



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:34 AM UTC

PDB ID : 2BFM / pdb_00002bfm
Title : Leishmania major pteridine reductase 1 in complex with NADP and trimethoprim
Authors : Schuettelkopf, A.W.; Hunter, W.N.
Deposited on : 2004-12-09
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

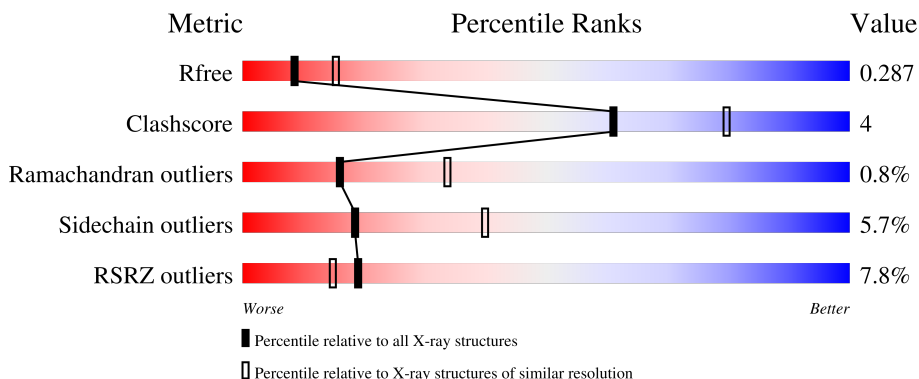
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	 8% 80% 12% • 8%
1	B	288	 10% 77% 13% • 8%
1	C	288	 6% 77% 10% • 12%
1	D	288	 5% 76% 12% • 11%

2 Entry composition [i](#)

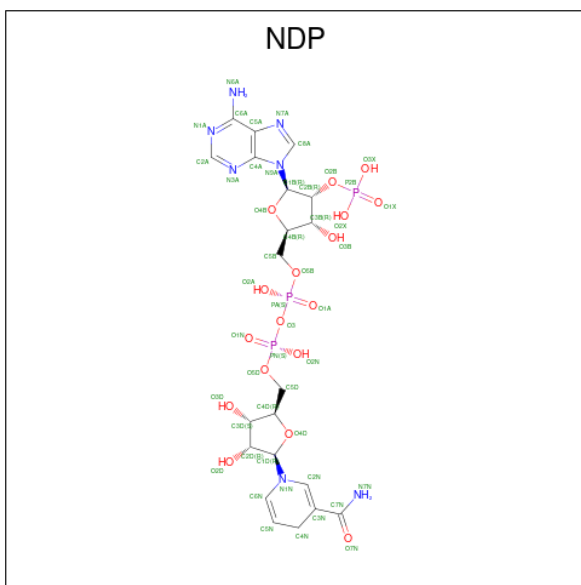
There are 4 unique types of molecules in this entry. The entry contains 8188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PTERIDINE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	Total	C	N	O	S	0	0	0
			1984	1250	353	370	11			
1	B	266	Total	C	N	O	S	0	0	0
			1987	1253	354	369	11			
1	C	254	Total	C	N	O	S	0	0	0
			1892	1192	340	350	10			
1	D	256	Total	C	N	O	S	0	0	0
			1906	1201	342	353	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



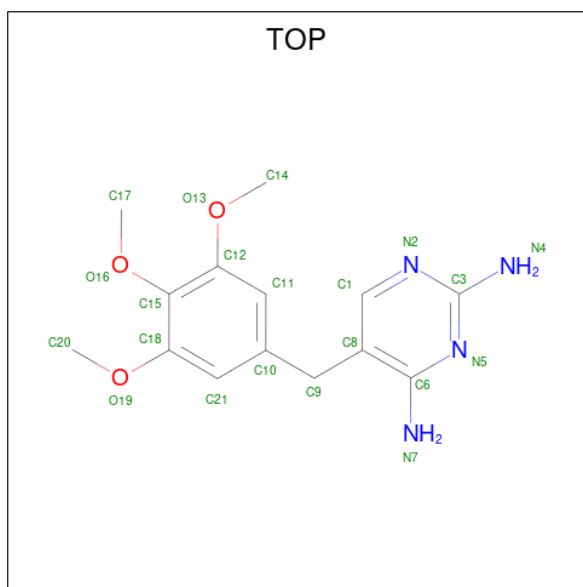
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

- Molecule 3 is TRIMETHOPRIM (CCD ID: TOP) (formula: C₁₄H₁₈N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	14	4	3		
3	B	1	Total	C	N	O	0	0
			21	14	4	3		

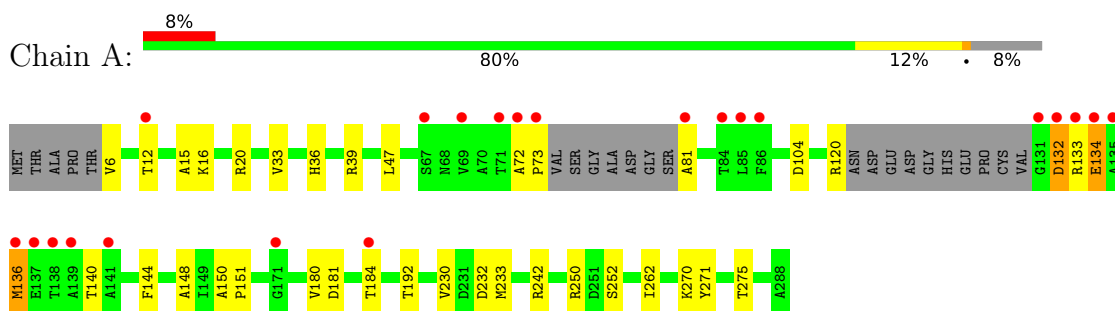
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	45	Total	O	0	0
			45	45		
4	C	44	Total	O	0	0
			44	44		
4	D	36	Total	O	0	0
			36	36		

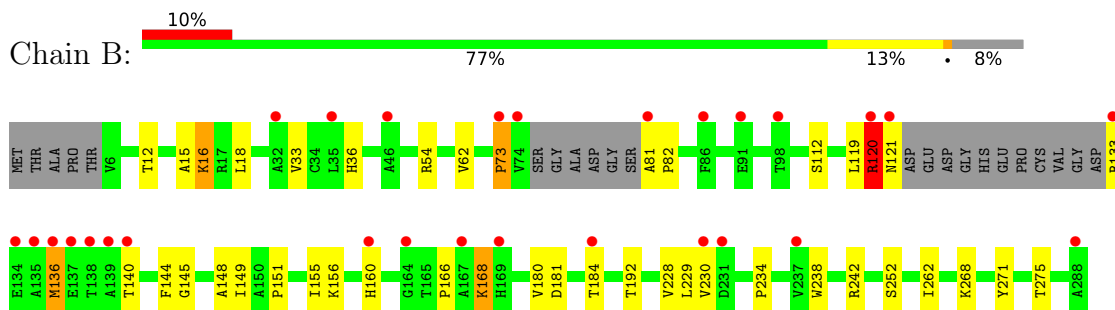
3 Residue-property plots [i](#)

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.

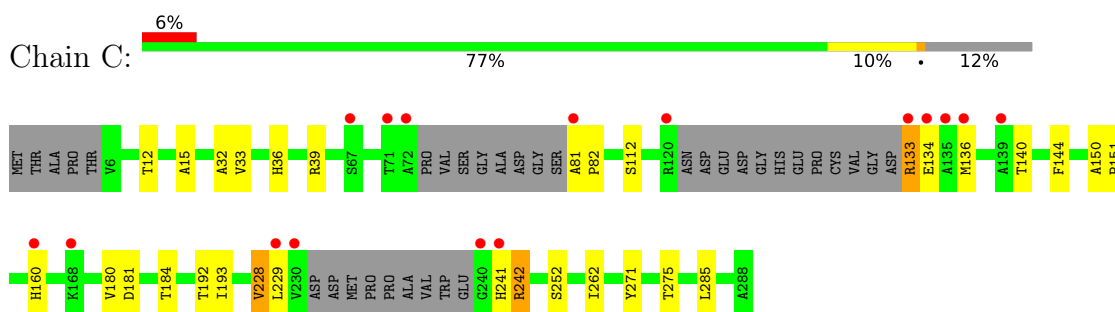
• Molecule 1: PTERIDINE REDUCTASE 1



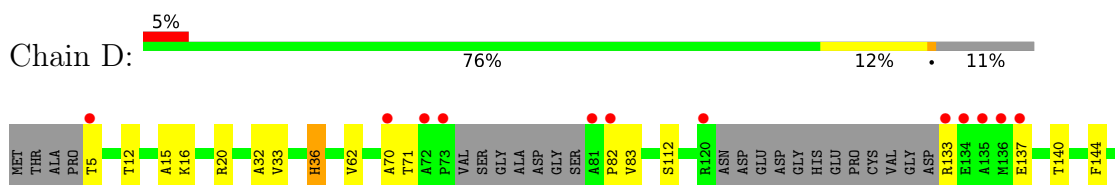
• Molecule 1: PTERIDINE REDUCTASE 1

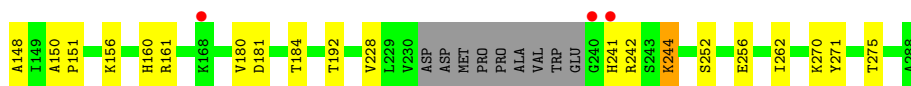


• Molecule 1: PTERIDINE REDUCTASE 1



• Molecule 1: PTERIDINE REDUCTASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.70Å 104.44Å 138.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.50 – 2.60 24.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.50-2.60) 97.5 (24.50-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.23 (at 2.60Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.253 , 0.288 0.253 , 0.287	Depositor DCC
R_{free} test set	2085 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8188	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.01 % 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 1.0083e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TOP, NDP

