



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:31 PM UTC

PDB ID : 1GRB / pdb_00001grb
Title : SUBSTRATE BINDING AND CATALYSIS BY GLUTATHIONE REDUCTASE AS DERIVED FROM REFINED ENZYME: SUBSTRATE CRYSTAL STRUCTURES AT 2 ANGSTROMS RESOLUTION
Authors : Karplus, P.A.; Schulz, G.E.
Deposited on : 1992-12-15
Resolution : 1.85 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

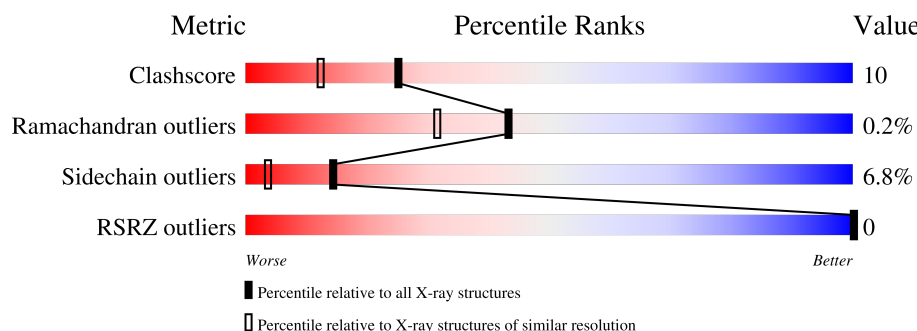
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	478	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	481	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4176 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
			Total	C	N	O	S			
1	A	461	3499	2212	603	660	24	5	0	0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



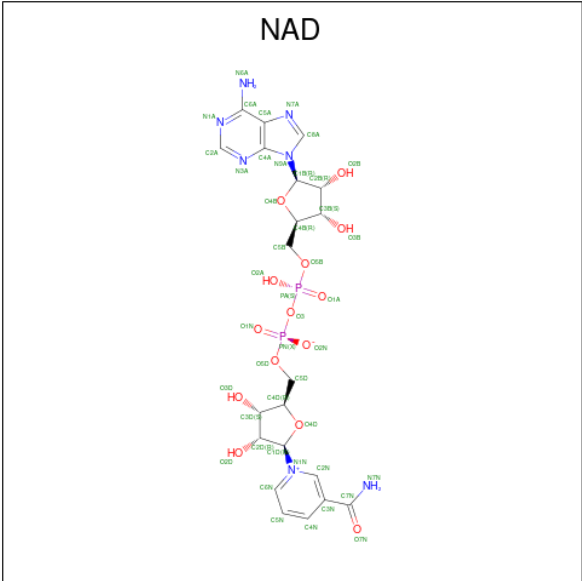
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

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



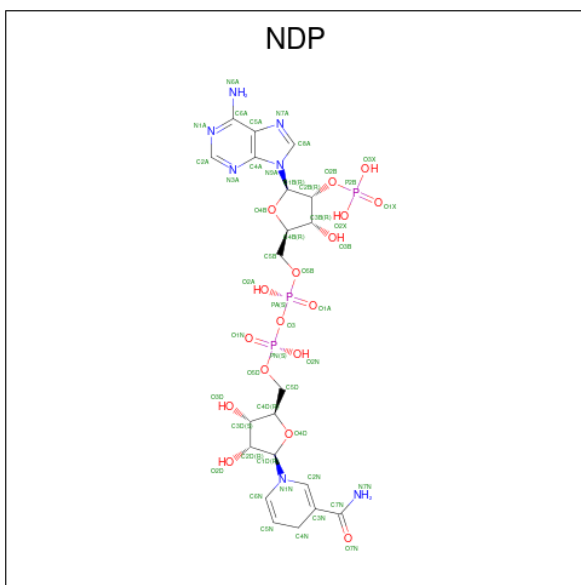
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	527	Total O 527 527	0	0

- Molecule 1: GLUTATHIONE REDUCTASE

E428	L289	S134	ALA
M435	V292	D135	CYS
L444	N293	P136	GLN
K457	N294	K137	GLU
A465	K296	P138	PRO
E472	L303	K146	GLN
E473	T307	H159	PRO
R478	H312	P160	GLY
	V315	P163	PRO
	D316	H164	PRO
	E317	Q167	ALA
	N320	F181	ALA
K324	G325	Q182	GLY
G326	I326	E186	ALA
D331	G334	R189	ALA
K335	A336	I198	ALA
L337	L338	M202	ALA
T339	P340	L205	ALA
R352	L353	K212	ALA
F354	E355	T213	ALA
S360	F372	V222	ALA
	L388	L223	ALA
E394	K397	K224	ALA
F403	V418	D227	ALA
P419	N421	S231	ALA
K426	F427	K247	ALA
		F248	ALA
		K252	ALA
		E253	ALA
		K256	ALA
		T257	ALA
		L258	ALA
		V266	ALA
		P270	ALA
		P274	ALA
		V275	ALA
		M276	ALA
		T277	ALA
		H282	ALA
		F87	ALA
		P88	ALA
		S89	ALA
		C90	ALA
		E91	ALA
		G92	ALA
		K93	ALA
		R97	ALA
		K100	ALA
		H122	ALA
		I123	ALA
		E124	ALA
		I125	ALA
		I126	ALA
		G128	ALA
		H129	ALA
		F132	ALA
		T133	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	119.80Å 84.50Å 63.20Å 90.00° 90.00° 58.70°	Depositor
Resolution (Å)	10.00 – 1.85 10.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.85) 81.7 (10.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.162 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 91.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4176	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 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NAD, NDP, FAD, PO4

