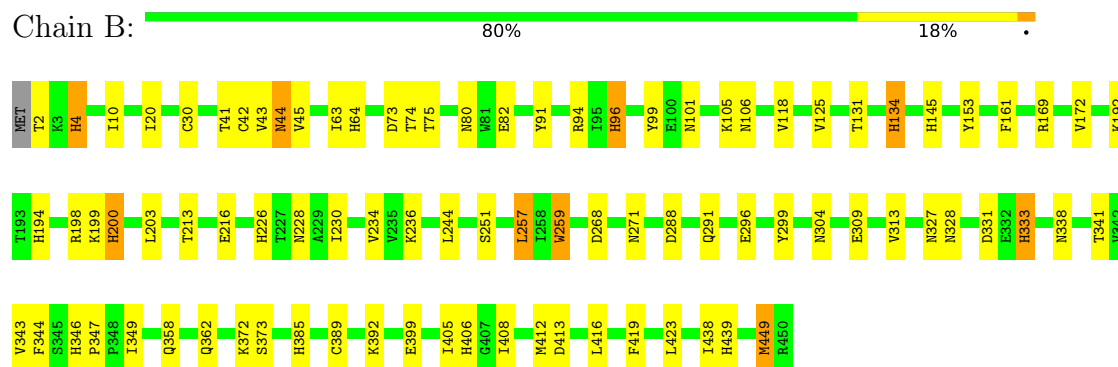
3 Residue-property plots

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 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: GLUTATHIONE REDUCTASE



• Molecule 1: GLUTATHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, α , β , γ	120.50Å 74.00Å 60.80Å 90.00° 90.00° 82.50°	Depositor
Resolution (Å)	7.00 – 2.00 7.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.00) 79.1 (7.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , (Not available) 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.9	EDS
L-test for twinning ¹	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3236e-03.*

¹Theoretical 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: FAD, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.10	20/3490 (0.6%)	1.71	54/4737 (1.1%)
1	B	1.15	21/3497 (0.6%)	1.75	52/4747 (1.1%)
All	All	1.12	41/6987 (0.6%)	1.73	106/9484 (1.1%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	HIS	CD2-NE2	-7.57	1.29	1.37
1	A	194	HIS	CD2-NE2	-7.44	1.29	1.37
1	B	194	HIS	CD2-NE2	-7.43	1.29	1.37
1	A	333	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	134	HIS	CD2-NE2	-6.96	1.30	1.37
1	B	412	MET	CA-CB	-6.78	1.42	1.53
1	B	226	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	145	HIS	CD2-NE2	-6.48	1.30	1.37
1	B	45	VAL	CA-CB	6.46	1.63	1.54
1	B	333	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	4	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	145	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	406	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	439	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	200	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	4	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	64	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	439	HIS	CG-ND1	-5.99	1.31	1.38
1	A	200	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	439	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	385	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	45	VAL	CA-CB	5.73	1.62	1.54
1	A	96	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	85	ILE	CA-CB	5.60	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	HIS	CG-ND1	-5.59	1.32	1.38
1	A	226	HIS	CG-ND1	-5.57	1.32	1.38
1	B	259	TRP	CA-CB	5.54	1.60	1.53
1	A	402	ILE	CA-CB	5.52	1.60	1.54
1	A	406	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	226	HIS	CD2-NE2	-5.41	1.31	1.37
1	B	64	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	385	HIS	CD2-NE2	-5.29	1.32	1.37
1	A	385	HIS	CG-ND1	-5.23	1.32	1.38
1	A	333	HIS	CG-ND1	-5.21	1.32	1.38
1	B	313	VAL	CA-CB	-5.16	1.47	1.54
1	B	96	HIS	CD2-NE2	-5.14	1.32	1.37
1	B	226	HIS	CG-ND1	-5.07	1.32	1.38
1	B	10	ILE	CA-CB	5.04	1.60	1.53
1	A	134	HIS	CG-ND1	-5.01	1.32	1.38
1	B	4	HIS	CG-ND1	-5.00	1.32	1.38
1	B	406	HIS	CG-ND1	-5.00	1.32	1.38