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	0.69	2/2023 (0.1%)	1.04	6/2755 (0.2%)
1	B	0.66	1/2026 (0.0%)	0.99	4/2760 (0.1%)
1	C	0.60	0/1925	1.00	5/2616 (0.2%)
1	D	0.62	0/1940	0.99	4/2638 (0.2%)
All	All	0.64	3/7914 (0.0%)	1.01	19/10769 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	PRO	CA-C	6.42	1.55	1.51
1	A	104	ASP	CG-OD2	-5.38	1.15	1.25
1	A	104	ASP	CG-OD1	-5.35	1.15	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASP	OD1-CG-OD2	-8.57	102.33	122.90
1	A	33	VAL	N-CA-C	6.88	117.75	108.11
1	B	192	THR	N-CA-C	6.73	119.18	111.11
1	C	33	VAL	N-CA-C	6.72	117.52	108.11
1	B	33	VAL	N-CA-C	6.44	117.13	108.11
1	D	33	VAL	N-CA-C	6.36	117.02	108.11
1	A	72	ALA	N-CA-C	6.16	116.68	109.60
1	A	15	ALA	N-CA-C	6.09	117.92	111.28
1	D	15	ALA	N-CA-C	6.06	117.89	111.28
1	C	15	ALA	N-CA-C	5.99	117.81	111.28
1	A	192	THR	N-CA-C	5.79	118.06	111.11
1	B	16	LYS	N-CA-C	5.73	115.67	108.45
1	D	192	THR	N-CA-C	5.69	117.94	111.11
1	A	104	ASP	CB-CG-OD2	5.68	131.45	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ALA	N-CA-C	5.33	117.09	111.28
1	D	32	ALA	N-CA-C	-5.07	101.45	109.96
1	C	229	LEU	N-CA-C	5.07	117.78	110.28
1	C	192	THR	N-CA-C	5.04	117.16	111.11
1	C	32	ALA	N-CA-C	-5.04	101.49	109.96

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	1984	0	1990	22	0
1	B	1987	0	1998	22	0
1	C	1892	0	1914	14	0
1	D	1906	0	1928	15	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	0	0
3	A	21	0	18	0	0
3	B	21	0	18	0	0
4	A	60	0	0	1	0
4	B	45	0	0	2	0
4	C	44	0	0	0	0
4	D	36	0	0	3	0
All	All	8188	0	7970	67	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 4.

All (67) 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:C:12:THR:HA	1:C:36:HIS:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:H	1:B:168:LYS:HD3	1.56	0.70
1:B:166:PRO:HB3	1:B:168:LYS:NZ	2.08	0.68
1:B:166:PRO:HB3	1:B:168:LYS:HZ1	1.59	0.67
1:B:156:LYS:HE2	4:B:2017:HOH:O	1.95	0.67
1:A:120:ARG:NH1	1:B:160:HIS:HB2	2.16	0.61
1:A:20:ARG:HE	1:A:47:LEU:HD13	1.65	0.60
1:B:229:LEU:HD23	1:B:238:TRP:CD1	2.36	0.60
1:A:120:ARG:CZ	1:B:160:HIS:HB2	2.32	0.58
1:B:12:THR:HA	1:B:36:HIS:HB3	1.85	0.57
1:C:39:ARG:HG2	1:C:39:ARG:HH11	1.69	0.57
1:C:133:ARG:O	1:C:136:MET:HG2	2.03	0.57
1:A:120:ARG:N	1:A:120:ARG:HD2	2.20	0.57
1:A:134:GLU:C	1:A:136:MET:H	2.12	0.57
1:A:252:SER:HB3	1:C:271:TYR:CE2	2.40	0.57
1:A:242:ARG:HB2	1:A:250:ARG:HA	1.86	0.57
1:C:81:ALA:HB3	1:C:82:PRO:HD3	1.87	0.56
1:D:181:ASP:HB3	1:D:184:THR:HG23	1.87	0.55
1:B:73:PRO:HD3	1:B:82:PRO:HA	1.86	0.55
1:C:181:ASP:HB3	1:C:184:THR:HG23	1.87	0.55
1:B:136:MET:HE3	1:B:136:MET:HA	1.91	0.53
1:D:140:THR:O	1:D:144:PHE:HB2	2.09	0.53
1:A:271:TYR:CE2	1:C:252:SER:HB3	2.44	0.52
1:A:73:PRO:HA	1:A:81:ALA:O	2.09	0.52
4:B:2025:HOH:O	1:C:285:LEU:HD23	2.09	0.52
1:D:161:ARG:NH1	4:D:2013:HOH:O	2.42	0.52
1:D:156:LYS:HG2	1:D:160:HIS:HE1	1.75	0.52
1:C:150:ALA:HB3	1:C:151:PRO:HD3	1.91	0.52
1:A:181:ASP:HB3	1:A:184:THR:HG23	1.92	0.50
1:B:252:SER:HB3	1:D:271:TYR:CE2	2.45	0.50
1:D:150:ALA:HB3	1:D:151:PRO:HD3	1.93	0.50
1:A:20:ARG:NH2	4:A:2001:HOH:O	2.43	0.50
1:B:73:PRO:HG3	1:B:81:ALA:O	2.12	0.49
1:B:168:LYS:H	1:B:168:LYS:CD	2.19	0.48
1:B:271:TYR:CE2	1:D:252:SER:HB3	2.49	0.47
1:C:39:ARG:HG2	1:C:39:ARG:NH1	2.28	0.47
1:D:156:LYS:HG2	1:D:160:HIS:CE1	2.50	0.47
1:D:148:ALA:C	1:D:151:PRO:HD2	2.41	0.46
1:B:181:ASP:HB3	1:B:184:THR:HG23	1.98	0.46
1:C:140:THR:O	1:C:144:PHE:HB2	2.16	0.45
1:D:71:THR:O	1:D:83:VAL:N	2.47	0.45
1:C:242:ARG:H	1:C:242:ARG:HG3	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:HIS:HB2	4:D:2012:HOH:O	2.16	0.45
1:B:145:GLY:HA2	1:B:149:ILE:HB	1.97	0.45
1:D:12:THR:HA	1:D:36:HIS:HB3	1.99	0.45
1:B:119:LEU:O	1:B:121:ASN:N	2.49	0.45
1:A:134:GLU:C	1:A:136:MET:N	2.75	0.45
1:A:120:ARG:N	1:A:120:ARG:CD	2.81	0.44
1:A:148:ALA:C	1:A:151:PRO:HD2	2.43	0.44
1:B:140:THR:O	1:B:144:PHE:HB2	2.17	0.44
1:B:151:PRO:O	1:B:155:ILE:HG13	2.18	0.44
1:D:70:ALA:HB1	1:D:82:PRO:HB2	1.99	0.43
1:B:148:ALA:C	1:B:151:PRO:HD2	2.44	0.43
1:B:238:TRP:CE2	1:B:242:ARG:HD2	2.54	0.43
1:A:133:ARG:HA	1:A:136:MET:HB3	1.99	0.42
1:B:119:LEU:HB3	1:B:120:ARG:H	1.52	0.42
1:D:244:LYS:HD3	1:D:244:LYS:HA	1.59	0.42
1:A:12:THR:HA	1:A:36:HIS:HB3	2.01	0.42
1:A:150:ALA:HB3	1:A:151:PRO:HD3	2.02	0.42
1:D:256:GLU:HA	4:D:2029:HOH:O	2.21	0.41
1:A:120:ARG:CD	1:A:120:ARG:H	2.33	0.41
1:A:132:ASP:C	1:A:134:GLU:H	2.28	0.40
1:A:232:ASP:O	1:A:232:ASP:CG	2.64	0.40
1:C:133:ARG:N	1:C:136:MET:HE3	2.36	0.40
1:A:140:THR:O	1:A:144:PHE:HB2	2.20	0.40
1:A:230:VAL:O	1:A:233:MET:HE3	2.21	0.40
1:D:36:HIS:ND1	1:D:36:HIS:C	2.77	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	260/288 (90%)	241 (93%)	18 (7%)	1 (0%)	30 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	260/288 (90%)	242 (93%)	14 (5%)	4 (2%)	8	18
1	C	246/288 (85%)	234 (95%)	10 (4%)	2 (1%)	16	34
1	D	248/288 (86%)	235 (95%)	12 (5%)	1 (0%)	30	51
All	All	1014/1152 (88%)	952 (94%)	54 (5%)	8 (1%)	16	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	ARG
1	B	136	MET
1	A	180	VAL
1	B	180	VAL
1	C	228	VAL
1	D	180	VAL
1	C	180	VAL
1	B	73	PRO

