



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:00 PM UTC

PDB ID : 4UP3 / pdb_00004up3
Title : Crystal structure of the mutant C140S,C286Q thioredoxin reductase from *Entamoeba histolytica*
Authors : Podust, L.M.; Vieira, D.F.
Deposited on : 2014-06-11
Resolution : 1.44 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

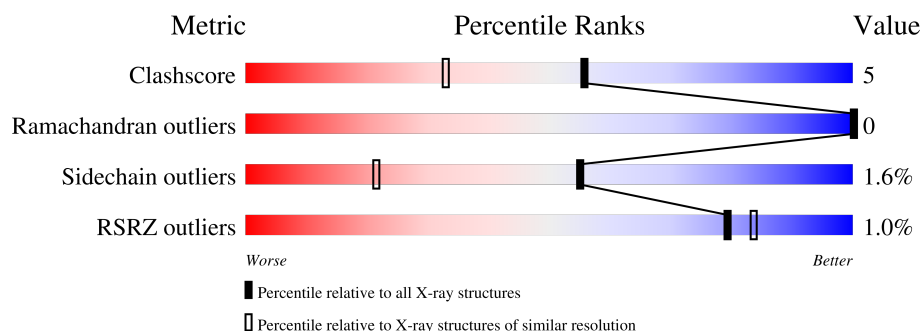
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	314	% 90% 10% .
1	B	314	% 89% 9% ..

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5812 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.

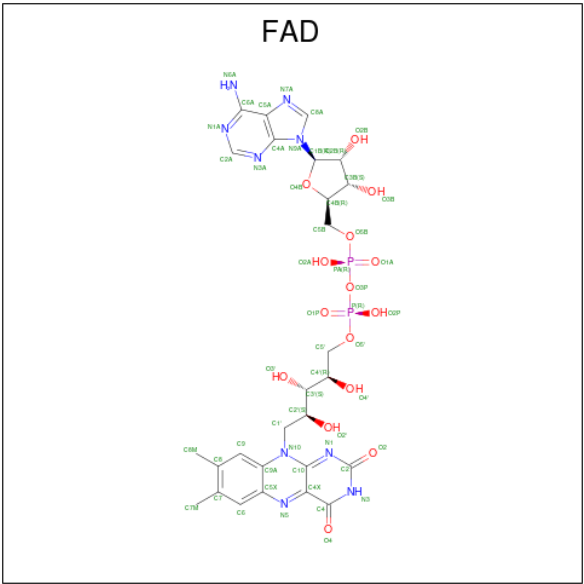
- Molecule 1 is a protein called THIOREDOXIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	9	0
			2420	1527	413	464	16			
1	B	312	Total	C	N	O	S	0	3	0
			2371	1500	408	449	14			

There are 4 discrepancies between the modelled and reference sequences:

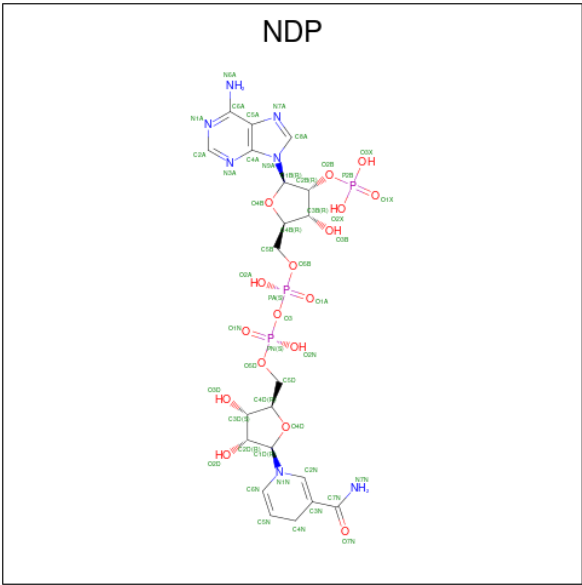
Chain	Residue	Modelled	Actual	Comment	Reference
A	140	SER	CYS	engineered mutation	UNP C4LW95
A	286	GLN	CYS	engineered mutation	UNP C4LW95
B	140	SER	CYS	engineered mutation	UNP C4LW95
B	286	GLN	CYS	engineered mutation	UNP C4LW95

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



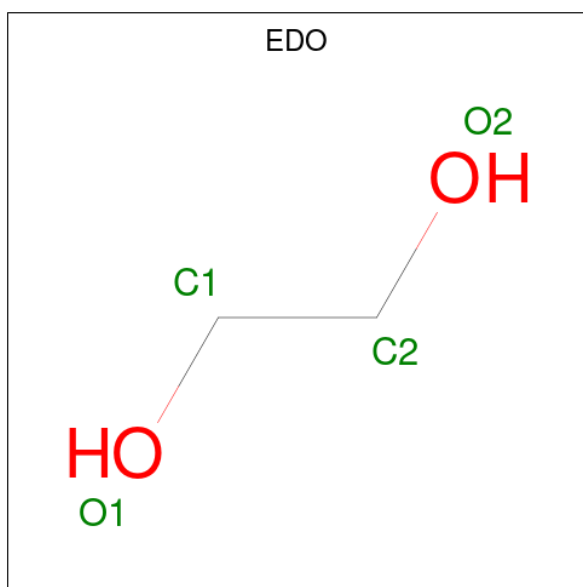
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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	1
			96	42	14	34	6		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

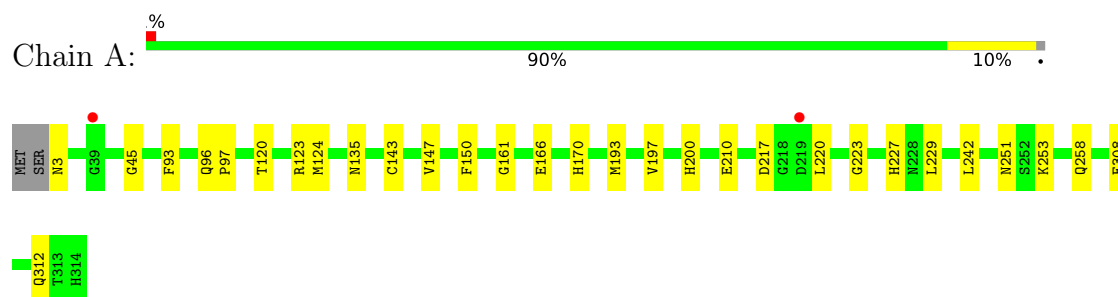
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	417	Total	O	0	0
			417	417		
5	B	350	Total	O	0	0
			350	350		

