



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:16 PM UTC

PDB ID : 1G0O / pdb_00001g0o
Title : STRUCTURE OF TRIHYDROXYNAPHTHALENE REDUCTASE IN
COMPLEX WITH NADPH AND PYROQUILON
Authors : Liao, D.; Basarab, G.S.; Gatenby, A.A.; Valent, B.; Jordan, D.B.
Deposited on : 2000-10-06
Resolution : 1.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

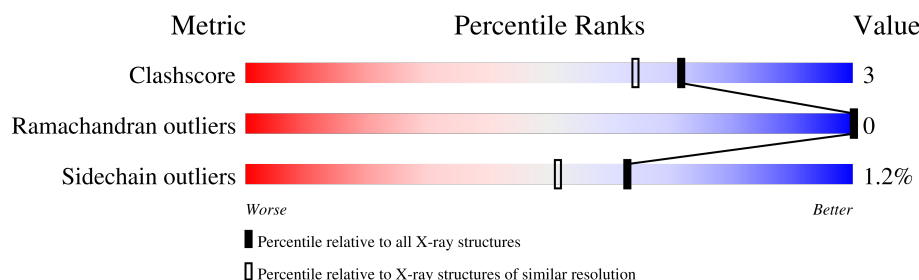
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	283	86% 10% .
1	B	283	88% 8% .
1	C	283	87% 11% ..
1	D	283	88% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9749 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 TRIHYDROXYNAPHTHALENE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2030	1276	356	383	15			
1	B	272	Total	C	N	O	S	0	0	0
			2030	1276	356	383	15			
1	C	281	Total	C	N	O	S	0	0	0
			2095	1314	369	397	15			
1	D	281	Total	C	N	O	S	0	0	0
			2095	1314	369	397	15			

There are 12 discrepancies between the modelled and reference sequences:

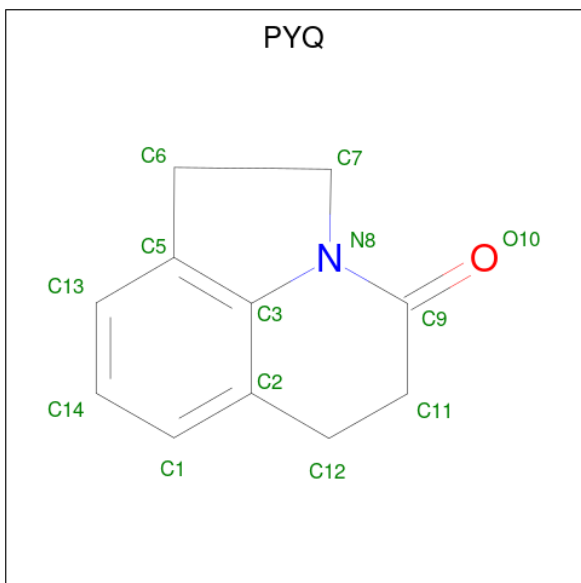
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	VAL	SER	engineered mutation	UNP Q12634
A	242	GLN	ALA	engineered mutation	UNP Q12634
A	247	ARG	HIS	engineered mutation	UNP Q12634
B	241	VAL	SER	engineered mutation	UNP Q12634
B	242	GLN	ALA	engineered mutation	UNP Q12634
B	247	ARG	HIS	engineered mutation	UNP Q12634
C	241	VAL	SER	engineered mutation	UNP Q12634
C	242	GLN	ALA	engineered mutation	UNP Q12634
C	247	ARG	HIS	engineered mutation	UNP Q12634
D	241	VAL	SER	engineered mutation	UNP Q12634
D	242	GLN	ALA	engineered mutation	UNP Q12634
D	247	ARG	HIS	engineered mutation	UNP Q12634

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 3 is PYROQUILON (CCD ID: PYQ) (formula: $C_{11}H_{11}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	11	1	1		
3	B	1	Total	C	N	O	0	0
			13	11	1	1		
3	C	1	Total	C	N	O	0	0
			13	11	1	1		
3	D	1	Total	C	N	O	0	0
			13	11	1	1		

- Molecule 4 is water.