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH2	-8.99	111.11	119.20
1	A	413	ASP	CA-CB-CG	8.99	121.59	112.60
1	B	194	HIS	CB-CG-CD2	-8.60	120.02	131.20
1	B	118	VAL	N-CA-C	-7.72	105.17	111.81
1	A	338	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	A	346	HIS	CB-CG-CD2	-7.64	121.27	131.20
1	A	268	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	119	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	433	ASP	N-CA-C	7.24	121.02	111.75
1	B	291	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	B	304	ASN	CA-CB-CG	7.16	119.76	112.60
1	A	413	ASP	N-CA-C	7.12	119.03	111.28
1	B	134	HIS	CB-CG-CD2	-7.08	122.00	131.20
1	A	212	GLU	CA-CB-CG	7.07	128.25	114.10
1	B	288	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	280	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	187	ASN	OD1-CG-ND2	-6.89	115.70	122.60
1	A	194	HIS	CB-CG-CD2	-6.74	122.43	131.20
1	A	13	GLY	N-CA-C	-6.74	102.97	112.60
1	A	134	HIS	CB-CG-CD2	-6.72	122.46	131.20
1	A	200	HIS	CB-CG-CD2	-6.66	122.54	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASP	N-CA-C	-6.54	105.46	113.50
1	B	389[A]	CYS	N-CA-C	-6.51	98.36	109.24
1	B	389[B]	CYS	N-CA-C	-6.51	98.36	109.24
1	B	106	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	B	94	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	346	HIS	CB-CG-ND1	6.27	132.10	122.70
1	B	172	VAL	N-CA-C	-6.21	99.41	108.11
1	A	235	VAL	N-CA-CB	-6.20	103.65	111.46
1	A	389[A]	CYS	N-CA-C	-6.16	98.96	109.24
1	A	389[B]	CYS	N-CA-C	-6.16	98.96	109.24
1	B	73	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	303	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	62	ALA	N-CA-C	-6.08	104.56	111.07
1	A	434	ASN	OD1-CG-ND2	-6.03	116.58	122.60
1	B	145	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	B	82	GLU	CB-CG-CD	6.01	122.81	112.60
1	B	362	GLN	N-CA-C	6.00	117.82	111.28
1	B	271	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	B	91	TYR	N-CA-C	-5.97	104.69	111.14
1	B	161	PHE	CA-CB-CG	-5.96	107.84	113.80
1	A	94	ARG	CG-CD-NE	-5.96	98.90	112.00
1	B	125	VAL	CB-CA-C	-5.95	100.88	110.28
1	A	271	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	335	ASP	CA-CB-CG	5.88	118.47	112.60
1	B	338	ASN	CA-C-N	-5.84	117.67	123.04
1	B	338	ASN	C-N-CA	-5.84	117.67	123.04
1	B	234	VAL	O-C-N	-5.83	117.02	123.20
1	B	194	HIS	CB-CG-ND1	5.80	131.40	122.70
1	B	327	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	48	VAL	N-CA-CB	-5.78	103.11	111.21
1	A	187	ASN	CB-CG-ND2	5.76	125.04	116.40
1	B	44	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	A	145	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	B	125	VAL	N-CA-C	-5.74	99.79	108.17
1	A	409	GLY	O-C-N	-5.73	118.22	123.78
1	A	327	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	B	268	ASP	N-CA-C	5.72	120.33	113.23
1	B	385	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	A	4	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	64	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	268	ASP	N-CA-C	5.64	118.28	111.40
1	A	291	GLN	OE1-CD-NE2	-5.61	116.99	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	405	ILE	O-C-N	-5.56	117.31	123.20
1	A	161	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	177	TYR	CB-CA-C	-5.54	102.10	110.92
1	B	2	THR	N-CA-CB	-5.54	102.09	111.50
1	B	296	GLU	CB-CG-CD	5.50	121.96	112.60
1	B	199	LYS	CA-CB-CG	-5.50	103.10	114.10
1	A	432	PHE	N-CA-C	-5.50	104.93	111.03
1	B	226	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	A	259	TRP	O-C-N	-5.48	116.63	123.04
1	B	343	VAL	O-C-N	-5.48	116.26	122.94
1	B	134	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	288	ASP	CA-CB-CG	5.42	118.03	112.60
1	A	200	HIS	CB-CG-ND1	5.42	130.82	122.70
1	B	413	ASP	N-CA-C	5.41	117.17	111.28
1	B	304	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	80	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	B	346	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	B	328	ASN	N-CA-C	5.35	119.00	111.52
1	A	96	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	B	416	LEU	N-CA-C	5.30	117.06	111.28
1	B	41	THR	CA-CB-OG1	-5.27	101.69	109.60
1	A	268	ASP	O-C-N	-5.26	115.81	122.17
1	B	230	ILE	CA-C-N	5.25	125.50	119.83
1	B	230	ILE	C-N-CA	5.25	125.50	119.83
1	A	180	VAL	N-CA-CB	-5.23	104.43	110.55
1	A	268	ASP	CA-C-O	-5.21	114.97	120.55
1	A	217	VAL	N-CA-C	-5.18	105.44	110.42
1	B	41	THR	CA-CB-CG2	5.17	119.28	110.50
1	A	406	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	B	358	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	35	ALA	N-CA-C	5.12	116.94	111.36
1	B	413	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	412	MET	CG-SD-CE	5.11	112.14	100.90
1	B	333	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	B	413	ASP	CA-C-O	5.08	125.93	120.55
1	B	42	CYS	N-CA-C	5.04	117.17	111.02
1	A	166	LEU	CA-C-N	5.04	125.02	120.03
1	A	166	LEU	C-N-CA	5.04	125.02	120.03
1	A	338	ASN	CB-CG-ND2	5.04	123.96	116.40
1	B	349	ILE	O-C-N	-5.02	117.76	123.18
1	B	64	HIS	CB-CG-CD2	-5.01	124.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	ILE	N-CA-C	-5.00	100.45	107.75