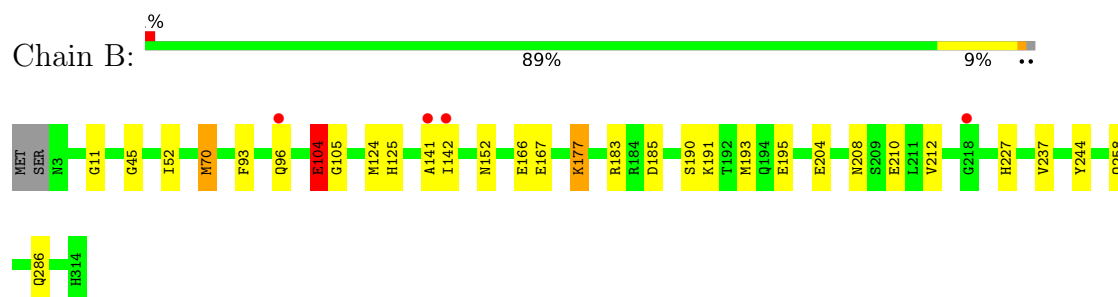
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: THIOREDOXIN REDUCTASE



- Molecule 1: THIOREDOXIN REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.78Å 92.05Å 102.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.62 – 1.44 68.62 – 1.44	Depositor EDS
% Data completeness (in resolution range)	80.8 (68.62-1.44) 80.8 (68.62-1.44)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.126 , 0.181 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5812	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: EDO, NDP, 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	1.18	2/2469 (0.1%)	1.07	4/3341 (0.1%)
1	B	1.23	3/2417 (0.1%)	1.08	5/3273 (0.2%)
All	All	1.20	5/4886 (0.1%)	1.08	9/6614 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	GLY	N-CA	6.01	1.53	1.45
1	A	161	GLY	N-CA	5.69	1.49	1.44
1	B	183	ARG	C-O	-5.41	1.16	1.24
1	B	237	VAL	CA-C	-5.31	1.49	1.53
1	A	223	GLY	C-O	-5.22	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	GLY	CA-C-O	-6.15	117.88	122.37
1	A	200	HIS	CA-C-N	-6.08	113.42	119.56
1	A	200	HIS	C-N-CA	-6.08	113.42	119.56
1	B	183	ARG	CG-CD-NE	-5.98	98.85	112.00
1	A	124	MET	CG-SD-CE	-5.78	88.18	100.90
1	B	212	VAL	N-CA-C	5.68	119.10	113.53
1	B	104	GLU	CA-C-N	-5.38	114.14	122.69
1	B	104	GLU	C-N-CA	-5.38	114.14	122.69
1	A	197	VAL	N-CA-C	5.08	115.31	110.53

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	2420	0	2398	18	0
1	B	2371	0	2359	30	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	48	0	26	0	0
3	B	96	0	52	1	0
4	B	4	0	6	0	0
5	A	417	0	0	6	0
5	B	350	0	0	8	0
All	All	5812	0	4903	47	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 (47) 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:B:96[A]:GLN:CA	1:B:96[A]:GLN:CB	2.05	1.34
1:A:308:GLU:HG2	5:A:2401:HOH:O	1.44	1.15
1:A:143[B]:CYS:SG	5:A:2229:HOH:O	2.37	0.82
1:B:52[B]:ILE:HD12	1:B:52[B]:ILE:O	1.85	0.75
1:A:120:THR:HB	1:A:251:ASN:HD21	1.53	0.73
1:B:93:PHE:H	1:B:258:GLN:HE21	1.44	0.66
1:A:93:PHE:H	1:A:258:GLN:HE21	1.45	0.65
1:B:210:GLU:OE2	1:B:227:HIS:HD2	1.81	0.63
1:A:3:ASN:HA	5:A:2001:HOH:O	2.00	0.60
1:B:70:MET:HG3	5:B:2072:HOH:O	2.03	0.59
1:A:308:GLU:OE2	1:B:190:SER:HB2	2.01	0.59
1:A:93:PHE:H	1:A:258:GLN:NE2	2.00	0.58
1:B:70:MET:O	1:B:70:MET:HE3	2.03	0.58
1:B:96[A]:GLN:CA	1:B:96[A]:GLN:CG	2.80	0.57
1:A:166:GLU:HG3	1:A:193:MET:HE2	1.87	0.56
1:A:210:GLU:OE2	1:A:227:HIS:HD2	1.88	0.55
1:B:93:PHE:H	1:B:258:GLN:NE2	2.05	0.55
1:B:191:LYS:HE3	1:B:195:GLU:OE2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLY:HA2	2:A:1315:FAD:O3B	2.06	0.55
1:B:166:GLU:CG	3:B:1316[B]:NDP:O7N	2.56	0.54
1:A:170:HIS:HE1	5:A:2226:HOH:O	1.90	0.53
1:B:125:HIS:HD2	5:B:2157:HOH:O	1.91	0.53
1:A:312:GLN:CD	5:A:2409:HOH:O	2.51	0.53
1:B:124:MET:HG3	1:B:244:TYR:CE1	2.44	0.53
1:B:141:ALA:N	1:B:167:GLU:OE1	2.37	0.52
1:A:147:VAL:HG22	1:A:150:PHE:CD2	2.44	0.52
1:B:70:MET:CG	5:B:2072:HOH:O	2.58	0.51
1:B:96[A]:GLN:NE2	5:B:2126:HOH:O	2.43	0.51
1:A:166:GLU:CG	1:A:193:MET:HE2	2.41	0.51
1:B:227:HIS:HE1	5:B:2245:HOH:O	1.94	0.51
1:A:253:LYS:HB2	5:A:2331:HOH:O	2.10	0.50
1:B:52[B]:ILE:O	1:B:52[B]:ILE:CD1	2.58	0.50
1:B:166:GLU:CG	1:B:193:MET:HE2	2.41	0.49
1:B:177:LYS:CE	1:B:204:GLU:OE1	2.61	0.48
1:A:217:ASP:OD1	1:A:217:ASP:C	2.56	0.46
1:B:52[B]:ILE:HD12	1:B:52[B]:ILE:C	2.40	0.46
1:A:210:GLU:CD	1:A:229[A]:LEU:HD21	2.40	0.46
1:B:185:ASP:HB3	1:B:208:ASN:HD21	1.79	0.46
1:B:52[B]:ILE:CD1	1:B:52[B]:ILE:C	2.90	0.45
1:B:141:ALA:CB	1:B:167:GLU:OE1	2.65	0.44
1:B:191:LYS:CE	1:B:195:GLU:OE2	2.66	0.43
1:B:152:ASN:ND2	5:B:2174:HOH:O	2.45	0.43
1:A:96:GLN:HA	1:A:97:PRO:C	2.45	0.42
1:B:45:GLY:HA2	2:B:1315:FAD:O3B	2.19	0.42
1:B:96[A]:GLN:CB	1:B:96[A]:GLN:N	2.75	0.41
1:B:104:GLU:HG2	5:B:2128:HOH:O	2.21	0.40
1:B:142:ILE:HG21	5:B:2055:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/314 (102%)	313 (98%)	6 (2%)	0	100	100
1	B	313/314 (100%)	307 (98%)	6 (2%)	0	100	100
All	All	632/628 (101%)	620 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	258/251 (103%)	254 (98%)	4 (2%)	55	21
1	B	250/251 (100%)	246 (98%)	4 (2%)	55	21
All	All	508/502 (101%)	500 (98%)	8 (2%)	55	21