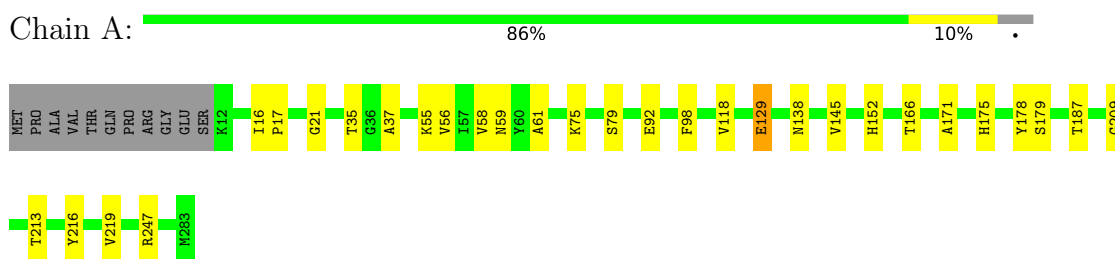
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	314	Total	O	0	0
			314	314		
4	C	286	Total	O	0	0
			286	286		
4	D	337	Total	O	0	0
			337	337		

3 Residue-property plots

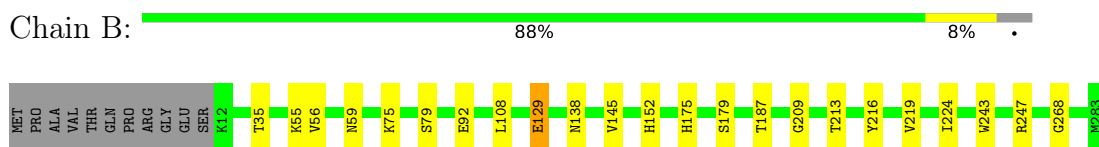
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

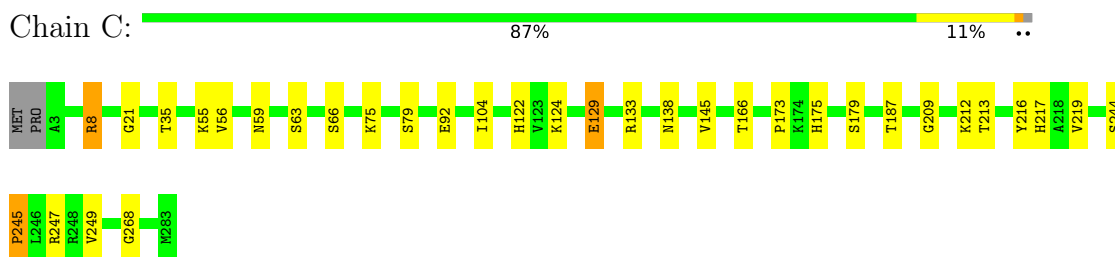
• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE



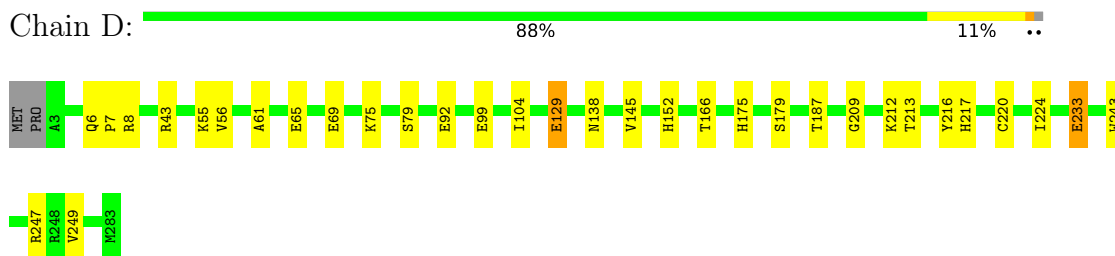
• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE



• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE



• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.00Å 143.30Å 141.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.176 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9749	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYQ, 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	0.59	0/2062	0.99	11/2782 (0.4%)
1	B	0.59	0/2062	1.00	10/2782 (0.4%)
1	C	0.59	0/2128	1.01	12/2872 (0.4%)
1	D	0.60	0/2128	1.01	9/2872 (0.3%)
All	All	0.59	0/8380	1.00	42/11308 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	LYS	N-CA-C	-8.01	96.50	109.96
1	C	55	LYS	N-CA-C	-7.61	97.18	109.96
1	C	209	GLY	N-CA-C	-7.36	99.60	112.55
1	A	55	LYS	N-CA-C	-7.26	97.76	109.96
1	B	145	VAL	N-CA-C	-7.24	103.41	110.72
1	D	55	LYS	N-CA-C	-7.20	97.50	109.46
1	B	56	VAL	N-CA-C	7.18	118.16	108.11
1	A	145	VAL	N-CA-C	-7.01	103.64	110.72
1	D	56	VAL	N-CA-C	6.99	118.54	108.48
1	B	209	GLY	N-CA-C	-6.95	100.33	112.55
1	A	209	GLY	N-CA-C	-6.80	100.58	112.55
1	C	145	VAL	N-CA-C	-6.69	103.96	110.72
1	D	209	GLY	N-CA-C	-6.62	100.90	112.55
1	D	138	ASN	N-CA-C	6.57	119.44	111.82
1	C	56	VAL	N-CA-C	6.39	117.98	108.46
1	B	138	ASN	N-CA-C	6.37	119.21	111.82
1	D	145	VAL	N-CA-C	-6.23	104.43	110.72
1	A	138	ASN	N-CA-C	6.23	119.04	111.82
1	A	56	VAL	N-CA-C	6.15	116.72	108.11
1	C	21	GLY	CA-C-N	6.06	126.50	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	GLY	C-N-CA	6.06	126.50	119.47
1	C	138	ASN	N-CA-C	5.98	118.76	111.82
1	D	247	ARG	N-CA-C	5.73	119.54	111.52
1	C	247	ARG	N-CA-C	5.70	119.50	111.52
1	D	243	TRP	N-CA-C	5.64	119.85	112.92
1	B	247	ARG	N-CA-C	5.59	118.95	111.24
1	D	104	ILE	N-CA-C	5.52	115.66	110.30
1	A	219	VAL	N-CA-C	5.52	120.82	109.34
1	C	219	VAL	N-CA-C	5.50	120.78	109.34
1	A	21	GLY	CA-C-N	5.38	126.56	119.84
1	A	21	GLY	C-N-CA	5.38	126.56	119.84
1	B	243	TRP	N-CA-C	5.26	119.39	112.92
1	A	171	ALA	CA-C-N	-5.24	119.04	122.60
1	A	171	ALA	C-N-CA	-5.24	119.04	122.60
1	A	247	ARG	N-CA-C	5.22	118.59	111.39
1	C	245	PRO	N-CA-C	-5.21	107.34	113.86
1	C	104	ILE	N-CA-C	5.18	115.33	110.30
1	B	219	VAL	N-CA-C	5.17	120.10	109.34
1	C	268	GLY	N-CA-C	5.15	119.11	112.83
1	D	224	ILE	N-CA-C	5.14	113.58	107.73
1	B	268	GLY	N-CA-C	5.07	119.02	112.83
1	B	224	ILE	N-CA-C	5.02	113.45	107.73

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	2030	0	2046	13	0
1	B	2030	0	2046	10	0
1	C	2095	0	2109	17	0
1	D	2095	0	2109	19	0
2	A	48	0	26	2	0
2	B	48	0	26	1	0
2	C	48	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	26	2	0
3	A	13	0	11	2	0
3	B	13	0	11	1	0
3	C	13	0	11	1	0
3	D	13	0	11	2	0
4	A	318	0	0	0	0
4	B	314	0	0	2	0
4	C	286	0	0	4	0
4	D	337	0	0	4	0
All	All	9749	0	8458	56	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 3.