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	206/223 (92%)	197 (96%)	9 (4%)	25	50
1	B	207/223 (93%)	194 (94%)	13 (6%)	16	36
1	C	196/223 (88%)	187 (95%)	9 (5%)	24	49
1	D	198/223 (89%)	183 (92%)	15 (8%)	12	27
All	All	807/892 (90%)	761 (94%)	46 (6%)	18	40

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	16	LYS
1	A	39	ARG

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Mol	Chain	Res	Type
1	A	132	ASP
1	A	134	GLU
1	A	136	MET
1	A	262	ILE
1	A	270	LYS
1	A	275	THR
1	B	16	LYS
1	B	18	LEU
1	B	54	ARG
1	B	62	VAL
1	B	112	SER
1	B	120	ARG
1	B	133	ARG
1	B	168	LYS
1	B	228	VAL
1	B	230	VAL
1	B	262	ILE
1	B	268	LYS
1	B	275	THR
1	C	112	SER
1	C	133	ARG
1	C	134	GLU
1	C	193	ILE
1	C	228	VAL
1	C	241	HIS
1	C	242	ARG
1	C	262	ILE
1	C	275	THR
1	D	5	THR
1	D	16	LYS
1	D	20	ARG
1	D	36	HIS
1	D	62	VAL
1	D	112	SER
1	D	133	ARG
1	D	137	GLU
1	D	228	VAL
1	D	241	HIS
1	D	242	ARG
1	D	244	LYS
1	D	262	ILE
1	D	270	LYS

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Mol	Chain	Res	Type
1	D	275	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	108	ASN
1	A	216	GLN
1	B	108	ASN
1	B	216	GLN
1	C	108	ASN
1	C	216	GLN
1	D	108	ASN
1	D	216	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	NDP	B	1289	-	51,52,52	1.66	7 (13%)	71,80,80	1.45	10 (14%)
3	TOP	B	1290	-	22,22,22	2.44	4 (18%)	30,30,30	2.40	13 (43%)
3	TOP	A	1290	-	22,22,22	2.40	3 (13%)	30,30,30	2.26	13 (43%)
2	NDP	C	1289	-	51,52,52	1.69	7 (13%)	71,80,80	1.58	12 (16%)
2	NDP	D	1289	-	51,52,52	1.66	8 (15%)	71,80,80	1.55	11 (15%)
2	NDP	A	1289	-	51,52,52	1.66	8 (15%)	71,80,80	1.48	10 (14%)

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	NDP	B	1289	-	-	3/34/77/77	0/5/5/5
3	TOP	B	1290	-	-	2/10/10/10	0/2/2/2
3	TOP	A	1290	-	-	2/10/10/10	0/2/2/2
2	NDP	C	1289	-	-	3/34/77/77	0/5/5/5
2	NDP	D	1289	-	-	2/34/77/77	0/5/5/5
2	NDP	A	1289	-	-	2/34/77/77	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1289	NDP	O7N-C7N	7.12	1.41	1.24
2	A	1289	NDP	O7N-C7N	7.12	1.41	1.24
2	B	1289	NDP	O7N-C7N	7.08	1.41	1.24
2	C	1289	NDP	O7N-C7N	7.04	1.40	1.24
3	A	1290	TOP	O13-C12	-6.62	1.26	1.37
3	B	1290	TOP	O13-C12	-6.42	1.26	1.37
3	B	1290	TOP	O19-C18	-6.34	1.26	1.37
3	B	1290	TOP	O16-C15	-6.15	1.27	1.38
3	A	1290	TOP	O19-C18	-6.13	1.27	1.37
3	A	1290	TOP	O16-C15	-5.84	1.27	1.38
2	B	1289	NDP	C4N-C3N	-5.75	1.39	1.50
2	A	1289	NDP	C4N-C3N	-5.61	1.39	1.50
2	C	1289	NDP	C4N-C3N	-5.51	1.39	1.50
2	D	1289	NDP	C4N-C3N	-5.42	1.39	1.50
2	C	1289	NDP	C2A-N1A	3.01	1.39	1.33
2	C	1289	NDP	PA-O3	3.00	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1289	NDP	PN-O3	2.89	1.62	1.59
2	D	1289	NDP	PA-O3	2.85	1.62	1.59
2	A	1289	NDP	C2A-N1A	2.71	1.38	1.33
2	C	1289	NDP	C2A-N3A	2.67	1.38	1.33
2	B	1289	NDP	PN-O3	2.66	1.62	1.59
2	A	1289	NDP	C5A-N7A	-2.58	1.34	1.39
2	B	1289	NDP	C2A-N1A	2.50	1.38	1.33
2	D	1289	NDP	C2A-N1A	2.41	1.38	1.33
2	D	1289	NDP	PN-O3	2.41	1.62	1.59
2	D	1289	NDP	C2A-N3A	2.40	1.38	1.33
2	B	1289	NDP	C2A-N3A	2.38	1.38	1.33
2	A	1289	NDP	C2A-N3A	2.27	1.38	1.33
2	B	1289	NDP	C5A-N7A	-2.25	1.35	1.39
2	B	1289	NDP	PA-O3	2.21	1.61	1.59
2	A	1289	NDP	C6N-C5N	2.11	1.39	1.33
3	B	1290	TOP	C8-C6	-2.10	1.39	1.42
2	A	1289	NDP	PA-O3	2.08	1.61	1.59
2	A	1289	NDP	PN-O3	2.07	1.61	1.59
2	C	1289	NDP	C8A-N7A	2.07	1.35	1.31
2	D	1289	NDP	C6N-C5N	2.05	1.39	1.33
2	D	1289	NDP	C5A-N7A	-2.04	1.35	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1289	NDP	N3A-C2A-N1A	-5.87	119.70	128.58
2	A	1289	NDP	N3A-C2A-N1A	-5.76	119.86	128.58
2	B	1289	NDP	N3A-C2A-N1A	-5.74	119.89	128.58
2	C	1289	NDP	N3A-C2A-N1A	-5.68	119.98	128.58
3	B	1290	TOP	N2-C3-N5	-5.07	120.06	125.70
3	A	1290	TOP	N2-C3-N5	-4.67	120.50	125.70
2	C	1289	NDP	C5A-C4A-N3A	-4.57	120.42	126.72
2	D	1289	NDP	C5A-C4A-N3A	-4.34	120.74	126.72
3	B	1290	TOP	C14-O13-C12	4.28	123.80	117.51
2	C	1289	NDP	N9A-C8A-N7A	-4.22	107.95	113.94
2	D	1289	NDP	N9A-C8A-N7A	-4.20	107.97	113.94
3	B	1290	TOP	O13-C12-C15	4.00	122.00	115.14
2	A	1289	NDP	C5A-C4A-N3A	-3.96	121.27	126.72
2	B	1289	NDP	C5A-C4A-N3A	-3.86	121.41	126.72
2	C	1289	NDP	C5A-N7A-C8A	3.85	109.50	103.45
2	D	1289	NDP	C5A-N7A-C8A	3.74	109.33	103.45
3	A	1290	TOP	C20-O19-C18	3.66	122.88	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1289	NDP	N9A-C8A-N7A	-3.64	108.77	113.94
2	A	1289	NDP	N9A-C8A-N7A	-3.62	108.81	113.94
3	A	1290	TOP	C17-O16-C15	3.59	124.50	114.74
2	C	1289	NDP	C2A-N3A-C4A	3.58	120.57	111.83
3	A	1290	TOP	O19-C18-C15	3.55	121.22	115.14
2	D	1289	NDP	C2A-N3A-C4A	3.54	120.47	111.83
3	A	1290	TOP	O13-C12-C15	3.46	121.07	115.14
3	B	1290	TOP	O13-C12-C11	-3.41	118.20	124.08
3	A	1290	TOP	O13-C12-C11	-3.40	118.22	124.08
3	B	1290	TOP	C20-O19-C18	3.39	122.48	117.51
3	B	1290	TOP	O19-C18-C15	3.34	120.87	115.14
3	A	1290	TOP	C8-C1-N2	-3.33	118.42	123.83
2	B	1289	NDP	C2A-N3A-C4A	3.30	119.89	111.83
2	A	1289	NDP	C2A-N3A-C4A	3.29	119.87	111.83
3	B	1290	TOP	C17-O16-C15	3.23	123.52	114.74
2	A	1289	NDP	C5A-N7A-C8A	3.23	108.53	103.45
2	B	1289	NDP	C5A-N7A-C8A	3.22	108.52	103.45
3	B	1290	TOP	C1-C8-C6	3.18	119.46	115.55
2	C	1289	NDP	C4A-C5A-N7A	-3.18	106.94	110.58
3	A	1290	TOP	C1-N2-C3	3.09	121.74	116.29
3	B	1290	TOP	N4-C3-N2	3.09	120.60	117.40
3	B	1290	TOP	C8-C1-N2	-3.09	118.81	123.83
3	A	1290	TOP	N4-C3-N2	3.06	120.57	117.40
3	B	1290	TOP	C1-N2-C3	3.00	121.56	116.29
3	A	1290	TOP	C14-O13-C12	2.99	121.89	117.51
2	C	1289	NDP	N3A-C4A-N9A	2.85	132.01	127.17
2	D	1289	NDP	C4A-C5A-N7A	-2.83	107.34	110.58
3	A	1290	TOP	C1-C8-C6	2.82	119.02	115.55
2	D	1289	NDP	N3A-C4A-N9A	2.75	131.85	127.17
2	A	1289	NDP	O2A-PA-O3	2.74	114.67	107.27
2	B	1289	NDP	O4B-C1B-N9A	2.73	113.34	108.09
2	B	1289	NDP	C6N-N1N-C2N	2.60	122.11	119.32
3	A	1290	TOP	O19-C18-C21	-2.53	119.72	124.08
2	B	1289	NDP	N3A-C4A-N9A	2.47	131.36	127.17
2	C	1289	NDP	C6N-N1N-C2N	2.46	121.95	119.32
3	B	1290	TOP	C3-N5-C6	2.46	120.23	117.28
2	A	1289	NDP	N3A-C4A-N9A	2.43	131.30	127.17
2	C	1289	NDP	O2A-PA-O3	2.40	113.75	107.27
2	D	1289	NDP	O2A-PA-O3	2.34	113.60	107.27
3	B	1290	TOP	O19-C18-C21	-2.31	120.10	124.08
2	A	1289	NDP	C4A-C5A-N7A	-2.30	107.95	110.58
2	A	1289	NDP	O4B-C1B-N9A	2.27	112.44	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1289	NDP	C6N-N1N-C2N	2.24	121.72	119.32
2	C	1289	NDP	C4A-N9A-C8A	2.18	108.03	105.74
2	C	1289	NDP	C2B-C1B-N9A	-2.13	110.24	113.75
2	D	1289	NDP	O4B-C1B-N9A	2.13	112.19	108.09
2	D	1289	NDP	C6N-N1N-C2N	2.12	121.59	119.32
2	B	1289	NDP	C4A-C5A-N7A	-2.11	108.17	110.58
2	B	1289	NDP	O2A-PA-O3	2.10	112.95	107.27
2	D	1289	NDP	C4A-N9A-C8A	2.10	107.94	105.74
3	A	1290	TOP	C3-N5-C6	2.07	119.76	117.28
2	C	1289	NDP	O4B-C1B-N9A	2.06	112.04	108.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