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	3415	0	3377	39	0
1	B	3422	0	3384	26	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	48	0	25	2	0
3	B	48	0	25	1	0
4	A	214	0	0	3	0
4	B	236	0	0	2	0
All	All	7489	0	6873	63	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 (63) 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:74:THR:HB	4:A:612:HOH:O	1.83	0.79
1:A:74:THR:HG21	1:B:63:ILE:HD13	1.67	0.76
1:A:63:ILE:HG12	1:B:63:ILE:HG12	1.67	0.75
1:A:4:HIS:HD2	1:A:131:THR:HG23	1.52	0.73
1:B:4:HIS:HD2	1:B:131:THR:HG23	1.54	0.71
4:A:612:HOH:O	1:B:74:THR:HB	1.95	0.65
1:A:377:ALA:HB2	1:A:389[A]:CYS:SG	2.37	0.64
1:A:177:TYR:OH	1:A:341:THR:HG21	2.01	0.61
1:A:63:ILE:HD13	1:B:74:THR:HG21	1.82	0.60
1:A:281:GLU:HB2	1:A:282:LYS:HE2	1.84	0.59
1:B:4:HIS:CD2	1:B:131:THR:HG23	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:CYS:HG	1:A:47:CYS:HG	1.50	0.57
1:A:437:ALA:HB1	1:A:444:GLU:HB2	1.87	0.56
1:B:101:ASN:OD1	1:B:105:LYS:HE2	2.07	0.55
1:A:343:VAL:HB	1:A:349:ILE:HB	1.89	0.55
1:B:373:SER:HB3	1:B:449:MET:HE2	1.89	0.54
1:A:4:HIS:CD2	1:A:131:THR:HG23	2.39	0.53
1:A:231:PRO:HB3	1:A:244:LEU:HD11	1.91	0.52
1:A:134:HIS:HB3	1:A:299:TYR:HE2	1.75	0.52
1:A:43:VAL:HG21	1:A:99:TYR:HE2	1.75	0.52
1:A:96:HIS:HD2	4:A:628:HOH:O	1.92	0.52
1:B:198:ARG:O	1:B:228:ASN:HA	2.11	0.50
1:A:169:ARG:HD3	1:A:255:ASP:OD2	2.10	0.50
1:A:146:PRO:O	1:A:151:VAL:HG21	2.12	0.49
1:B:44:ASN:OD1	1:B:96:HIS:HE1	1.94	0.49
1:B:153:TYR:CE1	1:B:236:LYS:HD2	2.47	0.49
1:A:9:ALA:HB3	1:A:32:LEU:HD12	1.94	0.49
1:A:291:GLN:HG3	1:A:301:VAL:HG12	1.95	0.48
1:A:198:ARG:O	1:A:228:ASN:HA	2.14	0.47
1:B:344:PHE:HE1	4:B:651:HOH:O	1.97	0.47
1:B:373:SER:CB	1:B:449:MET:HE2	2.45	0.47
1:A:331:ASP:O	1:A:333:HIS:HD2	1.97	0.46
1:B:331:ASP:O	1:B:333:HIS:HD2	1.98	0.46
1:B:347:PRO:HG2	1:B:408:ILE:HG12	1.98	0.46
1:B:257:LEU:HD21	1:B:259:TRP:CZ2	2.52	0.45
1:A:183:ALA:HB1	1:A:223:PRO:HG3	1.99	0.45
1:A:200:HIS:CE1	1:A:204:ARG:HG2	2.52	0.45
1:A:118:VAL:HB	1:A:122:THR:HB	1.99	0.45
1:B:134:HIS:HB3	1:B:299:TYR:HE2	1.82	0.45
1:A:36:LYS:O	1:A:112:LYS:HE2	2.16	0.45
1:A:171:ALA:HB2	1:A:254:VAL:HG11	1.99	0.45
1:A:323:GLU:HB3	1:A:329:LYS:HD2	1.98	0.45
1:B:44:ASN:OD1	1:B:96:HIS:CE1	2.70	0.44
1:A:375:PHE:CZ	1:A:445:GLU:HG3	2.52	0.44
1:B:20:ILE:HD11	1:B:30:CYS:HB3	2.00	0.43
1:B:372:LYS:HZ3	1:B:392:LYS:HE2	1.83	0.43
2:B:451:FAD:H9	2:B:451:FAD:H1'1	1.81	0.43
1:A:310:LEU:HD23	3:A:452:NAP:H2N	2.00	0.43
1:A:44:ASN:OD1	1:A:96:HIS:HE1	2.01	0.43
1:A:347:PRO:HB3	1:A:387:GLN:OE1	2.18	0.43
1:A:22:ARG:O	1:A:25:MET:HB2	2.18	0.42
1:A:7:TYR:HD1	1:A:134:HIS:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:O	1:B:251:SER:HA	2.20	0.41
1:B:309:GLU:O	3:B:452:NAP:H1D	2.20	0.41
1:B:43:VAL:HG21	1:B:99:TYR:HE2	1.85	0.41
1:A:208:PRO:O	1:A:212:GLU:HG3	2.21	0.41
1:B:200:HIS:HE1	4:B:584:HOH:O	2.03	0.41
1:A:242:LEU:O	1:A:253:THR:HA	2.19	0.41
1:A:5:TYR:O	1:A:132:ALA:HA	2.20	0.41
1:A:207:ASP:HA	1:A:208:PRO:HD3	1.86	0.40
1:A:204:ARG:HD3	3:A:452:NAP:O1X	2.21	0.40
1:B:405:ILE:HD13	1:B:419:PHE:HB3	2.03	0.40
1:B:213:THR:O	1:B:216:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

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	447/450 (99%)	427 (96%)	20 (4%)	0	100	100
1	B	448/450 (100%)	431 (96%)	17 (4%)	0	100	100
All	All	895/900 (99%)	858 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	361/362 (100%)	351 (97%)	10 (3%)	38	41
1	B	362/362 (100%)	353 (98%)	9 (2%)	42	45
All	All	723/724 (100%)	704 (97%)	19 (3%)	40	44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PRO
1	A	107	ASN
1	A	169	ARG
1	A	221	GLU
1	A	238	THR
1	A	278	LYS
1	A	282	LYS
1	A	312	PRO
1	A	341	THR
1	A	449	MET
1	B	75	THR
1	B	169	ARG
1	B	192	LYS
1	B	203	LEU
1	B	257	LEU
1	B	341	THR
1	B	399	GLU
1	B	423	LEU
1	B	449	MET

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

Mol	Chain	Res	Type
1	A	4	HIS
1	A	44	ASN
1	A	77	ASN
1	A	80	ASN
1	A	96	HIS
1	A	126	ASN
1	A	200	HIS
1	A	333	HIS
1	A	362	GLN
1	A	367	GLN
1	A	434	ASN

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Mol	Chain	Res	Type
1	B	4	HIS
1	B	64	HIS
1	B	77	ASN
1	B	96	HIS
1	B	200	HIS
1	B	237	ASN
1	B	327	ASN
1	B	333	HIS
1	B	385	HIS

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](#)