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	135	ASN
1	A	220	LEU
1	A	242	LEU
1	B	70	MET
1	B	104	GLU
1	B	177	LYS
1	B	286	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	71	ASN
1	A	170	HIS
1	A	194	GLN
1	A	227	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	251	ASN
1	A	258	GLN
1	B	3	ASN
1	B	61	ASN
1	B	66	ASN
1	B	125	HIS
1	B	152	ASN
1	B	170	HIS
1	B	194	GLN
1	B	208	ASN
1	B	227	HIS
1	B	248	HIS
1	B	258	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	1315	-	58,58,58	1.68	12 (20%)	85,89,89	1.57	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDP	A	1316	-	51,52,52	1.25	6 (11%)	71,80,80	1.72	13 (18%)
4	EDO	B	1317	-	3,3,3	0.17	0	2,2,2	0.69	0
3	NDP	B	1316[B]	-	51,52,52	1.36	5 (9%)	71,80,80	1.58	14 (19%)
3	NDP	B	1316[A]	-	51,52,52	1.33	4 (7%)	71,80,80	1.65	15 (21%)
2	FAD	B	1315	-	58,58,58	1.77	7 (12%)	85,89,89	1.57	14 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	1315	-	-	5/34/50/50	0/6/6/6
3	NDP	A	1316	-	-	4/34/77/77	0/5/5/5
4	EDO	B	1317	-	-	1/1/1/1	-
3	NDP	B	1316[B]	-	-	3/34/77/77	0/5/5/5
3	NDP	B	1316[A]	-	-	4/34/77/77	0/5/5/5
2	FAD	B	1315	-	-	5/34/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1315	FAD	C9A-C5X	6.41	1.51	1.41
2	B	1315	FAD	P-O3P	5.81	1.65	1.59
3	B	1316[B]	NDP	PN-O3	4.74	1.64	1.59
3	B	1316[A]	NDP	PN-O3	4.66	1.64	1.59
2	A	1315	FAD	C9A-C5X	4.51	1.48	1.41
2	B	1315	FAD	C4X-N5	4.51	1.40	1.30
2	B	1315	FAD	C5A-C4A	4.43	1.47	1.39
3	B	1316[A]	NDP	C5A-C4A	4.34	1.46	1.39
3	B	1316[B]	NDP	C5A-C4A	4.34	1.46	1.39
2	A	1315	FAD	C8A-N7A	3.68	1.38	1.31
2	A	1315	FAD	C1'-C2'	-3.68	1.47	1.52
2	A	1315	FAD	C5A-C4A	3.63	1.45	1.39
2	A	1315	FAD	P-O3P	3.43	1.63	1.59
3	A	1316	NDP	PN-O3	3.32	1.63	1.59
3	A	1316	NDP	C5A-C4A	3.30	1.45	1.39
3	A	1316	NDP	C4A-N9A	-3.06	1.31	1.37
2	B	1315	FAD	C10-N1	3.00	1.39	1.33
3	B	1316[A]	NDP	C4A-N9A	-2.71	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1316[B]	NDP	C4A-N9A	-2.69	1.32	1.37
2	A	1315	FAD	C8-C7	2.64	1.47	1.40
2	A	1315	FAD	C5'-C4'	2.59	1.55	1.51
2	A	1315	FAD	C4X-N5	2.58	1.36	1.30
3	A	1316	NDP	P2B-O2B	2.53	1.64	1.59
2	A	1315	FAD	C2A-N1A	2.52	1.38	1.33
2	A	1315	FAD	C5A-C6A	2.42	1.47	1.41
2	B	1315	FAD	C1'-C2'	-2.39	1.49	1.52
2	B	1315	FAD	C4-N3	-2.31	1.34	1.38
3	B	1316[B]	NDP	C6N-C5N	2.21	1.39	1.33
2	A	1315	FAD	P-O1P	-2.12	1.43	1.50
3	B	1316[A]	NDP	C6N-C5N	2.11	1.39	1.33
3	A	1316	NDP	C6N-C5N	2.10	1.39	1.33
3	A	1316	NDP	PA-O3	2.07	1.61	1.59
3	B	1316[B]	NDP	C2N-C3N	2.04	1.40	1.35
2	A	1315	FAD	O3B-C3B	2.03	1.48	1.43