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	0.98	0/3566	1.45	32/4824 (0.7%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	MET	CB-CA-C	-9.62	97.19	110.37
1	A	91	GLU	CA-C-N	-9.43	102.93	121.41
1	A	91	GLU	C-N-CA	-9.43	102.93	121.41
1	A	91	GLU	N-CA-C	8.38	122.79	112.23
1	A	55	GLY	N-CA-C	-8.14	105.00	114.69
1	A	52	HIS	CA-CB-CG	-7.91	105.89	113.80
1	A	444	LEU	N-CA-C	6.71	118.25	111.07
1	A	372	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	352	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A	181	PHE	CA-CB-CG	-6.12	107.69	113.80
1	A	189	ARG	CA-C-N	-5.96	113.33	122.62
1	A	189	ARG	C-N-CA	-5.96	113.33	122.62
1	A	354	PHE	CA-CB-CG	-5.93	107.87	113.80
1	A	97	ARG	N-CA-C	5.86	118.45	111.71
1	A	78	PHE	CA-CB-CG	-5.67	108.13	113.80
1	A	274	PRO	N-CA-CB	5.62	108.24	103.35
1	A	213	THR	N-CA-C	5.62	118.63	109.59
1	A	122	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	97	ARG	N-CA-CB	5.56	118.78	110.22
1	A	248	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	60	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	295	THR	CA-C-O	5.43	124.94	118.69
1	A	289	ILE	N-CA-C	5.43	117.42	111.77
1	A	93	LYS	N-CA-C	5.39	118.38	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ASN	N-CA-CB	-5.21	102.83	110.49
1	A	60	ASN	N-CA-C	5.17	117.71	111.40
1	A	135	ASP	CA-C-O	5.17	125.03	120.02
1	A	135	ASP	CA-C-N	5.16	126.29	119.84
1	A	135	ASP	C-N-CA	5.16	126.29	119.84
1	A	270	PRO	N-CA-CB	5.15	107.89	103.36
1	A	59	VAL	N-CA-C	5.03	115.26	110.53
1	A	163	PRO	N-CA-CB	5.02	108.00	103.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3499	0	3539	59	1
2	A	5	0	0	2	0
3	A	53	0	31	2	0
4	A	44	0	18	7	0
5	A	48	0	17	10	0
6	A	527	0	0	13	1
All	All	4176	0	3605	70	2

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 10.