4 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	NAP	B	452	-	50,52,52	1.33	6 (12%)	71,80,80	1.72	15 (21%)
2	FAD	A	451	-	58,58,58	1.18	5 (8%)	85,89,89	1.10	7 (8%)
3	NAP	A	452	-	50,52,52	1.38	6 (12%)	71,80,80	1.56	13 (18%)
2	FAD	B	451	-	58,58,58	1.31	5 (8%)	85,89,89	1.15	8 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	B	452	-	-	4/35/67/67	0/5/5/5
2	FAD	A	451	-	-	4/34/50/50	0/6/6/6
3	NAP	A	452	-	-	5/35/67/67	0/5/5/5
2	FAD	B	451	-	-	3/34/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	452	NAP	C2N-N1N	4.87	1.40	1.35
2	B	451	FAD	PA-O3P	-4.82	1.54	1.59
3	B	452	NAP	C2N-N1N	4.37	1.39	1.35
3	A	452	NAP	O4D-C1D	4.12	1.46	1.40
2	A	451	FAD	PA-O3P	-3.61	1.55	1.59
3	B	452	NAP	C5A-N7A	-3.49	1.32	1.39
3	A	452	NAP	C5A-N7A	-3.48	1.32	1.39
3	B	452	NAP	PN-O3	3.48	1.63	1.59
2	B	451	FAD	P-O3P	-3.37	1.55	1.59
2	B	451	FAD	C4X-N5	3.05	1.37	1.30
2	A	451	FAD	C4X-N5	2.80	1.36	1.30
3	B	452	NAP	O4D-C1D	2.77	1.44	1.40
3	A	452	NAP	C3N-C7N	2.67	1.54	1.50
2	A	451	FAD	C9-C9A	2.44	1.43	1.39
2	A	451	FAD	C4'-C3'	-2.37	1.49	1.53
3	A	452	NAP	C4A-N9A	-2.23	1.33	1.37
3	A	452	NAP	PN-O3	2.07	1.61	1.59
2	A	451	FAD	O5'-C5'	2.06	1.52	1.44
3	B	452	NAP	C4A-N9A	-2.06	1.33	1.37
2	B	451	FAD	C2B-C3B	2.05	1.58	1.53
3	B	452	NAP	C3N-C7N	2.04	1.53	1.50
2	B	451	FAD	C5X-N5	-2.02	1.35	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	452	NAP	N3A-C4A-N9A	5.41	136.36	127.17
3	B	452	NAP	C5A-C4A-N3A	-4.69	120.26	126.72
3	A	452	NAP	C6N-N1N-C2N	-4.64	117.93	121.88
3	A	452	NAP	N3A-C4A-N9A	4.57	134.94	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	452	NAP	C5A-C4A-N3A	-4.26	120.85	126.72
2	B	451	FAD	O2A-PA-O3P	4.07	118.26	107.27
3	B	452	NAP	C4D-O4D-C1D	-4.05	106.21	109.92
3	B	452	NAP	N3A-C2A-N1A	-3.91	122.66	128.58
3	A	452	NAP	N3A-C2A-N1A	-3.82	122.80	128.58
3	B	452	NAP	C6N-N1N-C2N	-3.60	118.82	121.88
3	B	452	NAP	C4A-N9A-C8A	3.20	109.10	105.74
2	A	451	FAD	O2A-PA-O3P	3.03	115.46	107.27
3	B	452	NAP	C6A-C5A-N7A	-2.95	126.39	132.09
2	B	451	FAD	C5A-C4A-N3A	-2.83	122.83	126.72
3	B	452	NAP	C2A-N3A-C4A	2.76	118.58	111.83
3	A	452	NAP	P2B-O2B-C2B	-2.74	116.11	123.43
3	A	452	NAP	O4B-C1B-N9A	2.65	113.18	108.09
3	A	452	NAP	C2A-N3A-C4A	2.65	118.31	111.83
3	B	452	NAP	P2B-O2B-C2B	-2.64	116.39	123.43
2	A	451	FAD	C4-N3-C2	-2.63	120.97	125.64
3	B	452	NAP	C4A-C5A-N7A	2.55	113.50	110.58
3	A	452	NAP	C4A-C5A-N7A	2.51	113.46	110.58
2	A	451	FAD	C10-C4X-N5	-2.48	119.75	124.81
3	A	452	NAP	C6A-C5A-N7A	-2.46	127.35	132.09
3	B	452	NAP	O7N-C7N-C3N	2.42	122.55	119.60
2	A	451	FAD	C10-N1-C2	2.35	121.94	116.85
3	A	452	NAP	O2B-P2B-O1X	-2.34	101.01	109.33
2	B	451	FAD	O2P-P-O1P	2.31	123.21	112.44
3	B	452	NAP	N9A-C8A-N7A	-2.29	110.69	113.94
2	B	451	FAD	C4-N3-C2	-2.29	121.58	125.64
3	B	452	NAP	C5A-C4A-N9A	-2.27	103.33	105.81
2	B	451	FAD	O3P-PA-O1A	-2.25	103.93	110.70
2	A	451	FAD	C4X-C10-N10	2.25	119.70	116.48
3	B	452	NAP	O2B-P2B-O1X	-2.20	101.50	109.33
3	A	452	NAP	C4D-O4D-C1D	-2.18	107.92	109.92
3	A	452	NAP	C4A-N9A-C8A	2.17	108.02	105.74
2	B	451	FAD	C10-N1-C2	2.11	121.42	116.85
2	B	451	FAD	O4'-C4'-C3'	2.11	114.19	109.25
2	B	451	FAD	C5A-N7A-C8A	2.07	106.70	103.45
3	B	452	NAP	C6A-C5A-C4A	2.06	119.98	117.18
2	A	451	FAD	C5A-C4A-N3A	-2.05	123.89	126.72
2	A	451	FAD	C4X-C10-N1	-2.03	119.62	124.59
3	A	452	NAP	O4D-C4D-C5D	2.01	115.76	109.33

There are no chirality outliers.