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1316	NDP	C6N-N1N-C2N	4.95	124.61	119.32
3	A	1316	NDP	C1D-N1N-C2N	-4.74	113.33	121.14
2	A	1315	FAD	C5A-C4A-N3A	-4.69	120.26	126.72
3	B	1316[A]	NDP	O4D-C1D-N1N	4.55	116.76	108.08
2	A	1315	FAD	C4'-C3'-C2'	-4.39	106.27	113.57
2	B	1315	FAD	C5A-C4A-N3A	-4.34	120.74	126.72
2	B	1315	FAD	C4'-C3'-C2'	-4.23	106.53	113.57
2	B	1315	FAD	C4A-C5A-N7A	-4.18	105.80	110.58
3	A	1316	NDP	C5A-C4A-N3A	-4.04	121.16	126.72
3	A	1316	NDP	C4A-C5A-N7A	-4.00	106.01	110.58
3	B	1316[A]	NDP	N3A-C2A-N1A	-3.94	122.61	128.58
3	B	1316[B]	NDP	N3A-C2A-N1A	-3.93	122.63	128.58
2	B	1315	FAD	C4A-N9A-C8A	3.62	109.54	105.74
3	B	1316[B]	NDP	O3-PN-O1N	-3.60	99.86	110.70
3	B	1316[A]	NDP	O3-PN-O1N	-3.53	100.08	110.70
2	A	1315	FAD	O2-C2-N1	-3.42	116.11	121.80
2	B	1315	FAD	N3A-C4A-N9A	3.36	132.89	127.17
3	B	1316[A]	NDP	C5A-C4A-N3A	-3.34	122.12	126.72
3	B	1316[B]	NDP	C5A-C4A-N3A	-3.34	122.12	126.72
2	A	1315	FAD	N3A-C4A-N9A	3.32	132.82	127.17
2	B	1315	FAD	C5A-N7A-C8A	3.16	108.41	103.45
3	A	1316	NDP	O2N-PN-O1N	3.15	127.11	112.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1316	NDP	O4D-C1D-N1N	3.13	114.04	108.08
3	B	1316[A]	NDP	C2A-N1A-C6A	3.11	123.85	118.73
2	B	1315	FAD	O2-C2-N1	-3.11	116.63	121.80
2	B	1315	FAD	N3-C2-N1	3.11	126.11	119.50
3	B	1316[A]	NDP	C2A-N3A-C4A	3.08	119.36	111.83
3	B	1316[B]	NDP	C2A-N3A-C4A	3.08	119.36	111.83
3	B	1316[B]	NDP	C2A-N1A-C6A	3.08	123.79	118.73
2	B	1315	FAD	O4-C4-C4X	-3.03	118.54	126.53
2	B	1315	FAD	N9A-C8A-N7A	-2.97	109.73	113.94
3	B	1316[B]	NDP	O2A-PA-O1A	2.90	125.94	112.44
3	B	1316[A]	NDP	O2A-PA-O1A	2.89	125.87	112.44
2	A	1315	FAD	O4-C4-C4X	-2.84	119.04	126.53
2	A	1315	FAD	C4-C4X-N5	2.83	122.11	118.21
2	A	1315	FAD	C4A-N9A-C8A	2.82	108.70	105.74
3	B	1316[A]	NDP	C4A-N9A-C8A	2.81	108.69	105.74
3	B	1316[B]	NDP	C4A-N9A-C8A	2.80	108.68	105.74
3	B	1316[B]	NDP	N3A-C4A-N9A	2.73	131.82	127.17
3	B	1316[A]	NDP	N3A-C4A-N9A	2.73	131.81	127.17
2	A	1315	FAD	C4A-C5A-N7A	-2.66	107.54	110.58
2	A	1315	FAD	C1'-N10-C9A	2.62	125.73	120.63
2	A	1315	FAD	C4X-C10-N10	2.58	120.17	116.48
2	B	1315	FAD	O3P-P-O1P	-2.52	103.13	110.70
2	A	1315	FAD	N9A-C8A-N7A	-2.50	110.39	113.94
3	A	1316	NDP	C5A-N7A-C8A	2.47	107.33	103.45
3	A	1316	NDP	N6A-C6A-N1A	2.44	123.80	118.38
2	A	1315	FAD	C6A-C5A-C4A	2.42	120.48	117.18
3	B	1316[A]	NDP	N6A-C6A-N1A	2.39	123.70	118.38
3	A	1316	NDP	N9A-C8A-N7A	-2.38	110.56	113.94
2	B	1315	FAD	C1'-N10-C9A	2.38	125.25	120.63
3	B	1316[B]	NDP	N6A-C6A-N1A	2.35	123.62	118.38
3	B	1316[B]	NDP	O3-PA-O1A	-2.35	103.64	110.70
3	B	1316[A]	NDP	O3-PA-O1A	-2.34	103.65	110.70
3	B	1316[B]	NDP	C4A-C5A-N7A	-2.34	107.91	110.58
3	B	1316[A]	NDP	C4A-C5A-N7A	-2.32	107.93	110.58
3	B	1316[A]	NDP	C1D-N1N-C6N	-2.30	115.92	120.77
2	A	1315	FAD	O4'-C4'-C5'	-2.30	104.92	109.99
2	A	1315	FAD	N3-C2-N1	2.20	124.17	119.50
3	A	1316	NDP	C4A-N9A-C8A	2.20	108.04	105.74
2	A	1315	FAD	C4A-N9A-C1B	-2.19	121.52	126.63
2	A	1315	FAD	O2P-P-O1P	2.18	122.59	112.44
3	B	1316[B]	NDP	C6A-C5A-N7A	2.18	136.29	132.09
3	B	1316[A]	NDP	C6A-C5A-N7A	2.17	136.27	132.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1316[A]	NDP	O2A-PA-O3	2.16	113.10	107.27
3	A	1316	NDP	C2A-N3A-C4A	2.13	117.04	111.83
3	A	1316	NDP	N3A-C4A-N9A	2.13	130.78	127.17
2	A	1315	FAD	O3P-P-O1P	-2.11	104.37	110.70
3	B	1316[B]	NDP	O2A-PA-O3	2.09	112.92	107.27
3	A	1316	NDP	C5A-C4A-N9A	2.06	108.06	105.81
2	B	1315	FAD	C4X-C10-N10	2.04	119.41	116.48
3	B	1316[B]	NDP	O4D-C1D-N1N	2.03	111.96	108.08
2	B	1315	FAD	O4-C4-N3	2.02	123.91	120.11

There are no chirality outliers.

All (22) torsion outliers are listed below:

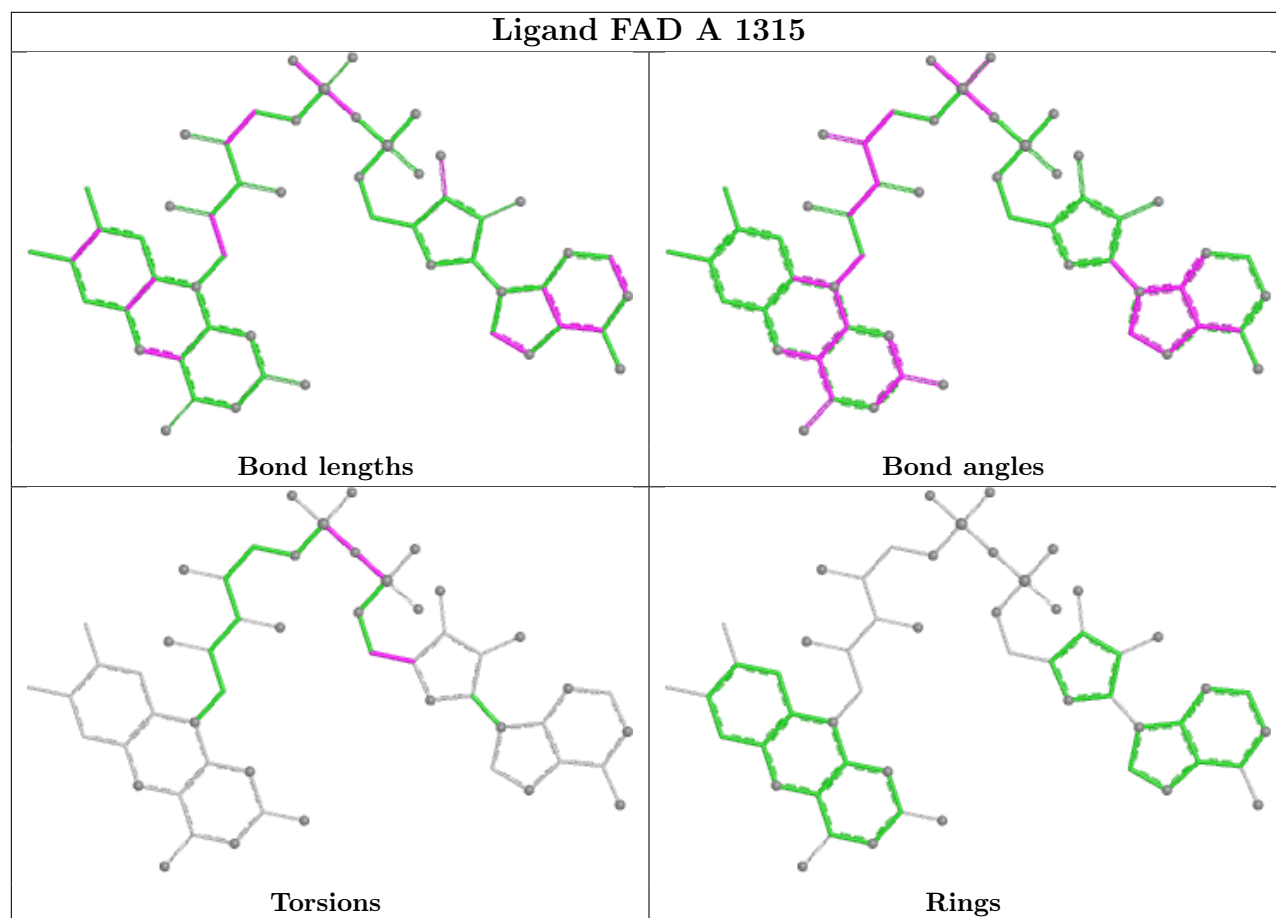
Mol	Chain	Res	Type	Atoms
3	A	1316	NDP	O4D-C1D-N1N-C6N
3	B	1316[A]	NDP	O4D-C1D-N1N-C6N
3	B	1316[B]	NDP	O4D-C1D-N1N-C2N
3	A	1316	NDP	C3B-C2B-O2B-P2B
3	B	1316[A]	NDP	C3B-C2B-O2B-P2B
3	B	1316[B]	NDP	C3B-C2B-O2B-P2B
3	A	1316	NDP	C1B-C2B-O2B-P2B
2	B	1315	FAD	C3B-C4B-C5B-O5B
2	B	1315	FAD	PA-O3P-P-O1P
2	A	1315	FAD	C3B-C4B-C5B-O5B
2	A	1315	FAD	PA-O3P-P-O5'
2	B	1315	FAD	PA-O3P-P-O5'
3	B	1316[A]	NDP	C1B-C2B-O2B-P2B
3	B	1316[B]	NDP	C1B-C2B-O2B-P2B
2	A	1315	FAD	O4B-C4B-C5B-O5B
2	A	1315	FAD	PA-O3P-P-O1P
2	B	1315	FAD	P-O3P-PA-O2A
2	B	1315	FAD	O4B-C4B-C5B-O5B
4	B	1317	EDO	O1-C1-C2-O2
3	B	1316[A]	NDP	C2D-C1D-N1N-C2N
2	A	1315	FAD	P-O3P-PA-O2A
3	A	1316	NDP	O4B-C4B-C5B-O5B

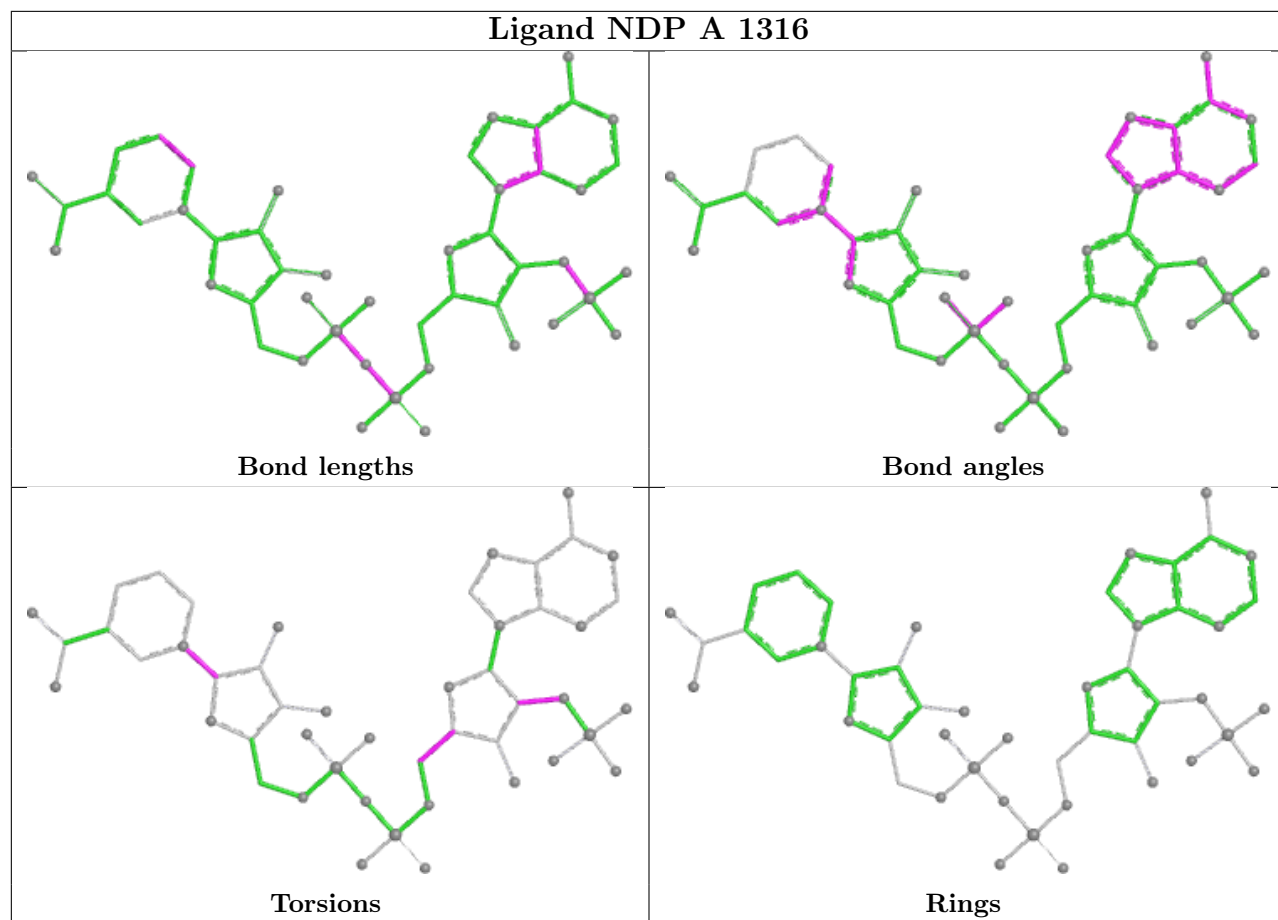
There are no ring outliers.