All (56) 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:D:99:GLU:HG2	4:D:1741:HOH:O	1.77	0.83
1:D:75:LYS:HA	1:D:79:SER:O	1.91	0.69
1:C:8:ARG:HG3	1:D:217:HIS:CG	2.29	0.68
1:B:75:LYS:HA	1:B:79:SER:O	1.95	0.66
1:C:133:ARG:HD3	4:C:1589:HOH:O	1.97	0.65
1:D:220:CYS:HB3	4:D:1669:HOH:O	1.99	0.62
1:C:75:LYS:HA	1:C:79:SER:O	2.00	0.62
2:B:1401:NDP:H41N	3:B:1405:PYQ:C9	2.37	0.55
1:C:217:HIS:CG	1:D:8:ARG:HG3	2.44	0.52
1:C:166:THR:HG23	3:C:1406:PYQ:H112	1.92	0.52
1:C:133:ARG:NH2	4:C:1564:HOH:O	2.43	0.51
2:A:1400:NDP:H41N	3:A:1404:PYQ:C9	2.41	0.50
1:A:129:GLU:CD	1:A:129:GLU:H	2.18	0.50
1:C:212:LYS:HG3	1:C:249:VAL:HG11	1.93	0.50
1:A:92:GLU:H	1:A:92:GLU:CD	2.20	0.49
1:D:61:ALA:HB2	2:D:1403:NDP:C2A	2.43	0.49
1:B:213:THR:H	1:B:216:TYR:HB3	1.78	0.49
1:B:152:HIS:CE1	4:B:1485:HOH:O	2.67	0.48
1:A:75:LYS:HA	1:A:79:SER:O	2.14	0.48
1:D:152:HIS:HE1	4:D:1529:HOH:O	1.97	0.47
1:B:35:THR:HA	1:B:59:ASN:HB3	1.95	0.47
1:B:129:GLU:H	1:B:129:GLU:CD	2.21	0.47
1:D:212:LYS:HG3	1:D:249:VAL:HG11	1.97	0.47
4:C:1424:HOH:O	1:D:8:ARG:HG2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1403:NDP:H41N	3:D:1407:PYQ:C9	2.45	0.46
1:C:122:HIS:ND1	1:C:124:LYS:HG2	2.30	0.46
1:D:233:GLU:H	1:D:233:GLU:CD	2.23	0.45
1:D:65:GLU:O	1:D:69:GLU:HG3	2.15	0.45
1:D:92:GLU:H	1:D:92:GLU:CD	2.25	0.45
1:D:166:THR:HG23	3:D:1407:PYQ:H112	1.99	0.45
1:B:92:GLU:H	1:B:92:GLU:CD	2.25	0.45
1:A:61:ALA:HB2	2:A:1400:NDP:C2A	2.47	0.45
1:D:213:THR:H	1:D:216:TYR:HB3	1.83	0.44
1:C:129:GLU:H	1:C:129:GLU:CD	2.24	0.44
1:D:43:ARG:NH1	4:D:1537:HOH:O	2.51	0.44
1:A:187:THR:HG21	1:D:179:SER:C	2.43	0.43
1:A:166:THR:HG23	3:A:1404:PYQ:H112	2.01	0.43
1:C:213:THR:H	1:C:216:TYR:HB3	1.83	0.43
1:D:129:GLU:H	1:D:129:GLU:CD	2.24	0.43
1:B:187:THR:HG21	1:C:179:SER:C	2.45	0.42
1:C:35:THR:HA	1:C:59:ASN:HB3	2.01	0.42
1:A:35:THR:HA	1:A:59:ASN:HB3	2.01	0.42
1:B:108:LEU:HD12	1:B:108:LEU:HA	1.95	0.42
1:A:118:VAL:HA	1:A:178:TYR:CD1	2.55	0.42
1:C:63:SER:HB3	1:C:66:SER:HB2	2.02	0.42
1:C:244:SER:HA	1:C:245:PRO:HD3	1.95	0.41
1:A:179:SER:C	1:D:187:THR:HG21	2.45	0.41
1:A:37:ALA:HB3	1:A:58:VAL:HG13	2.01	0.41
1:A:98:PHE:HB3	1:A:152:HIS:CD2	2.56	0.41
1:B:152:HIS:HE1	4:B:1485:HOH:O	2.01	0.41
1:B:179:SER:C	1:C:187:THR:HG21	2.46	0.41
1:D:6:GLN:HA	1:D:7:PRO:HD3	1.96	0.41
1:C:92:GLU:H	1:C:92:GLU:CD	2.28	0.41
1:A:213:THR:H	1:A:216:TYR:HB3	1.85	0.40
1:A:16:ILE:HA	1:A:17:PRO:HD3	1.88	0.40
1:C:173:PRO:HG3	4:C:1449:HOH:O	2.22	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	270/283 (95%)	265 (98%)	5 (2%)	0	100	100
1	B	270/283 (95%)	265 (98%)	5 (2%)	0	100	100
1	C	279/283 (99%)	275 (99%)	4 (1%)	0	100	100
1	D	279/283 (99%)	274 (98%)	5 (2%)	0	100	100
All	All	1098/1132 (97%)	1079 (98%)	19 (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	212/221 (96%)	210 (99%)	2 (1%)	70	62
1	B	212/221 (96%)	210 (99%)	2 (1%)	70	62
1	C	219/221 (99%)	216 (99%)	3 (1%)	59	46
1	D	219/221 (99%)	216 (99%)	3 (1%)	59	46
All	All	862/884 (98%)	852 (99%)	10 (1%)	63	51