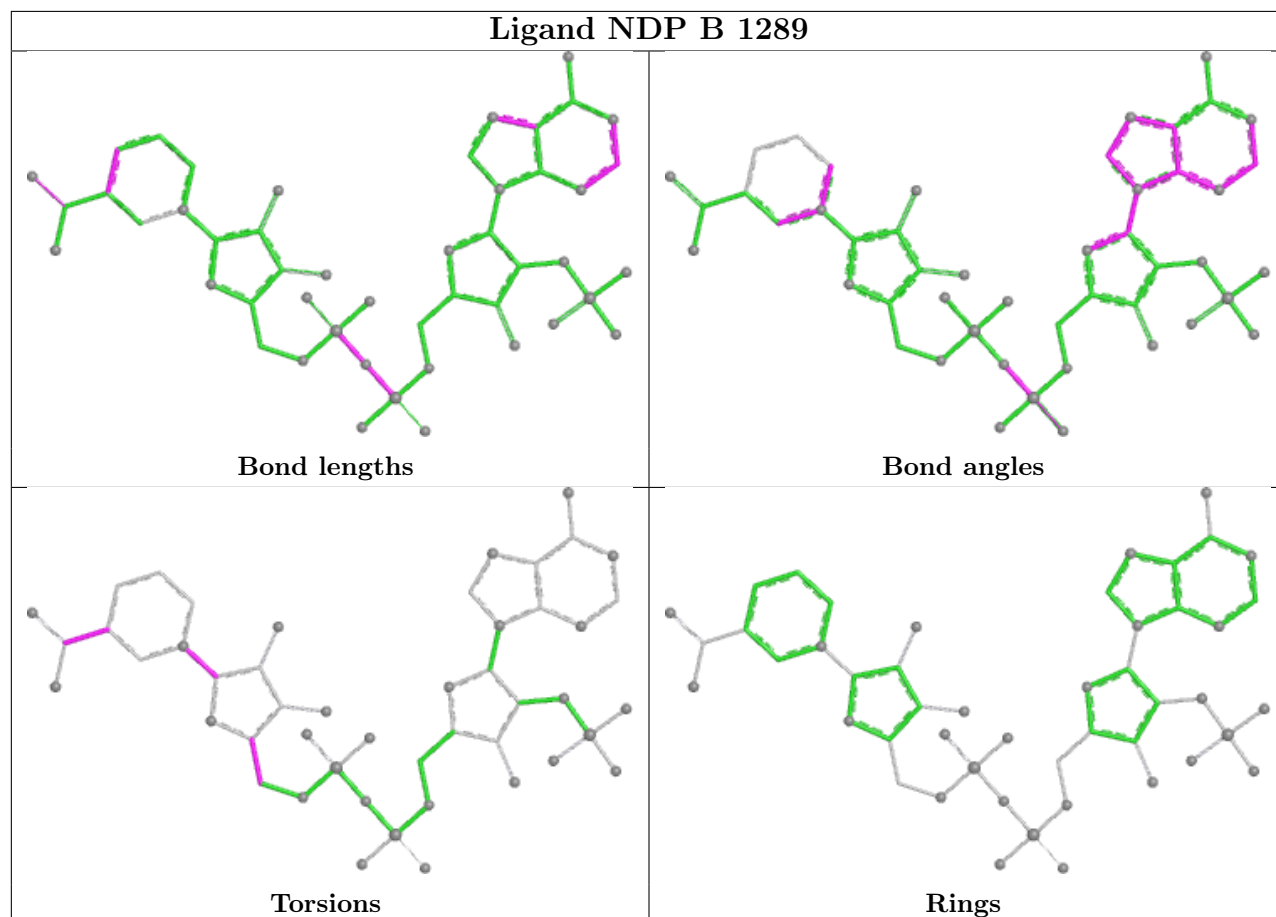
Mol	Chain	Res	Type	Atoms
3	A	1290	TOP	C15-C12-O13-C14
2	A	1289	NDP	O4D-C1D-N1N-C6N
2	B	1289	NDP	O4D-C1D-N1N-C6N
2	C	1289	NDP	O4D-C1D-N1N-C6N
2	D	1289	NDP	O4D-C1D-N1N-C6N
3	A	1290	TOP	C11-C12-O13-C14
3	B	1290	TOP	C11-C12-O13-C14
3	B	1290	TOP	C15-C12-O13-C14
2	A	1289	NDP	C2N-C3N-C7N-N7N
2	B	1289	NDP	C2N-C3N-C7N-N7N
2	C	1289	NDP	C2N-C3N-C7N-N7N
2	D	1289	NDP	C2N-C3N-C7N-N7N
2	B	1289	NDP	O4D-C4D-C5D-O5D
2	C	1289	NDP	O4D-C4D-C5D-O5D