All (70) 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)
3:A:479:FAD:O5'	3:A:479:FAD:C5'	1.65	1.45
4:A:480:NAD:O3B	5:A:483:NDP:O2B	1.71	1.00
1:A:202:MET:HA	1:A:202:MET:HE2	1.42	0.97
1:A:296:LYS:HB2	6:A:583:HOH:O	1.85	0.75
1:A:331:ASP:HA	1:A:337:LEU:HD22	1.73	0.70
1:A:93:LYS:O	1:A:93:LYS:HG2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HD2	6:A:721:HOH:O	1.93	0.68
3:A:479:FAD:C5'	3:A:479:FAD:P	2.86	0.64
1:A:292:VAL:HG23	1:A:293:PRO:HD2	1.80	0.63
1:A:78:PHE:HB3	6:A:958:HOH:O	1.98	0.61
1:A:293:PRO:HG3	1:A:312:HIS:CD2	2.36	0.61
1:A:222:VAL:O	1:A:231:SER:HB2	2.02	0.60
4:A:480:NAD:C3B	5:A:483:NDP:O3B	1.81	0.60
2:A:481:PO4:O2	5:A:483:NDP:H1B	2.02	0.60
1:A:185:GLU:HG3	6:A:799:HOH:O	2.01	0.59
1:A:403:PHE:CE1	1:A:473:GLU:HG3	2.39	0.58
1:A:45:ARG:NH2	1:A:124:GLU:OE1	2.38	0.57
1:A:202:MET:HE2	1:A:202:MET:CA	2.26	0.57
1:A:135:ASP:HB3	1:A:136:PRO:HD2	1.86	0.56
1:A:266:VAL:HG22	1:A:276:MET:HG2	1.89	0.54
1:A:388:ILE:HG23	1:A:393:ILE:HG12	1.89	0.54
1:A:167:GLN:HG2	6:A:646:HOH:O	2.08	0.53
4:A:480:NAD:C3B	5:A:483:NDP:HO3A	2.07	0.53
1:A:100:LYS:HG2	1:A:100:LYS:O	2.06	0.53
1:A:159:MET:HB3	1:A:160:PRO:HD2	1.91	0.52
1:A:202:MET:HA	1:A:202:MET:CE	2.28	0.52
1:A:159:MET:HB3	1:A:160:PRO:CD	2.41	0.51
1:A:125:ILE:HG22	1:A:127:ARG:HD3	1.94	0.49
1:A:247:LYS:NZ	6:A:660:HOH:O	2.45	0.49
4:A:480:NAD:C4N	5:A:483:NDP:H41N	0.97	0.49
1:A:334:GLY:HA2	1:A:337:LEU:HD21	1.95	0.49
4:A:480:NAD:H4N	5:A:483:NDP:C4N	0.97	0.49
4:A:480:NAD:C4N	5:A:483:NDP:H42N	0.97	0.48
1:A:164:HIS:HB2	6:A:912:HOH:O	2.13	0.48
1:A:198:ILE:O	1:A:202:MET:HG2	2.13	0.48
1:A:138:PRO:HB3	1:A:326:ILE:HD11	1.95	0.48
1:A:307:THR:HA	1:A:312:HIS:O	2.13	0.48
1:A:227:ASP:OD2	1:A:420:LYS:HE2	2.14	0.48
1:A:421:MET:SD	1:A:457:LYS:HD3	2.54	0.47
1:A:224:ARG:NH1	6:A:970:HOH:O	2.42	0.47
1:A:418:VAL:O	1:A:435:MET:HA	2.16	0.46
1:A:315:VAL:HA	1:A:320:ASN:O	2.16	0.46
1:A:82:HIS:CD2	1:A:87:PHE:CB	2.98	0.46
1:A:352:ARG:HB2	1:A:360:SER:HB3	1.98	0.46
1:A:91:GLU:HG2	1:A:92:GLY:N	2.31	0.46
1:A:427:GLU:OE1	1:A:427:GLU:N	2.46	0.46
1:A:182:GLN:HE21	1:A:182:GLN:HB3	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HG2	6:A:1006:HOH:O	2.16	0.45
1:A:135:ASP:CB	1:A:136:PRO:HD2	2.44	0.45
1:A:82:HIS:CD2	1:A:87:PHE:HB3	2.52	0.45
1:A:465:ALA:HB1	1:A:472:GLU:HB2	1.98	0.45
1:A:202:MET:CE	1:A:205:ILE:HD12	2.48	0.43
1:A:324:LYS:HE2	6:A:748:HOH:O	2.17	0.43
1:A:138:PRO:HA	6:A:582:HOH:O	2.19	0.42
2:A:481:PO4:O2	5:A:483:NDP:C1B	2.65	0.42
1:A:135:ASP:HA	1:A:136:PRO:HD3	1.72	0.42
1:A:65:PRO:HB2	1:A:181:PHE:CE1	2.54	0.42
1:A:339:THR:HB	1:A:340:PRO:HD3	2.02	0.42
1:A:129:HIS:CD2	1:A:129:HIS:C	2.98	0.42
1:A:337:LEU:O	5:A:483:NDP:H1D	2.19	0.41
1:A:355:GLU:O	1:A:355:GLU:HG2	2.20	0.41
1:A:78:PHE:HD1	1:A:78:PHE:HA	1.69	0.41
1:A:132:PHE:CD1	1:A:303:LEU:HD12	2.55	0.41
1:A:278:MET:HE2	1:A:278:MET:HB2	1.95	0.41
1:A:188:GLY:HA3	6:A:927:HOH:O	2.20	0.41
1:A:223:LEU:O	1:A:231:SER:HB3	2.20	0.41
5:A:483:NDP:H1B	6:A:594:HOH:O	2.20	0.41
1:A:337:LEU:O	4:A:480:NAD:H1D	2.19	0.41
1:A:427:GLU:O	1:A:428:GLU:HB2	2.21	0.40
1:A:258:LEU:HA	1:A:258:LEU:HD23	1.86	0.40

All (2) 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)
6:A:580:HOH:O	6:A:580:HOH:O[2_665]	0.76	1.44
1:A:90:CYS:SG	1:A:90:CYS:SG[2_665]	1.62	0.58

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	459/478 (96%)	440 (96%)	18 (4%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	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	382/393 (97%)	356 (93%)	26 (7%)	14	4

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	89	SER
1	A	90	CYS
1	A	91	GLU
1	A	93	LYS
1	A	134	SER
1	A	146	LYS
1	A	159	MET
1	A	167	GLN
1	A	185	GLU
1	A	202	MET
1	A	212	LYS
1	A	252	LYS
1	A	253	GLU
1	A	256	LYS
1	A	275	VAL
1	A	276	MET
1	A	292	VAL
1	A	296	LYS

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Mol	Chain	Res	Type
1	A	317	GLU
1	A	335	LYS
1	A	393	ILE
1	A	394	GLU
1	A	397	LYS
1	A	426	LYS
1	A	478	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	82	HIS
1	A	117	ASN
1	A	129	HIS
1	A	182	GLN
1	A	233	ASN
1	A	306	GLN
1	A	365	ASN
1	A	366	ASN
1	A	425	ASN
1	A	436	GLN