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	GLU
1	A	175	HIS
1	B	129	GLU
1	B	175	HIS
1	C	8	ARG
1	C	129	GLU
1	C	175	HIS
1	D	129	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	175	HIS
1	D	233	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	ASN
1	B	242	GLN
1	C	62	ASN
1	D	226	ASN
1	D	242	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	D	1403	-	51,52,52	1.39	8 (15%)	71,80,80	1.92	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	B	1401	-	51,52,52	1.32	5 (9%)	71,80,80	1.94	20 (28%)
3	PYQ	C	1406	-	15,15,15	3.00	6 (40%)	20,22,22	1.88	6 (30%)
2	NDP	A	1400	-	51,52,52	1.42	7 (13%)	71,80,80	1.91	17 (23%)
3	PYQ	B	1405	-	15,15,15	2.81	6 (40%)	20,22,22	1.85	5 (25%)
3	PYQ	A	1404	-	15,15,15	2.89	6 (40%)	20,22,22	1.86	7 (35%)
3	PYQ	D	1407	-	15,15,15	2.87	7 (46%)	20,22,22	1.90	6 (30%)
2	NDP	C	1402	-	51,52,52	1.39	6 (11%)	71,80,80	1.92	18 (25%)

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	D	1403	-	-	8/34/77/77	0/5/5/5
2	NDP	B	1401	-	-	5/34/77/77	0/5/5/5
3	PYQ	C	1406	-	-	-	0/3/3/3
2	NDP	A	1400	-	-	8/34/77/77	0/5/5/5
3	PYQ	B	1405	-	-	-	0/3/3/3
3	PYQ	A	1404	-	-	-	0/3/3/3
3	PYQ	D	1407	-	-	-	0/3/3/3
2	NDP	C	1402	-	-	8/34/77/77	0/5/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1406	PYQ	C12-C2	-6.20	1.40	1.51
3	C	1406	PYQ	C7-N8	-6.03	1.39	1.47
3	A	1404	PYQ	C12-C2	-6.01	1.41	1.51
3	D	1407	PYQ	C12-C2	-5.75	1.41	1.51
3	B	1405	PYQ	C7-N8	-5.55	1.39	1.47
3	B	1405	PYQ	C12-C2	-5.53	1.41	1.51
3	A	1404	PYQ	C7-N8	-5.49	1.40	1.47
3	D	1407	PYQ	C7-N8	-5.24	1.40	1.47
2	C	1402	NDP	C4N-C3N	-4.77	1.41	1.50