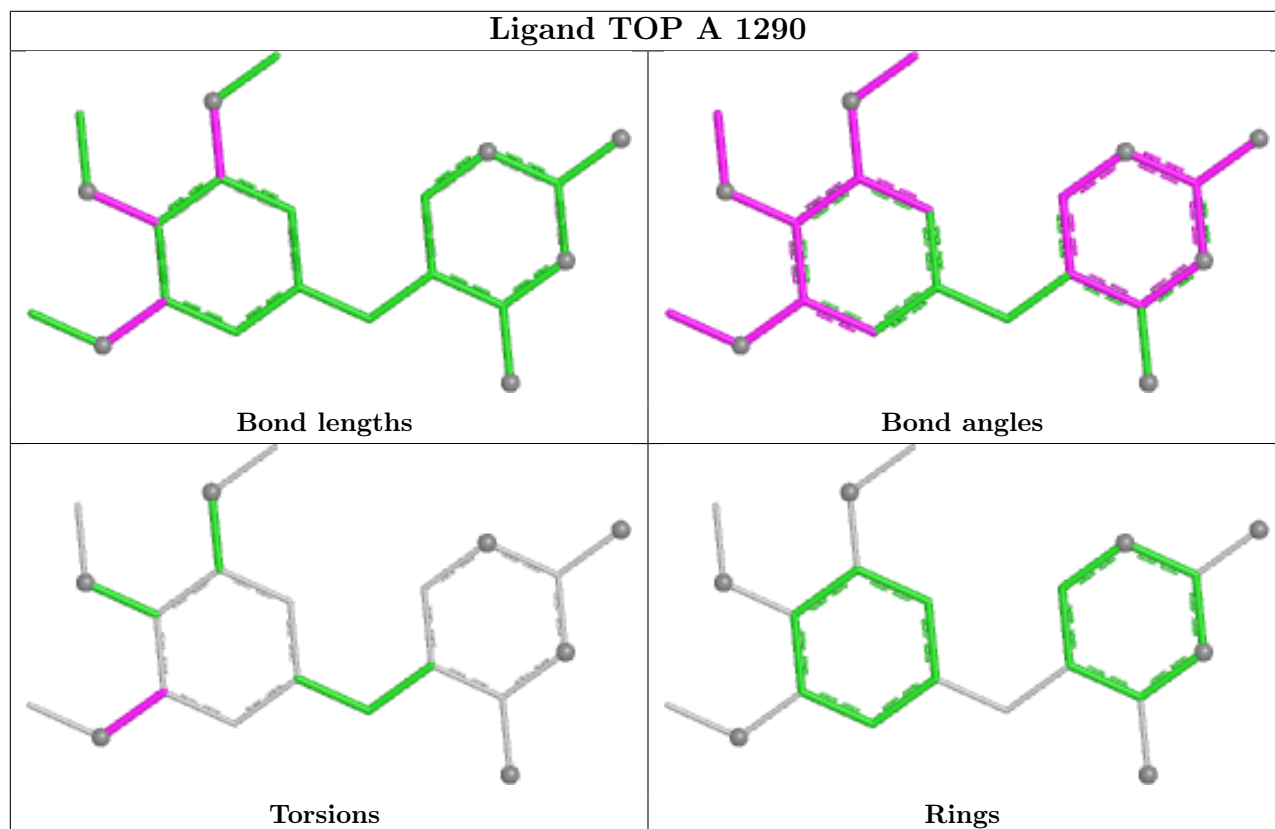
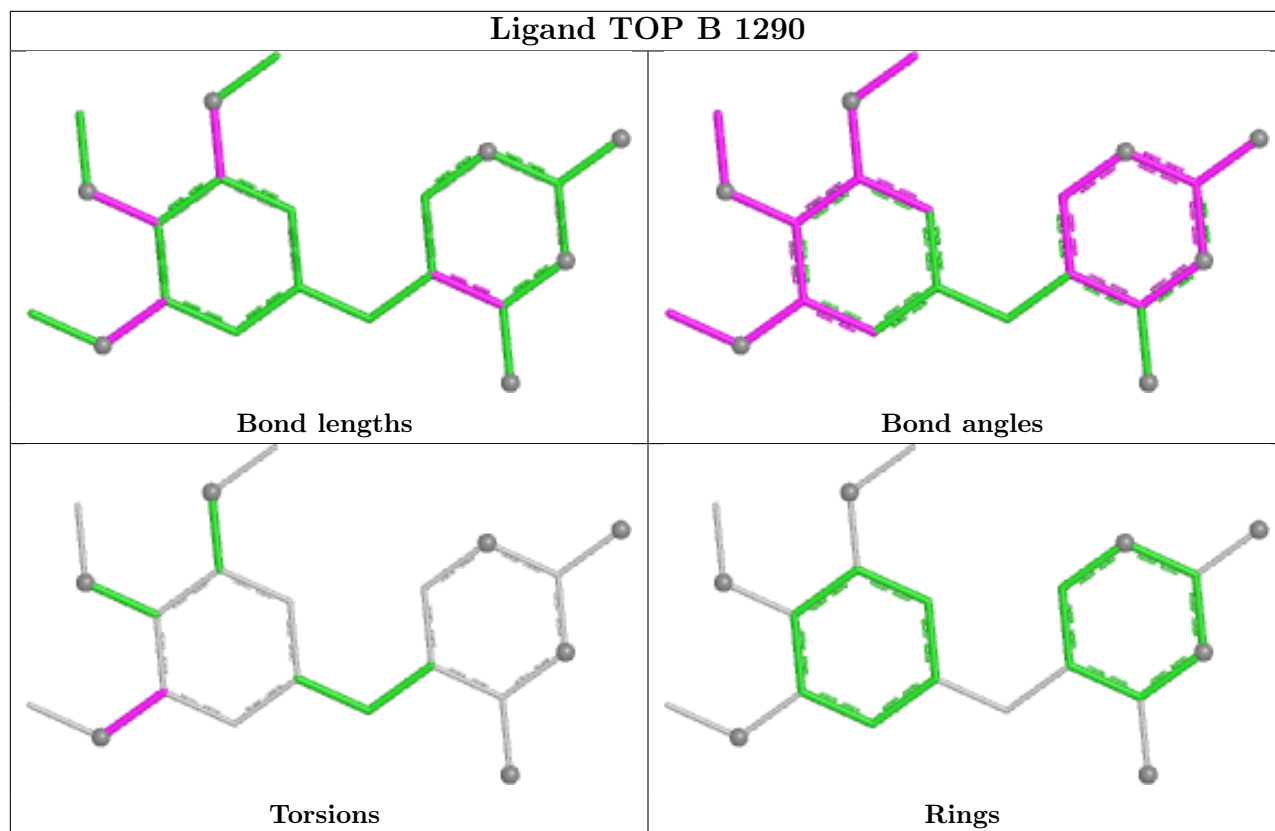
There are no ring outliers.