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	FAD	A	479	-	58,58,58	1.63	7 (12%)	85,89,89	1.17	7 (8%)
2	PO4	A	481	-	4,4,4	1.47	0	6,6,6	1.65	1 (16%)
4	NAD	A	480	-	46,48,48	1.62	6 (13%)	64,73,73	1.56	12 (18%)
5	NDP	A	483	-	51,52,52	1.72	12 (23%)	71,80,80	1.33	9 (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
3	FAD	A	479	-	-	5/34/50/50	0/6/6/6
4	NAD	A	480	-	-	7/30/62/62	0/5/5/5
5	NDP	A	483	-	-	7/34/77/77	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	479	FAD	P-O3P	-6.11	1.52	1.59
4	A	480	NAD	O4D-C1D	5.77	1.48	1.40
3	A	479	FAD	O5'-C5'	5.43	1.65	1.44
5	A	483	NDP	C4N-C3N	-4.30	1.41	1.50
3	A	479	FAD	C5'-C4'	3.76	1.56	1.51
5	A	483	NDP	PA-O5B	3.58	1.73	1.59
4	A	480	NAD	PN-O3	3.34	1.63	1.59
5	A	483	NDP	PN-O3	3.29	1.63	1.59
5	A	483	NDP	P2B-O2B	3.21	1.65	1.59
5	A	483	NDP	PA-O3	3.00	1.62	1.59
4	A	480	NAD	PA-O3	2.99	1.62	1.59
5	A	483	NDP	C6N-C5N	2.98	1.42	1.33
4	A	480	NAD	O4B-C1B	2.92	1.48	1.42
3	A	479	FAD	O4B-C1B	2.89	1.48	1.42
5	A	483	NDP	O4D-C1D	2.79	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	483	NDP	O4B-C1B	2.63	1.48	1.42
4	A	480	NAD	C5N-C4N	2.56	1.43	1.38
3	A	479	FAD	P-O2P	-2.52	1.43	1.55
4	A	480	NAD	C2N-N1N	2.40	1.37	1.35
3	A	479	FAD	O5B-C5B	2.35	1.53	1.44
5	A	483	NDP	C8A-N9A	2.31	1.41	1.37
5	A	483	NDP	C7N-C3N	2.24	1.53	1.48
5	A	483	NDP	C2A-N1A	2.21	1.37	1.33
5	A	483	NDP	C4N-C5N	-2.21	1.43	1.49
3	A	479	FAD	C1'-C2'	2.06	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	480	NAD	C6N-N1N-C2N	-5.88	116.88	121.88
3	A	479	FAD	C5'-C4'-C3'	-4.05	104.57	112.22
3	A	479	FAD	O4B-C1B-N9A	-3.74	100.90	108.09
4	A	480	NAD	O2N-PN-O1N	3.26	127.63	112.44
5	A	483	NDP	O2N-PN-O1N	3.26	127.63	112.44
4	A	480	NAD	C6N-N1N-C1D	3.00	125.62	119.73
4	A	480	NAD	C5N-C4N-C3N	-2.98	117.43	120.36
3	A	479	FAD	O5B-C5B-C4B	-2.98	98.84	108.99
5	A	483	NDP	O2A-PA-O1A	2.96	126.21	112.44
4	A	480	NAD	O2A-PA-O1A	2.96	126.21	112.44
3	A	479	FAD	O2P-P-O1P	2.81	125.51	112.44
5	A	483	NDP	C2A-N1A-C6A	2.81	123.34	118.73
4	A	480	NAD	O4D-C4D-C3D	-2.77	99.66	105.15
5	A	483	NDP	O4D-C4D-C3D	-2.77	99.66	105.15
4	A	480	NAD	O7N-C7N-C3N	-2.65	116.35	119.60
3	A	479	FAD	O2A-PA-O1A	2.62	124.62	112.44
5	A	483	NDP	O7N-C7N-C3N	-2.42	116.34	120.90
4	A	480	NAD	O5B-C5B-C4B	-2.32	101.08	108.99
5	A	483	NDP	C1D-N1N-C6N	2.29	125.62	120.77
5	A	483	NDP	C6N-N1N-C2N	-2.28	116.88	119.32
5	A	483	NDP	C1D-N1N-C2N	-2.23	117.46	121.14
2	A	481	PO4	O4-P-O1	-2.22	103.12	110.95
3	A	479	FAD	O4B-C1B-C2B	-2.10	102.11	106.62
3	A	479	FAD	C2A-N1A-C6A	2.10	122.18	118.73
4	A	480	NAD	O3-PN-O1N	-2.07	104.47	110.70
4	A	480	NAD	C4A-C5A-N7A	2.07	112.95	110.58
5	A	483	NDP	O3-PN-O1N	-2.07	104.49	110.70
4	A	480	NAD	O2B-C2B-C3B	-2.04	105.29	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	480	NAD	C2A-N1A-C6A	2.03	122.07	118.73