3	C	1406	PYQ	C12-C11	-4.38	1.41	1.52
2	B	1401	NDP	C4N-C3N	-4.32	1.41	1.50
3	D	1407	PYQ	C12-C11	-4.24	1.41	1.52
2	D	1403	NDP	C4N-C3N	-4.18	1.42	1.50
3	A	1404	PYQ	C11-C9	-4.13	1.42	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1405	PYQ	C12-C11	-4.12	1.41	1.52
2	A	1400	NDP	C4N-C3N	-4.05	1.42	1.50
3	D	1407	PYQ	C11-C9	-4.02	1.42	1.51
3	C	1406	PYQ	C11-C9	-3.97	1.42	1.51
3	A	1404	PYQ	C12-C11	-3.90	1.42	1.52
3	B	1405	PYQ	C11-C9	-3.79	1.43	1.51
2	D	1403	NDP	C5A-N7A	-3.57	1.32	1.39
2	A	1400	NDP	C5A-N7A	-3.53	1.32	1.39
2	C	1402	NDP	C5A-N7A	-3.33	1.33	1.39
2	B	1401	NDP	C5A-N7A	-3.20	1.33	1.39
2	C	1402	NDP	C4N-C5N	-3.20	1.40	1.49
2	A	1400	NDP	C4N-C5N	-3.10	1.41	1.49
2	A	1400	NDP	C7N-C3N	3.09	1.55	1.48
2	B	1401	NDP	C4N-C5N	-2.90	1.41	1.49
2	A	1400	NDP	C4A-N9A	-2.85	1.31	1.37
2	D	1403	NDP	C4N-C5N	-2.84	1.41	1.49
3	A	1404	PYQ	C3-N8	-2.76	1.34	1.40
3	C	1406	PYQ	C3-N8	-2.63	1.35	1.40
3	C	1406	PYQ	O10-C9	2.61	1.28	1.23
3	D	1407	PYQ	C3-N8	-2.61	1.35	1.40
3	B	1405	PYQ	O10-C9	2.44	1.28	1.23
3	B	1405	PYQ	C3-N8	-2.40	1.35	1.40
2	C	1402	NDP	PA-O3	2.39	1.62	1.59
3	D	1407	PYQ	O10-C9	2.38	1.28	1.23
2	D	1403	NDP	C7N-C3N	2.38	1.53	1.48
2	C	1402	NDP	C4A-N9A	-2.38	1.32	1.37
3	A	1404	PYQ	O10-C9	2.35	1.28	1.23
2	A	1400	NDP	C6N-C5N	2.35	1.40	1.33
2	C	1402	NDP	C6N-C5N	2.34	1.40	1.33
2	A	1400	NDP	C6N-N1N	2.31	1.42	1.37
2	D	1403	NDP	C6N-C5N	2.30	1.40	1.33
2	D	1403	NDP	PN-O3	2.29	1.62	1.59
2	D	1403	NDP	C4A-N9A	-2.22	1.33	1.37
2	D	1403	NDP	PA-O3	2.22	1.61	1.59
2	B	1401	NDP	C7N-C3N	2.21	1.53	1.48
2	B	1401	NDP	C4A-N9A	-2.20	1.33	1.37
3	D	1407	PYQ	C14-C1	2.02	1.42	1.38