All (16) torsion outliers are listed below:

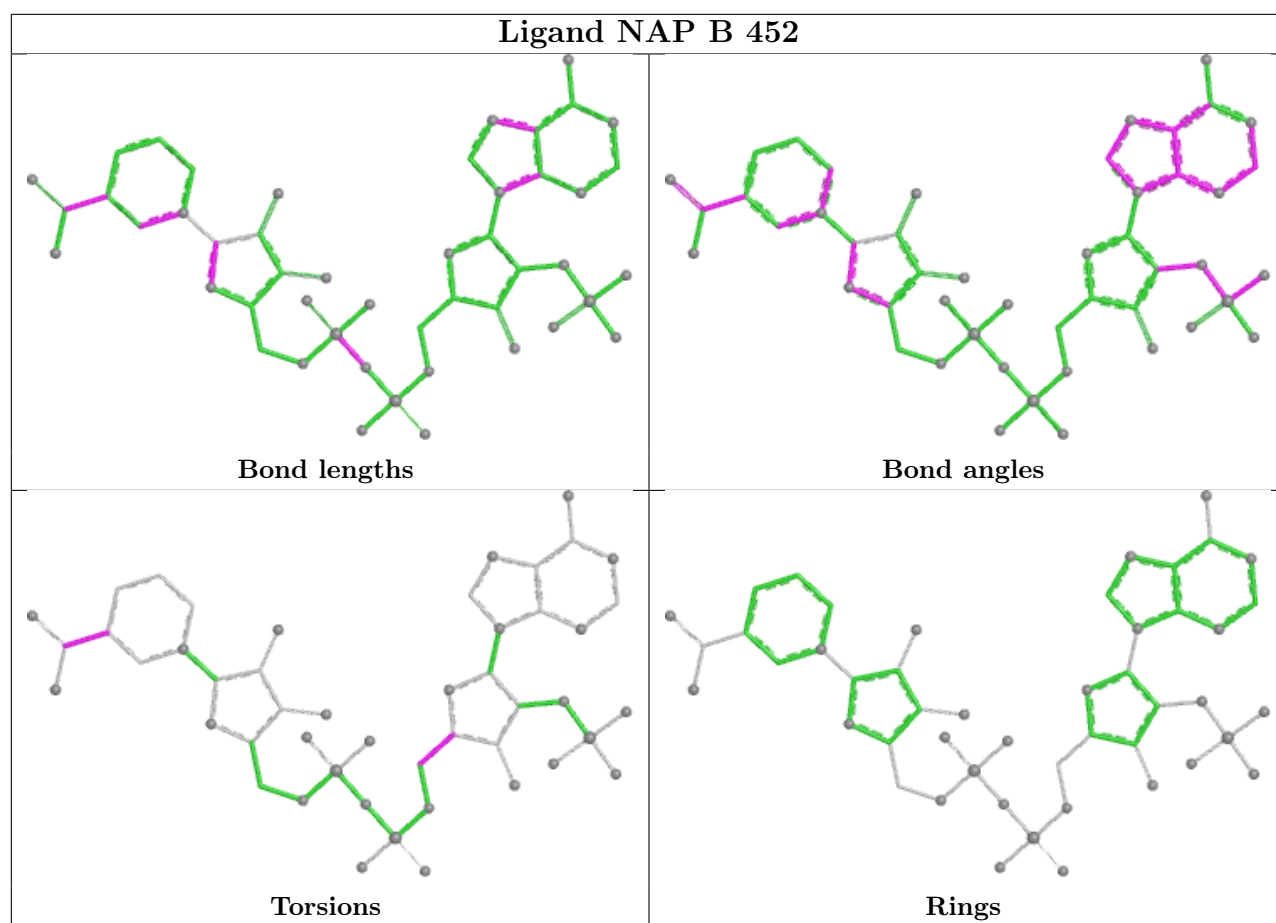
Mol	Chain	Res	Type	Atoms
2	B	451	FAD	PA-O3P-P-O5'
3	A	452	NAP	C5D-O5D-PN-O1N
3	A	452	NAP	C5D-O5D-PN-O2N
3	A	452	NAP	O4B-C4B-C5B-O5B
3	A	452	NAP	C3B-C4B-C5B-O5B
2	B	451	FAD	P-O3P-PA-O1A
2	A	451	FAD	PA-O3P-P-O5'
2	A	451	FAD	O4B-C4B-C5B-O5B
3	A	452	NAP	C5D-O5D-PN-O3
3	B	452	NAP	C2N-C3N-C7N-O7N
3	B	452	NAP	C2N-C3N-C7N-N7N
3	B	452	NAP	C3B-C4B-C5B-O5B
3	B	452	NAP	O4B-C4B-C5B-O5B
2	B	451	FAD	P-O3P-PA-O2A
2	A	451	FAD	C3B-C4B-C5B-O5B
2	A	451	FAD	P-O3P-PA-O2A