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	479	FAD	PA-O3P-P-O5'
5	A	483	NDP	O4D-C1D-N1N-C2N
5	A	483	NDP	O4B-C4B-C5B-O5B
5	A	483	NDP	C3B-C4B-C5B-O5B
3	A	479	FAD	O4B-C4B-C5B-O5B
4	A	480	NAD	C3D-C4D-C5D-O5D
5	A	483	NDP	C3D-C4D-C5D-O5D
4	A	480	NAD	C2B-C1B-N9A-C8A
3	A	479	FAD	C3B-C4B-C5B-O5B
3	A	479	FAD	P-O3P-PA-O2A
5	A	483	NDP	C2B-C1B-N9A-C8A
3	A	479	FAD	P-O3P-PA-O1A
4	A	480	NAD	O4B-C1B-N9A-C8A
4	A	480	NAD	O4D-C4D-C5D-O5D
5	A	483	NDP	O4D-C4D-C5D-O5D
4	A	480	NAD	C2B-C1B-N9A-C4A
4	A	480	NAD	PA-O3-PN-O2N
5	A	483	NDP	PA-O3-PN-O2N
4	A	480	NAD	O4B-C4B-C5B-O5B

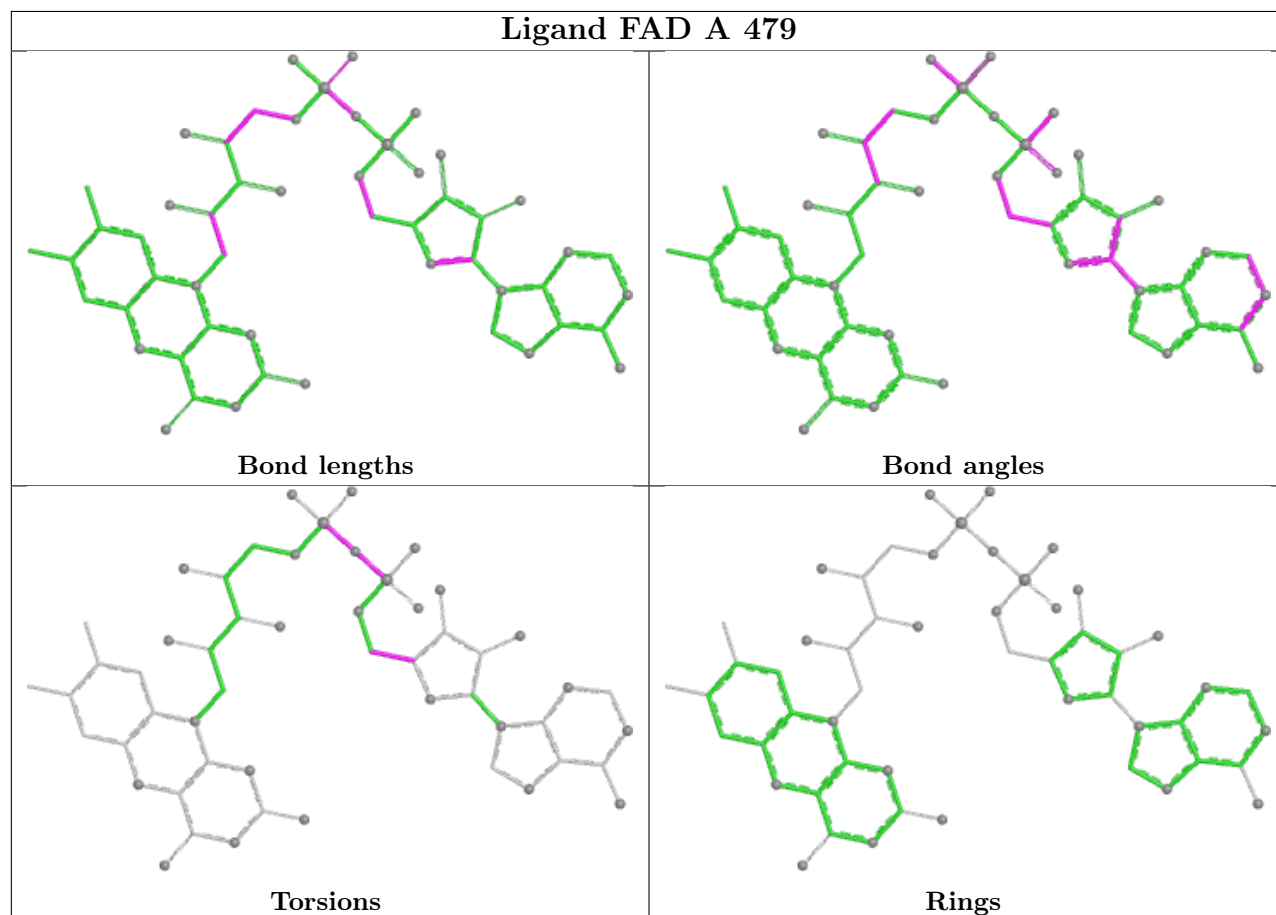
There are no ring outliers.