3 monomers are involved in 3 short contacts:

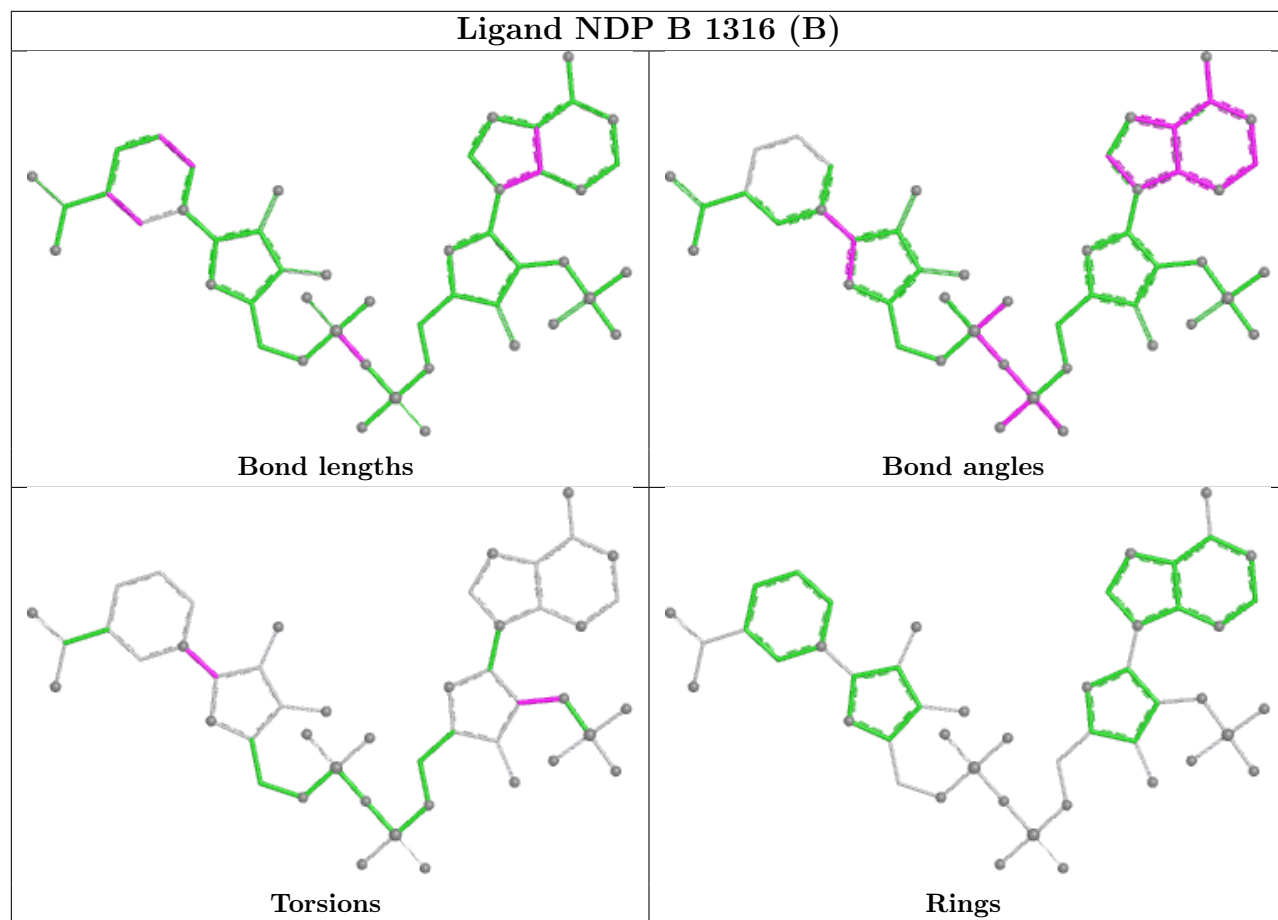
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1315	FAD	1	0
3	B	1316[B]	NDP	1	0
2	B	1315	FAD	1	0

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.