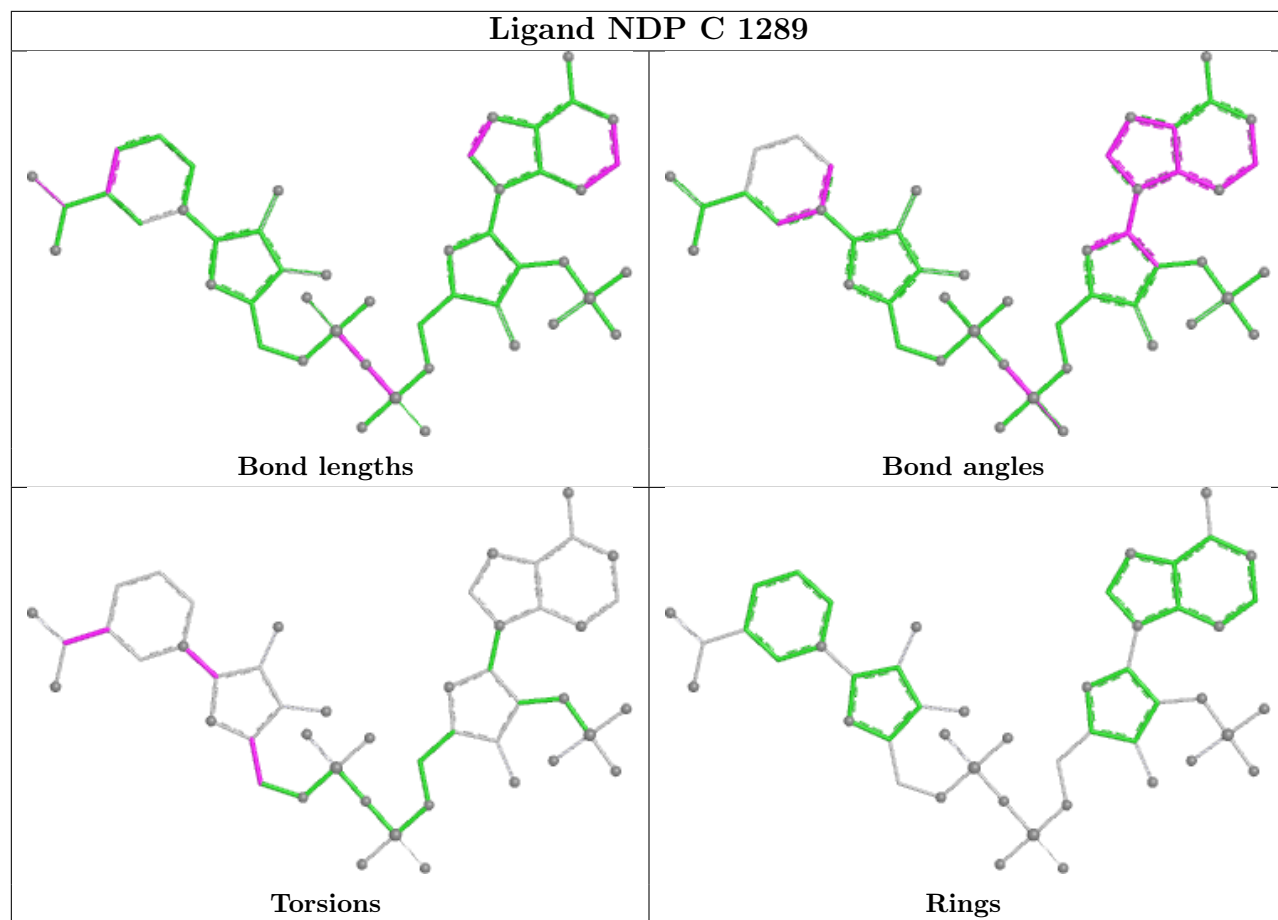
No monomer is involved in short contacts.

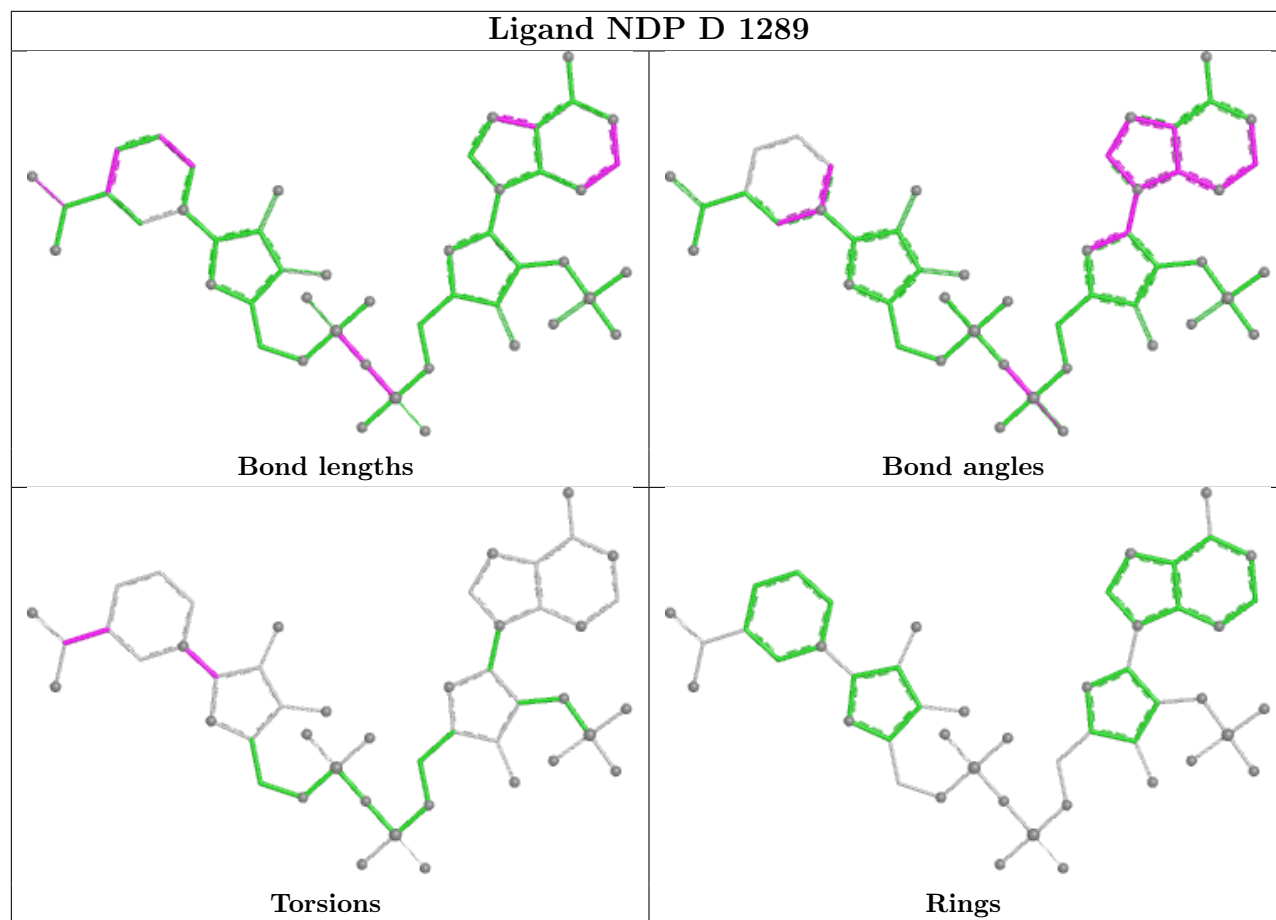
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