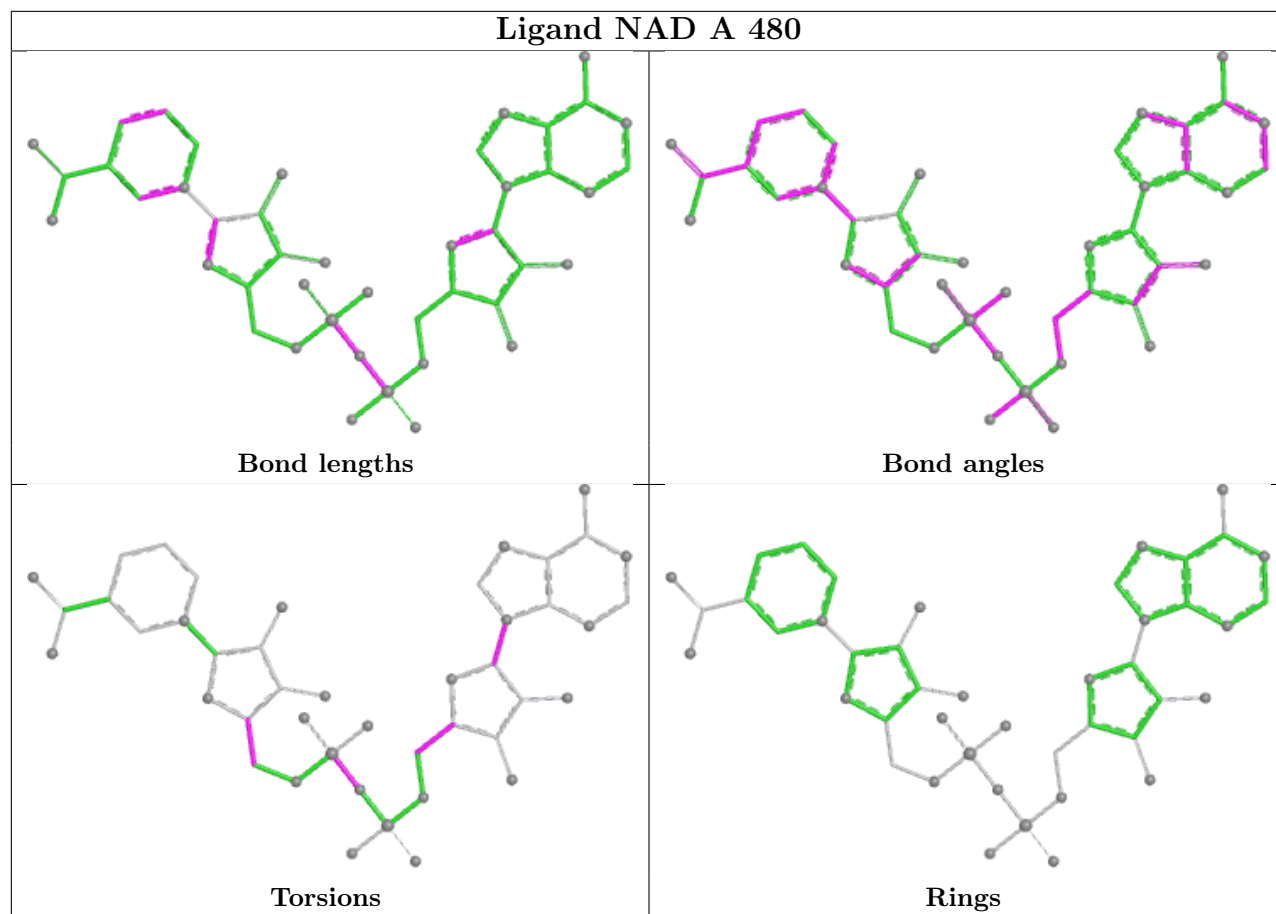
4 monomers are involved in 13 short contacts:

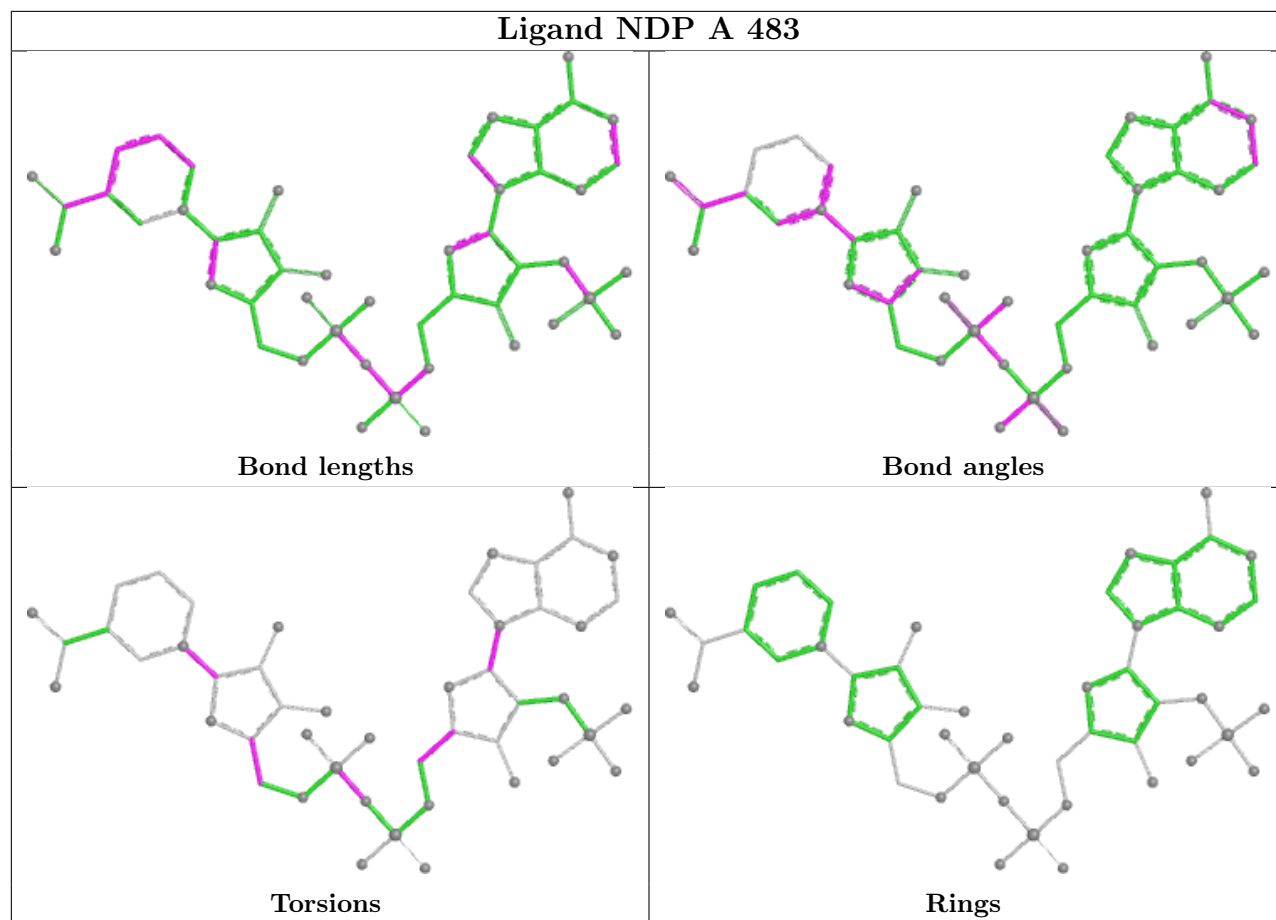
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	479	FAD	2	0
2	A	481	PO4	2	0
4	A	480	NAD	7	0
5	A	483	NDP	10	0

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	461/478 (96%)	-0.63	0 100 100	7, 18, 44, 70	1 (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](#)

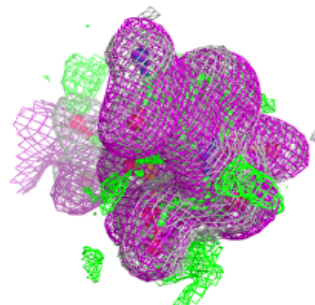
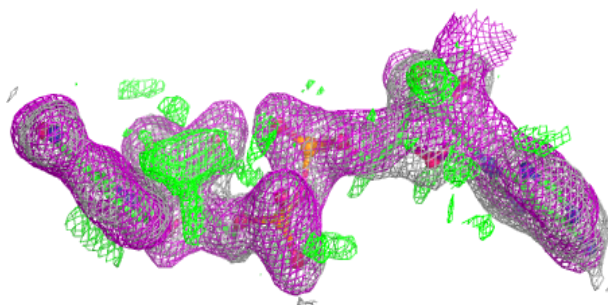
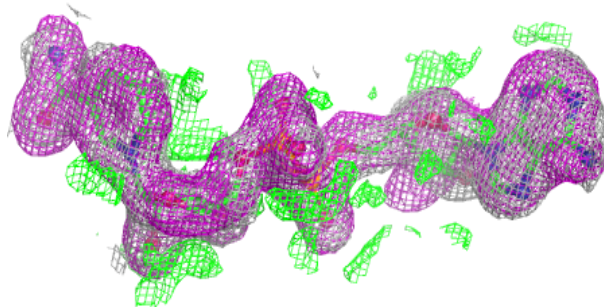
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAD	A	480	44/44	0.71	0.12	8,17,27,40	0
5	NDP	A	483	48/48	0.89	0.10	8,18,29,40	0
2	PO4	A	481	5/5	0.93	0.24	21,30,34,38	0
3	FAD	A	479	53/53	0.98	0.04	5,12,19,21	0