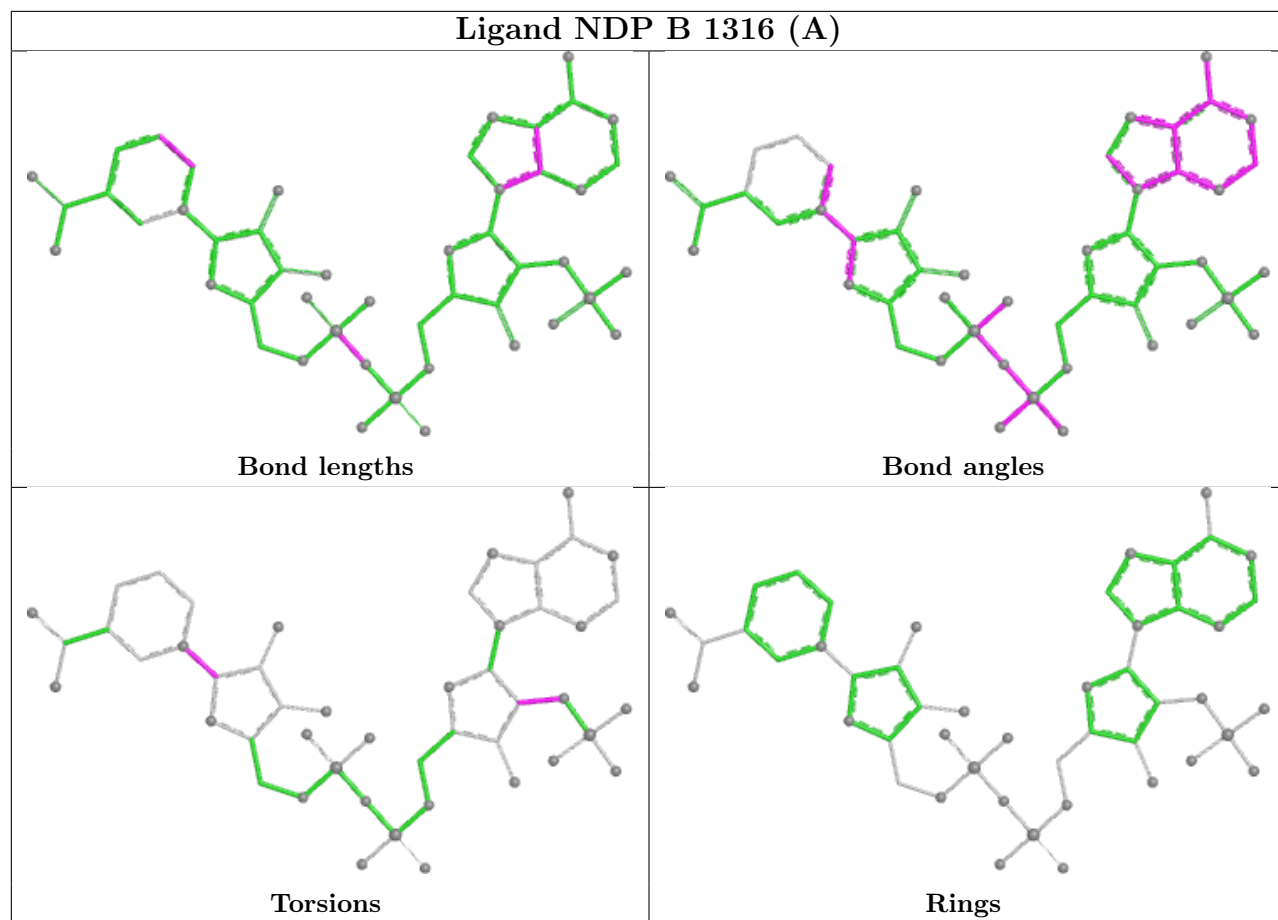


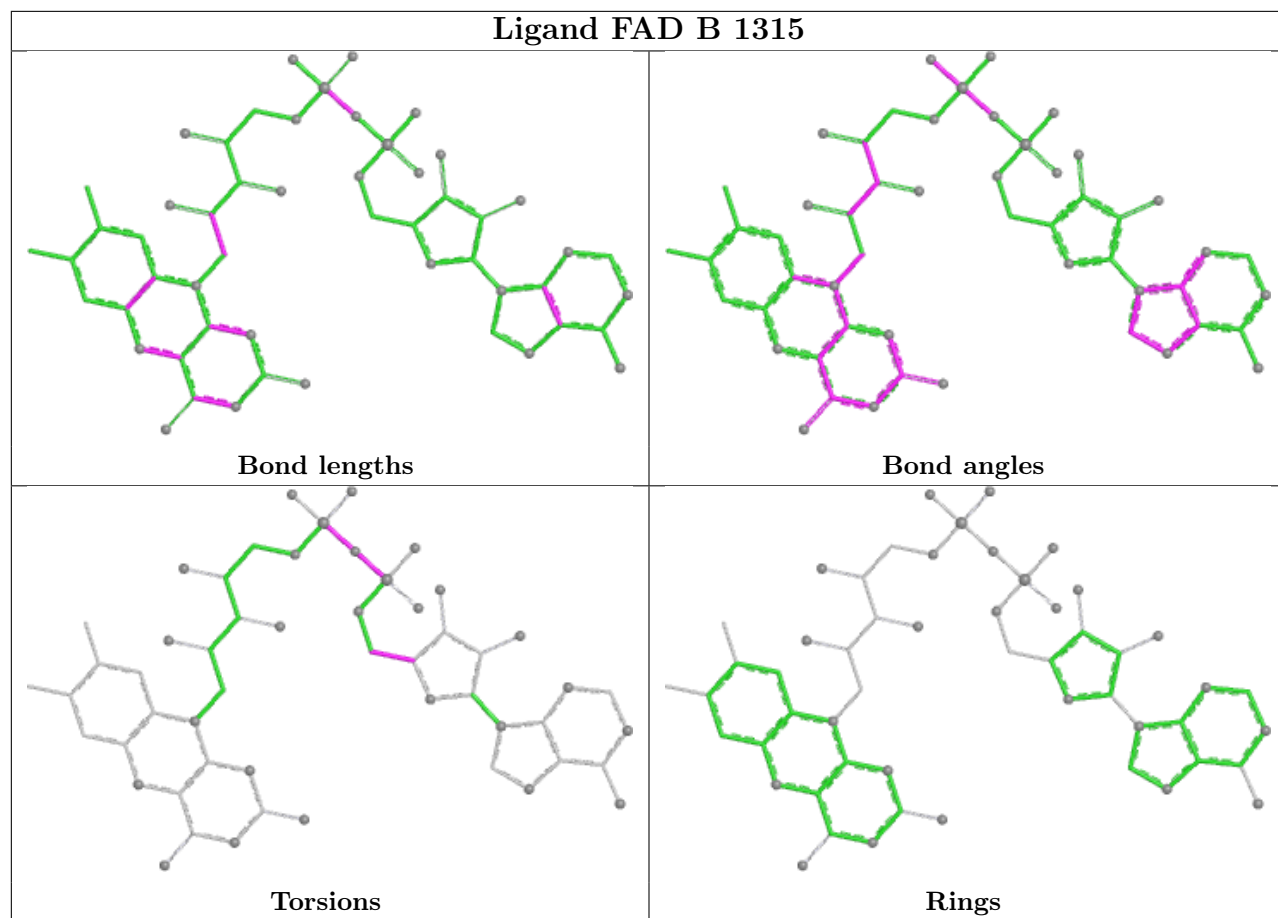


Ligand NDP B 1316 (B)



Ligand NDP B 1316 (A)





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	312/314 (99%)	-0.29	2 (0%) 85 89	10, 20, 34, 61	9 (2%)
1	B	312/314 (99%)	-0.11	4 (1%) 75 79	8, 22, 42, 63	4 (1%)
All	All	624/628 (99%)	-0.20	6 (0%) 79 84	8, 21, 39, 63	13 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	ASP	4.5
1	A	39	GLY	3.1
1	B	218	GLY	2.6
1	B	142	ILE	2.5
1	B	96[A]	GLN	2.5
1	B	141	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

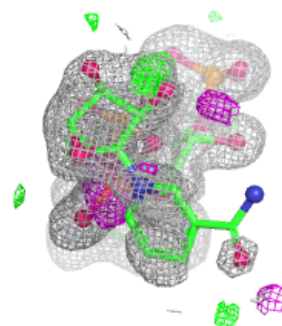
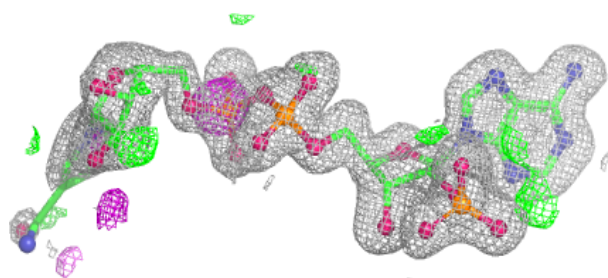
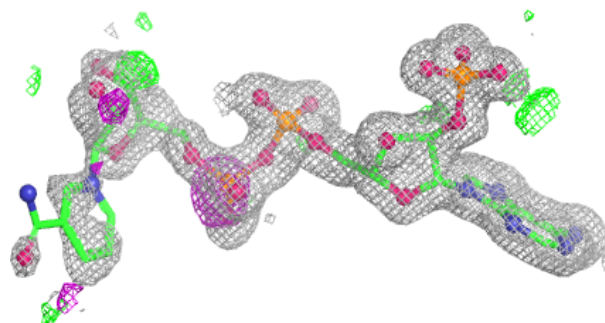
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	1317	4/4	0.87	0.12	38,43,46,49	0
3	NDP	B	1316[B]	48/48	0.96	0.09	17,25,56,65	48
3	NDP	B	1316[A]	48/48	0.96	0.09	17,25,68,71	48
2	FAD	B	1315	53/53	0.97	0.06	17,24,30,31	0
3	NDP	A	1316	48/48	0.98	0.07	13,22,70,80	0
2	FAD	A	1315	53/53	0.98	0.05	14,20,28,31	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.