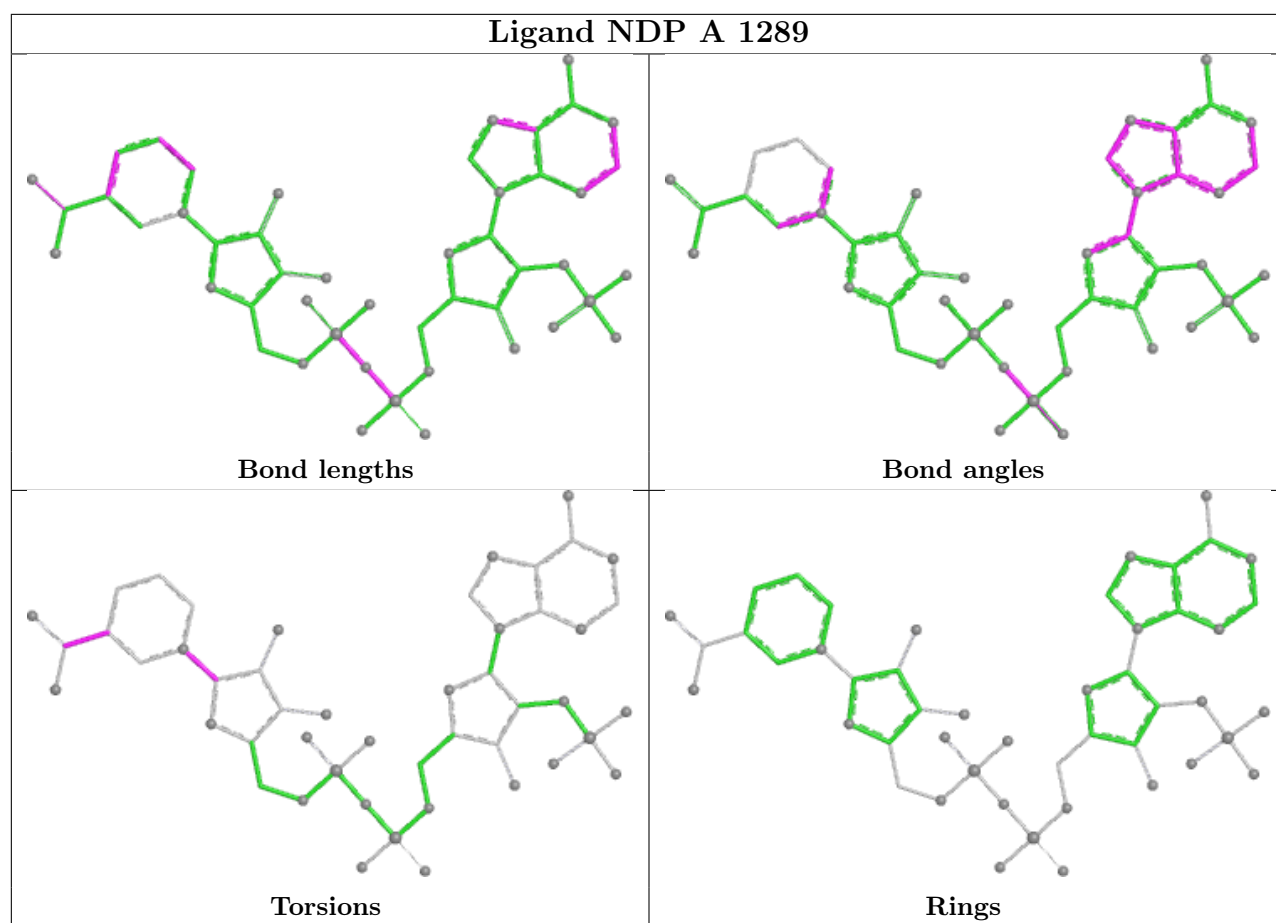
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	266/288 (92%)	0.77	22 (8%) 17 13	17, 27, 40, 74	1 (0%)
1	B	266/288 (92%)	0.84	28 (10%) 11 9	17, 27, 43, 66	1 (0%)
1	C	254/288 (88%)	0.41	16 (6%) 26 20	17, 27, 42, 71	3 (1%)
1	D	256/288 (88%)	0.50	15 (5%) 28 23	17, 27, 44, 71	3 (1%)
All	All	1042/1152 (90%)	0.63	81 (7%) 19 15	17, 27, 42, 74	8 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	GLU	11.3
1	C	133	ARG	11.3
1	D	120	ARG	9.0
1	D	134	GLU	8.7
1	B	120	ARG	8.5
1	C	120	ARG	8.5
1	A	131	GLY	5.4
1	A	184	THR	5.3
1	A	133	ARG	4.9
1	B	137	GLU	4.8
1	A	72	ALA	4.6
1	C	134	GLU	4.5
1	C	136	MET	4.5
1	A	132	ASP	4.5
1	B	74	VAL	4.4
1	B	184	THR	4.4
1	A	134	GLU	4.4
1	A	136	MET	4.3
1	B	135	ALA	4.2
1	D	168	LYS	4.2
1	C	72	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	135	ALA	4.1
1	C	168	LYS	3.9
1	B	73	PRO	3.8
1	B	138	THR	3.7
1	D	81	ALA	3.6
1	A	135	ALA	3.5
1	C	81	ALA	3.4
1	D	136	MET	3.2
1	B	164	GLY	3.2
1	B	136	MET	3.2
1	C	230	VAL	3.2
1	D	133	ARG	3.2
1	A	73	PRO	3.1
1	B	237	VAL	3.1
1	B	133	ARG	3.1
1	C	240	GLY	3.1
1	C	160	HIS	3.1
1	D	73	PRO	3.1
1	D	137	GLU	3.1
1	A	67	SER	3.0
1	B	86	PHE	3.0
1	B	139	ALA	2.9
1	D	240	GLY	2.9
1	A	138	THR	2.9
1	A	81	ALA	2.8
1	B	230	VAL	2.8
1	C	241	HIS	2.7
1	B	231	ASP	2.7
1	D	72	ALA	2.7
1	D	5	THR	2.7
1	C	67	SER	2.7
1	A	139	ALA	2.7
1	A	86	PHE	2.6
1	A	71	THR	2.6
1	B	160	HIS	2.6
1	C	71	THR	2.5
1	A	141	ALA	2.5
1	D	241	HIS	2.5
1	D	70	ALA	2.4
1	D	82	PRO	2.4
1	A	69	VAL	2.3
1	C	139	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	229	LEU	2.3
1	B	169	HIS	2.3
1	B	81	ALA	2.2
1	A	171	GLY	2.2
1	B	46	ALA	2.2
1	B	288	ALA	2.2
1	D	135	ALA	2.2
1	B	98	THR	2.2
1	A	85	LEU	2.2
1	B	32	ALA	2.1
1	B	134	GLU	2.1
1	B	91	GLU	2.1
1	B	140	THR	2.1
1	B	121	ASN	2.1
1	B	167	ALA	2.0
1	A	12	THR	2.0
1	A	84	THR	2.0
1	B	35	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

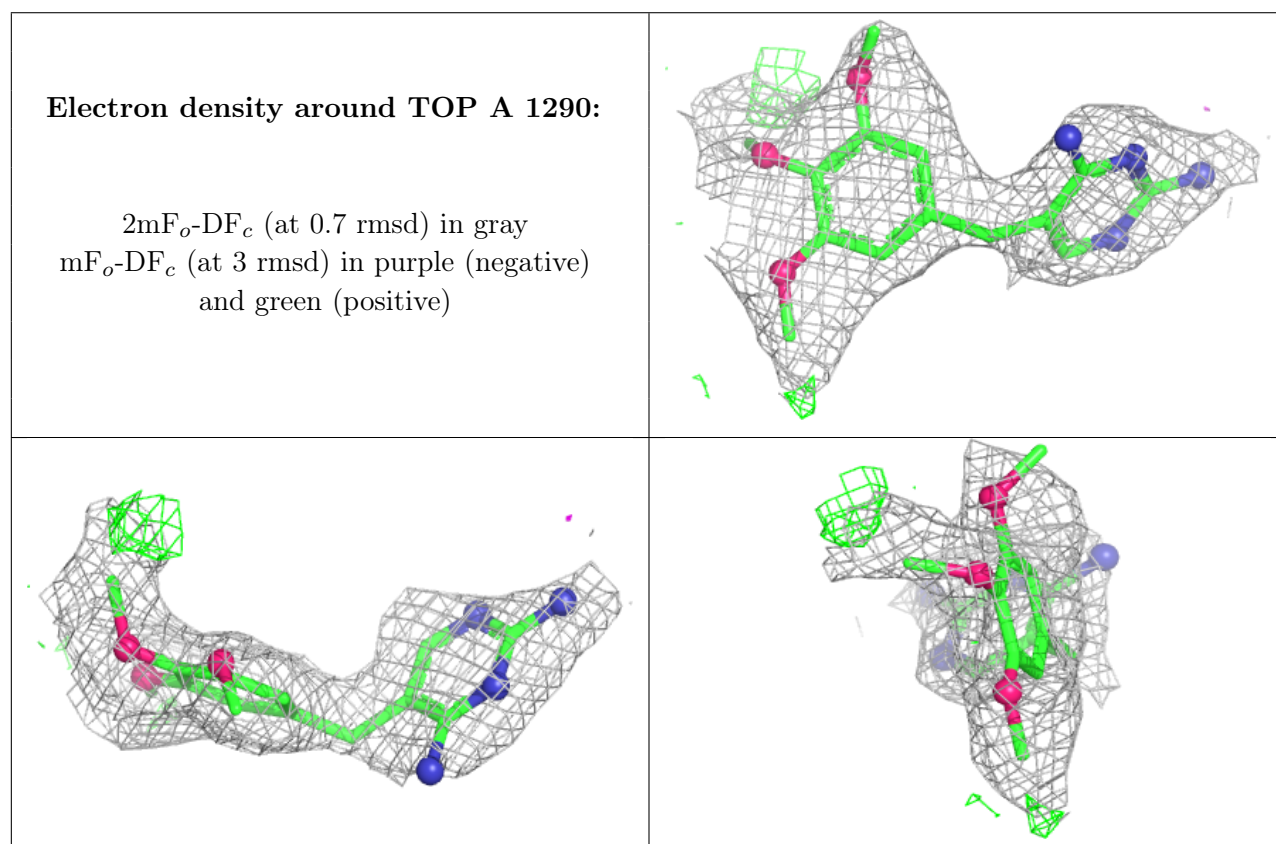
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TOP	A	1290	21/21	0.72	0.20	42,50,54,57	0
3	TOP	B	1290	21/21	0.77	0.20	48,54,58,59	0
2	NDP	A	1289	48/48	0.93	0.14	37,40,44,44	0
2	NDP	C	1289	48/48	0.93	0.12	37,40,44,44	0
2	NDP	B	1289	48/48	0.94	0.13	37,40,44,44	0