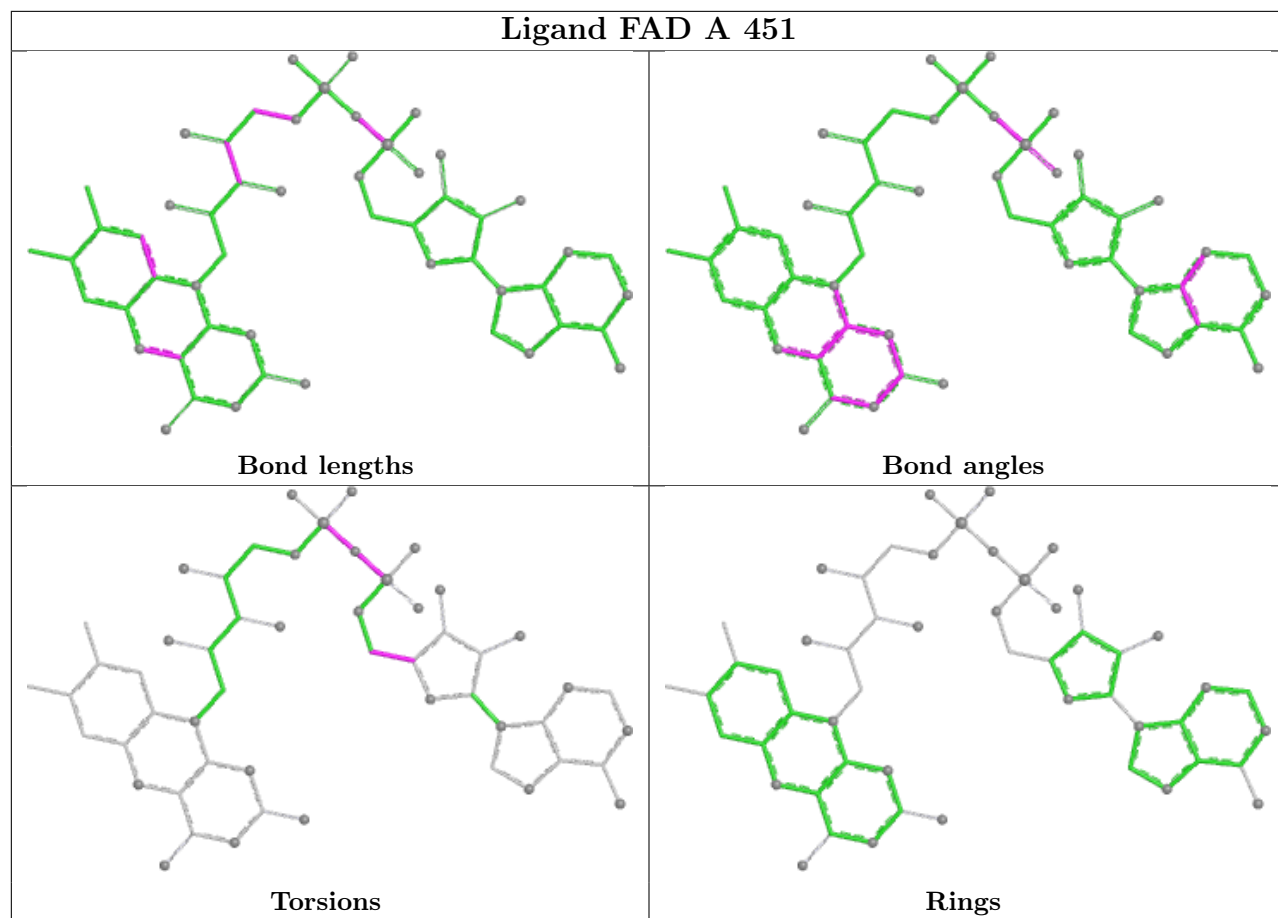
There are no ring outliers.

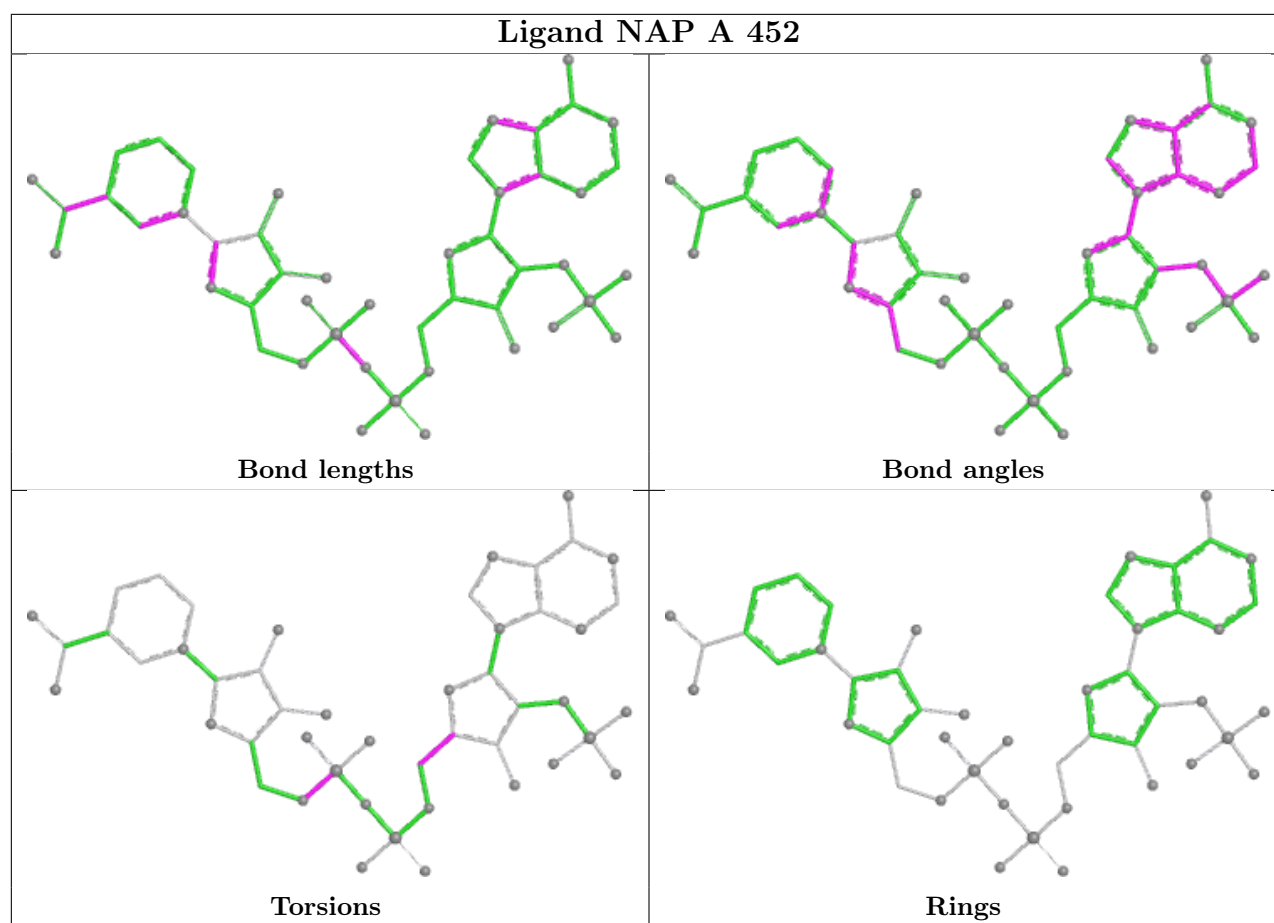
3 monomers are involved in 4 short contacts:

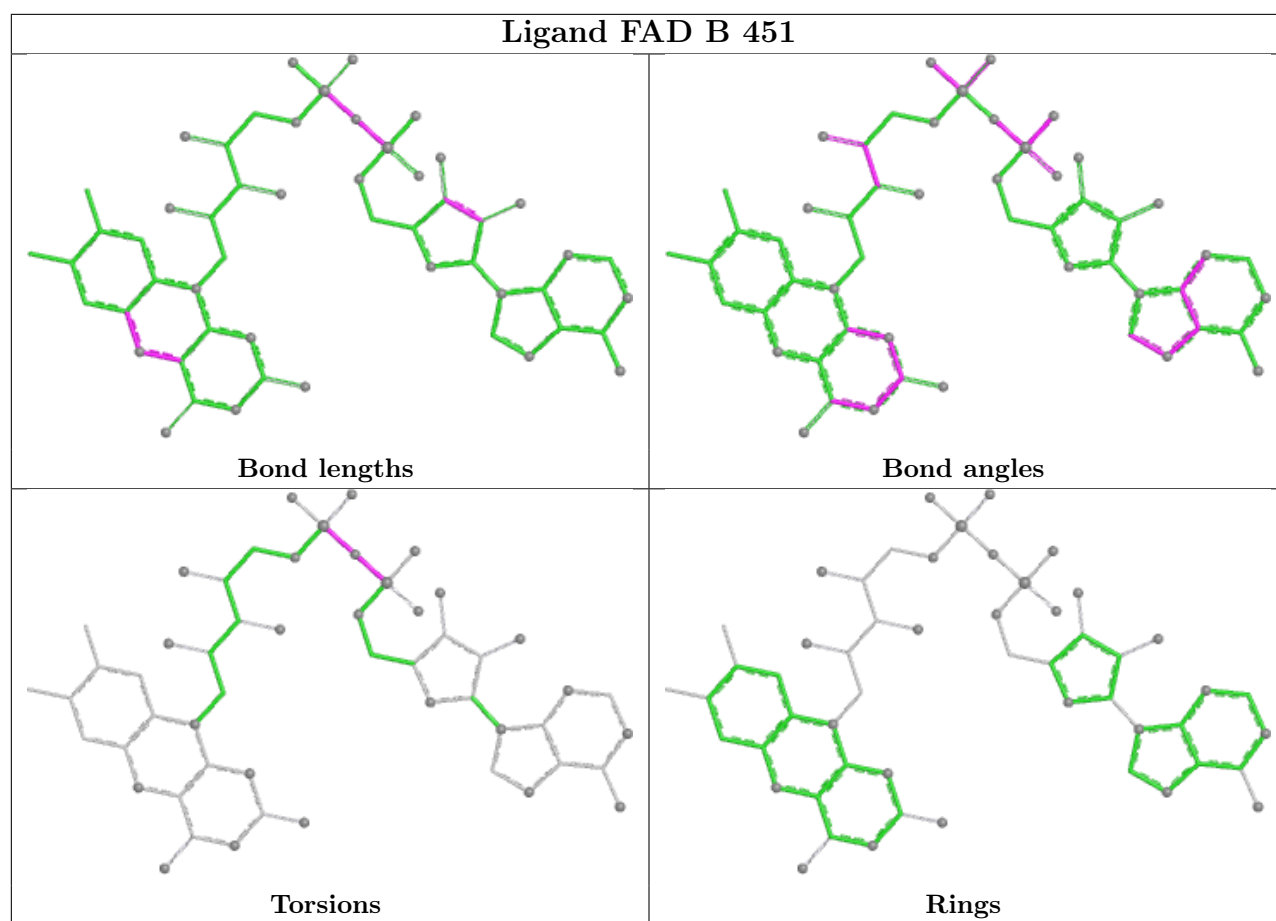
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	452	NAP	1	0
3	A	452	NAP	2	0
2	B	451	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	448/450 (99%)	-0.66	0 100 100	4, 18, 44, 63	1 (0%)
1	B	449/450 (99%)	-0.78	0 100 100	4, 16, 37, 67	1 (0%)
All	All	897/900 (99%)	-0.72	0 100 100	4, 17, 41, 67	2 (0%)

There are no RSRZ outliers to report.

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.