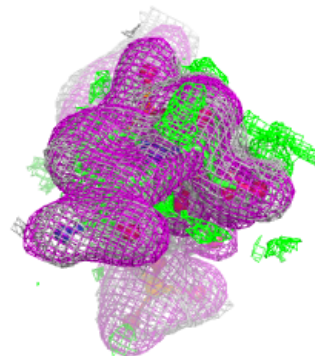
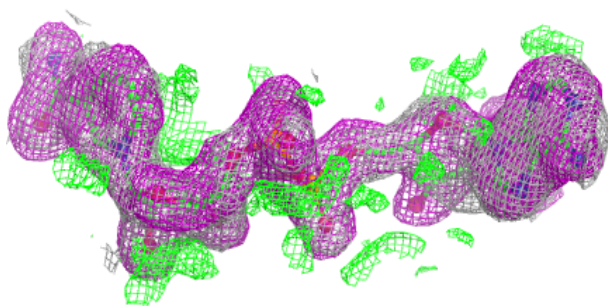
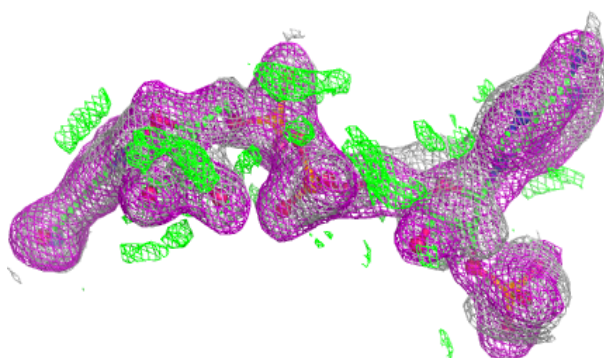
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

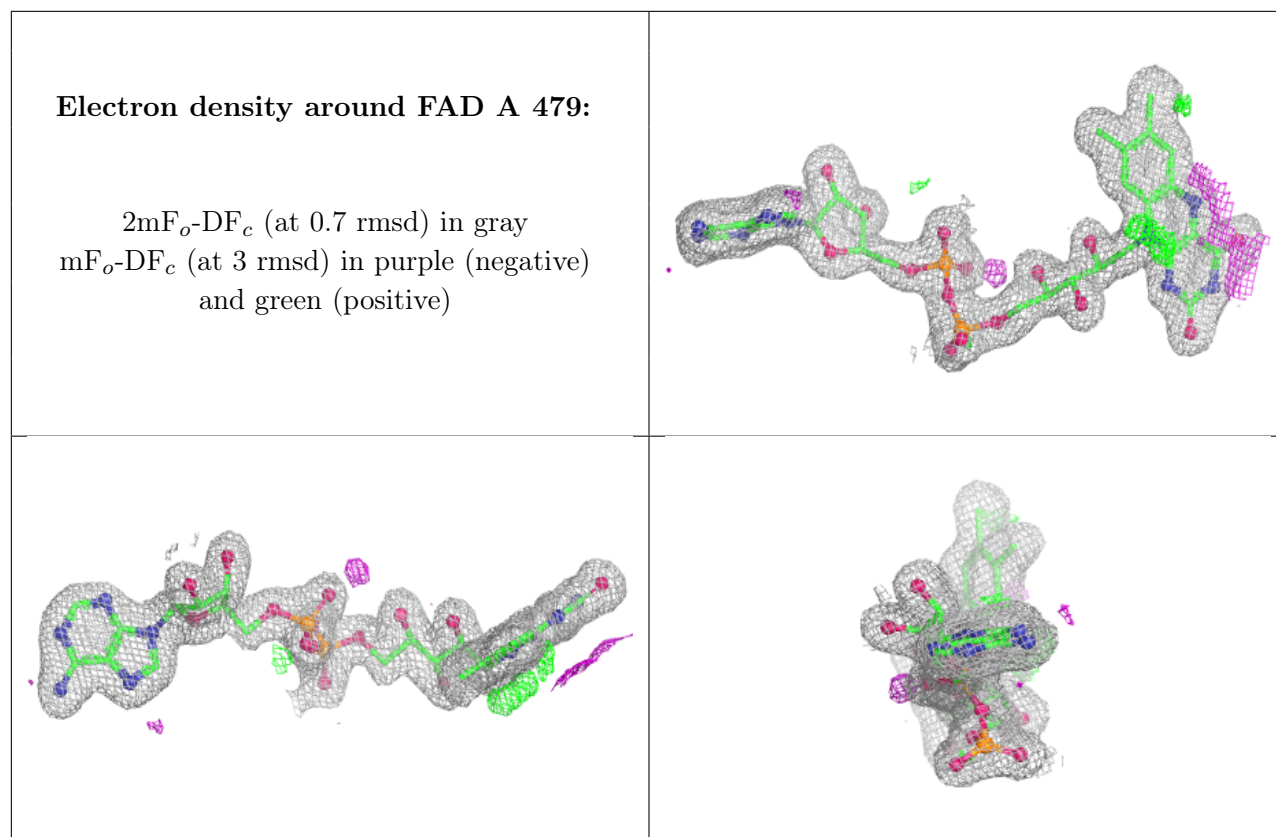
Electron density around NAD A 480:

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

**Electron density around NDP A 483:**

$2mF_o-DF_c$ (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.