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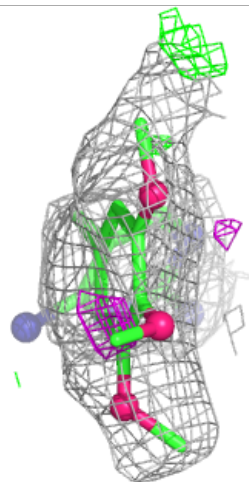
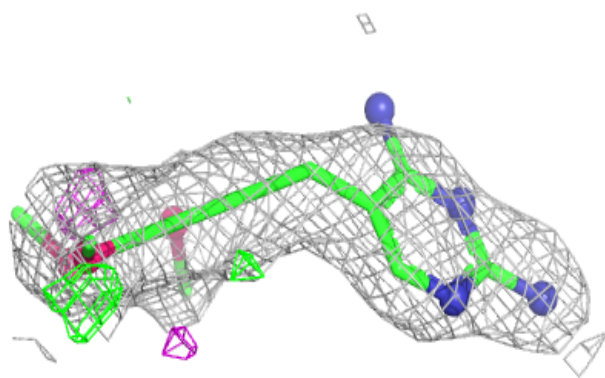
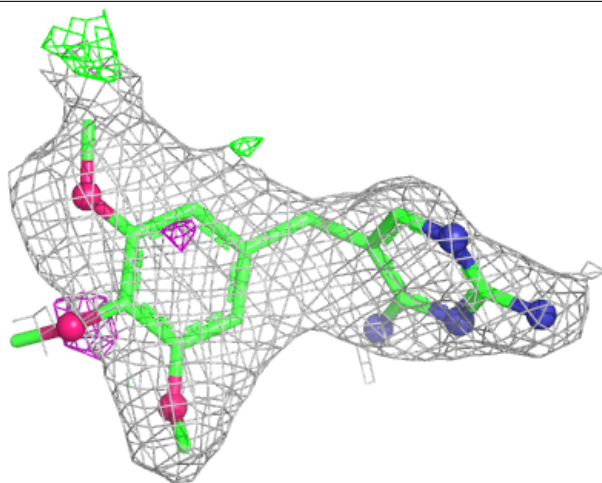
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NDP	D	1289	48/48	0.94	0.11	37,40,44,45	0

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.



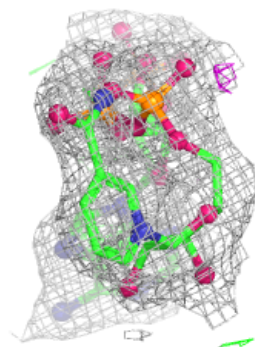
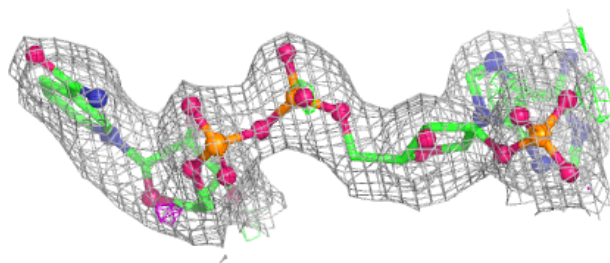
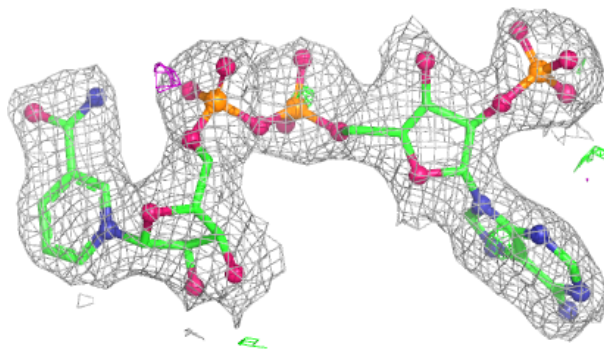
Electron density around TOP B 1290:

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

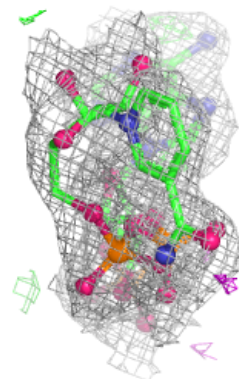
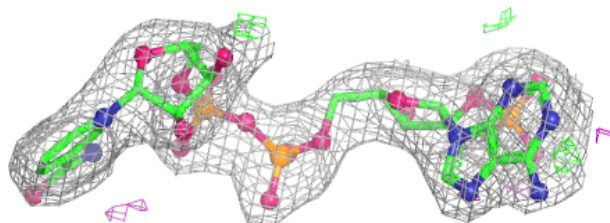
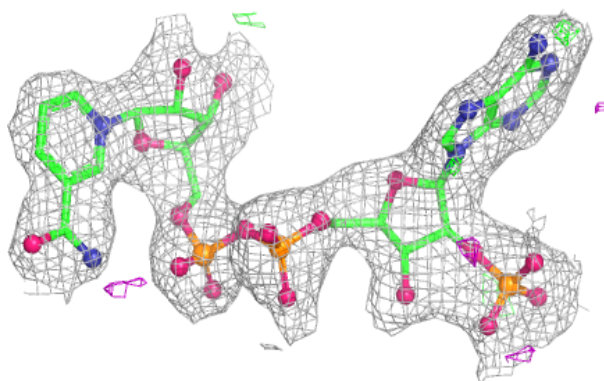


Electron density around NDP A 1289:

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

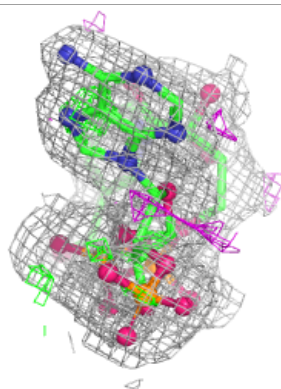
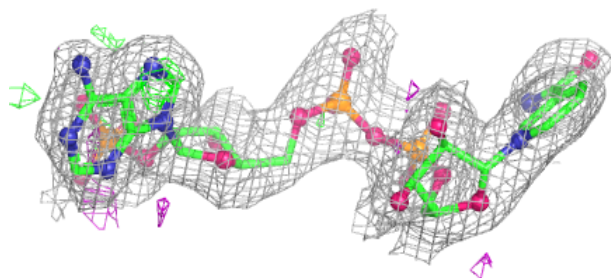
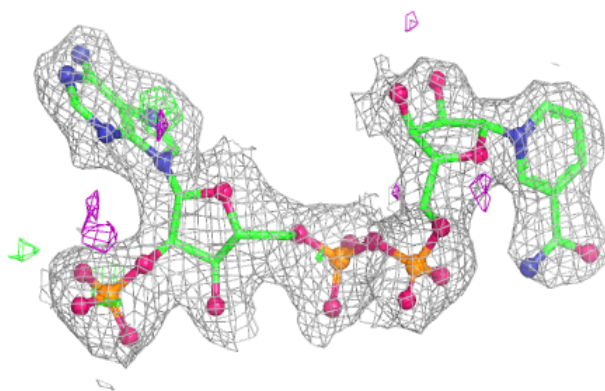
**Electron density around NDP C 1289:**

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

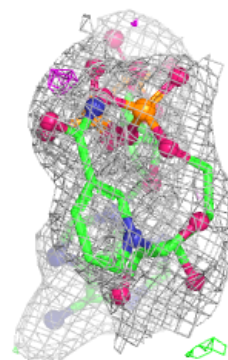
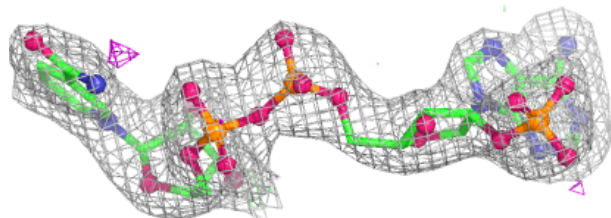
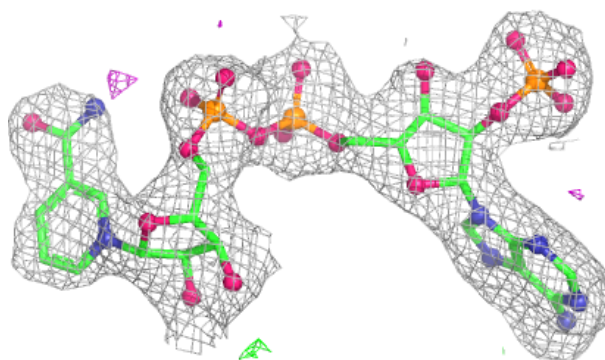


Electron density around NDP B 1289:

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

**Electron density around NDP D 1289:**

$2mF_o-DF_c$ (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.