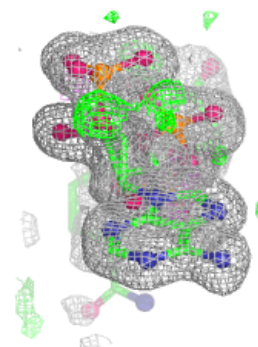
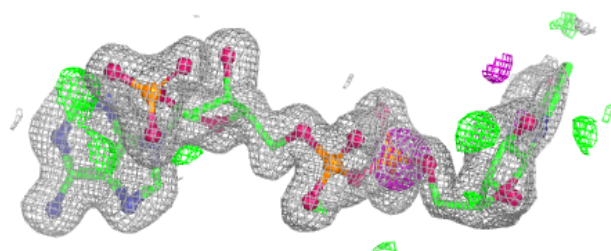
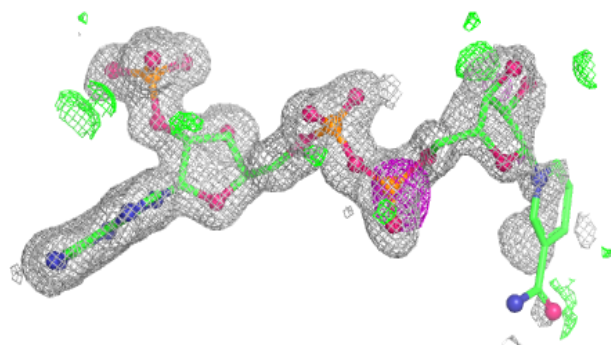
Electron density around NDP B 1316 (B):

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

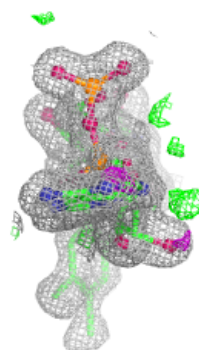
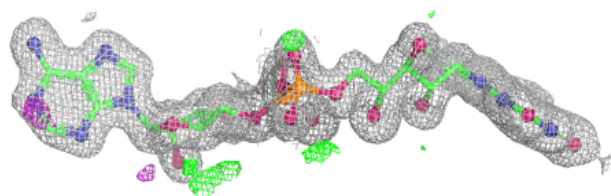
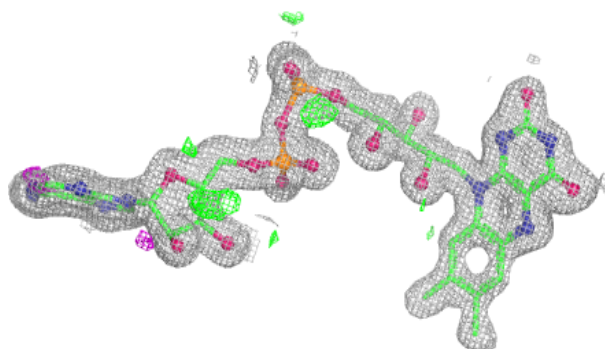


Electron density around NDP B 1316 (A):

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

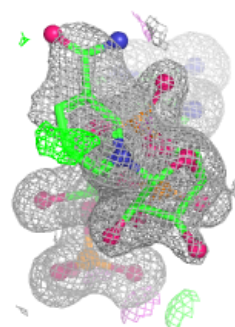
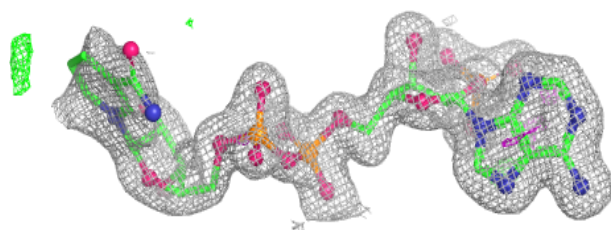
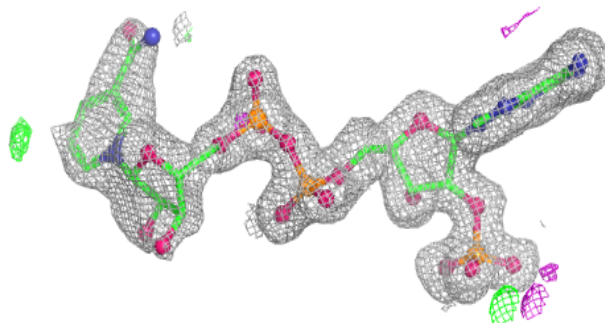
**Electron density around FAD B 1315:**

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

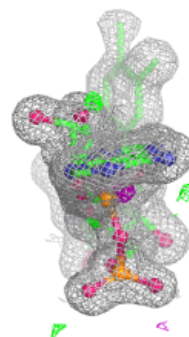
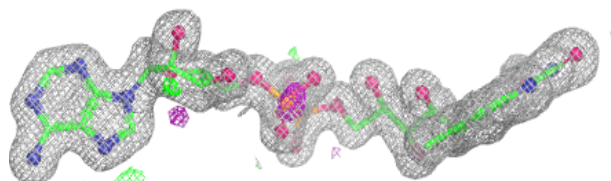
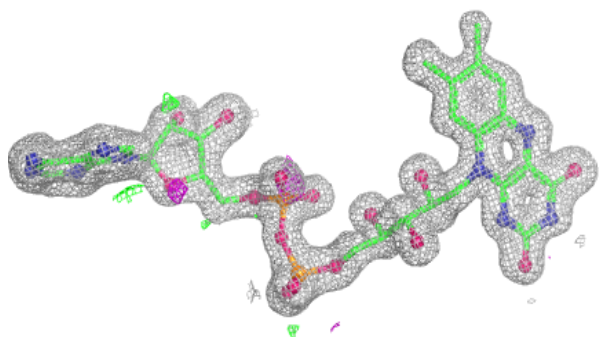


Electron density around NDP A 1316:

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

**Electron density around FAD A 1315:**

$2mF_o-DF_c$ (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.