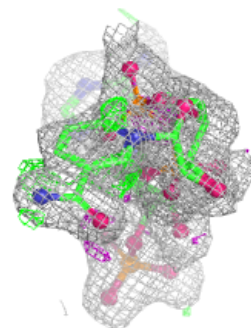
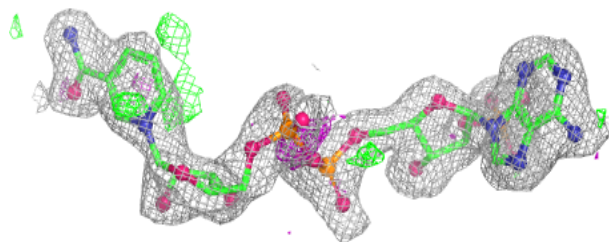
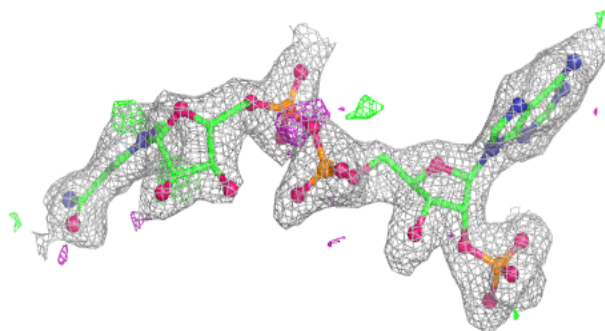
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	A	452	48/48	0.95	0.07	12,25,42,45	0
3	NAP	B	452	48/48	0.95	0.07	11,26,48,50	0
2	FAD	A	451	53/53	0.97	0.05	2,14,23,25	0
2	FAD	B	451	53/53	0.98	0.04	2,8,16,23	0

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.

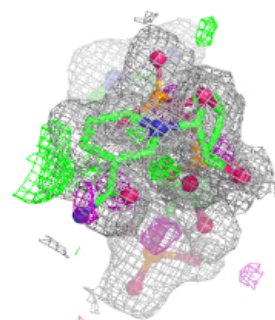
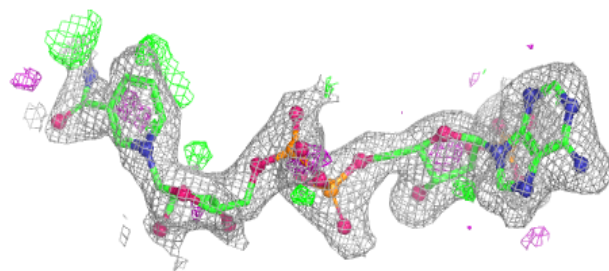
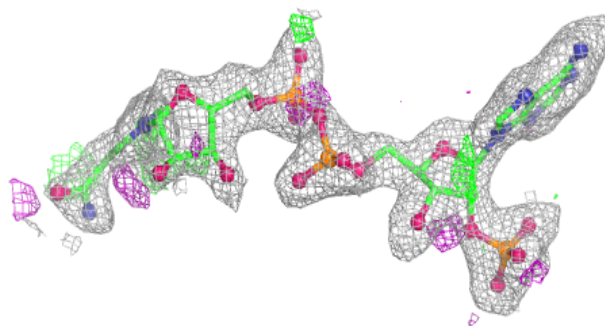
Electron density around NAP A 452:

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



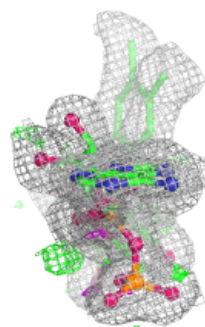
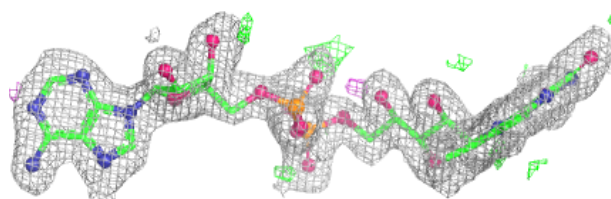
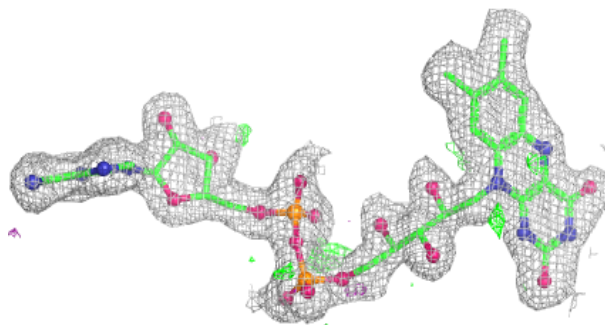
Electron density around NAP B 452:

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

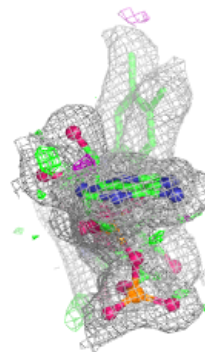
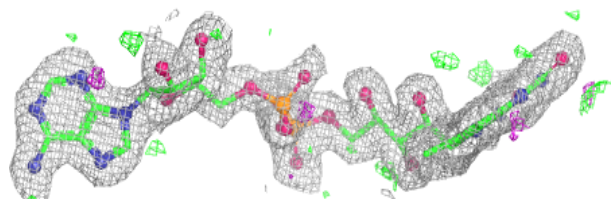
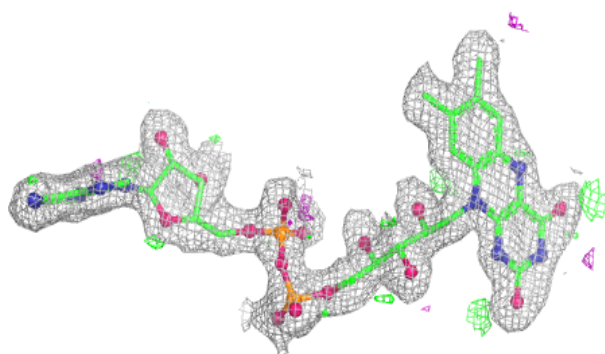


Electron density around FAD A 451:

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

**Electron density around FAD B 451:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.