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1402	NDP	N3A-C4A-N9A	6.44	138.11	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1403	NDP	N3A-C4A-N9A	6.33	137.93	127.17
2	B	1401	NDP	N3A-C4A-N9A	6.32	137.92	127.17
2	A	1400	NDP	N3A-C4A-N9A	6.19	137.70	127.17
2	D	1403	NDP	C5A-C4A-N3A	-5.97	118.50	126.72
2	C	1402	NDP	C5A-C4A-N3A	-5.95	118.52	126.72
2	B	1401	NDP	C5A-C4A-N3A	-5.87	118.64	126.72
2	A	1400	NDP	C5A-C4A-N3A	-5.78	118.76	126.72
2	D	1403	NDP	N3A-C2A-N1A	-4.74	121.41	128.58
2	A	1400	NDP	O4B-C1B-N9A	4.64	116.99	108.09
2	C	1402	NDP	N3A-C2A-N1A	-4.63	121.58	128.58
2	A	1400	NDP	N3A-C2A-N1A	-4.62	121.59	128.58
2	B	1401	NDP	N3A-C2A-N1A	-4.61	121.60	128.58
2	C	1402	NDP	O4B-C1B-N9A	4.42	116.57	108.09
2	D	1403	NDP	O4B-C1B-N9A	4.22	116.19	108.09
3	B	1405	PYQ	C3-N8-C9	-4.21	119.72	123.40
2	B	1401	NDP	O4B-C1B-N9A	4.20	116.15	108.09
3	C	1406	PYQ	C3-N8-C9	-4.13	119.80	123.40
3	D	1407	PYQ	C3-N8-C9	-3.99	119.92	123.40
2	D	1403	NDP	C6A-C5A-C4A	3.90	122.51	117.18
2	C	1402	NDP	C6A-C5A-C4A	3.86	122.45	117.18
2	A	1400	NDP	C6A-C5A-C4A	3.86	122.45	117.18
2	B	1401	NDP	C4A-N9A-C8A	3.84	109.77	105.74
2	A	1400	NDP	C4A-N9A-C8A	3.82	109.75	105.74
3	A	1404	PYQ	C3-N8-C9	-3.82	120.07	123.40
2	C	1402	NDP	C4A-N9A-C8A	3.64	109.56	105.74
2	B	1401	NDP	C6A-C5A-C4A	3.52	121.99	117.18
2	D	1403	NDP	C4A-N9A-C8A	3.50	109.42	105.74
3	C	1406	PYQ	C11-C12-C2	3.43	118.80	111.97
3	A	1404	PYQ	C11-C12-C2	3.38	118.69	111.97
3	D	1407	PYQ	C11-C12-C2	3.34	118.61	111.97
2	B	1401	NDP	C2A-N3A-C4A	3.31	119.90	111.83
3	B	1405	PYQ	C11-C12-C2	3.29	118.51	111.97
2	C	1402	NDP	C6A-C5A-N7A	-3.28	125.77	132.09
2	D	1403	NDP	C6A-C5A-N7A	-3.28	125.78	132.09
2	D	1403	NDP	C2A-N3A-C4A	3.26	119.79	111.83
2	A	1400	NDP	C2A-N3A-C4A	3.26	119.79	111.83
2	A	1400	NDP	C6A-C5A-N7A	-3.18	125.95	132.09
2	C	1402	NDP	C2A-N3A-C4A	3.16	119.55	111.83
2	B	1401	NDP	C6A-C5A-N7A	-3.06	126.19	132.09
3	B	1405	PYQ	C12-C2-C1	2.83	126.95	121.05
3	D	1407	PYQ	C12-C2-C1	2.80	126.90	121.05
3	A	1404	PYQ	C12-C2-C1	2.77	126.83	121.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1405	PYQ	C12-C11-C9	2.75	121.10	113.16
3	C	1406	PYQ	C12-C2-C1	2.73	126.74	121.05
2	D	1403	NDP	O5B-C5B-C4B	2.71	118.22	108.99
2	A	1400	NDP	C4B-O4B-C1B	-2.70	103.50	109.47
3	C	1406	PYQ	C12-C11-C9	2.70	120.93	113.16
3	D	1407	PYQ	C12-C11-C9	2.69	120.93	113.16
2	C	1402	NDP	C4B-O4B-C1B	-2.69	103.52	109.47
2	D	1403	NDP	C4B-O4B-C1B	-2.68	103.54	109.47
2	D	1403	NDP	N9A-C8A-N7A	-2.68	110.13	113.94
2	B	1401	NDP	N9A-C8A-N7A	-2.68	110.14	113.94
2	A	1400	NDP	N9A-C8A-N7A	-2.62	110.22	113.94
3	A	1404	PYQ	C12-C11-C9	2.58	120.60	113.16
3	D	1407	PYQ	O10-C9-N8	-2.57	118.86	122.47
3	A	1404	PYQ	O10-C9-N8	-2.57	118.86	122.47
2	B	1401	NDP	C3N-C2N-N1N	-2.54	119.47	123.20
2	C	1402	NDP	O5B-C5B-C4B	2.54	117.65	108.99
2	B	1401	NDP	O5B-C5B-C4B	2.50	117.49	108.99
2	A	1400	NDP	O5B-C5B-C4B	2.49	117.46	108.99
2	A	1400	NDP	C3N-C2N-N1N	-2.47	119.58	123.20
2	C	1402	NDP	N9A-C8A-N7A	-2.46	110.44	113.94
2	A	1400	NDP	O3B-C3B-C2B	-2.44	104.36	111.19
2	B	1401	NDP	C1D-N1N-C6N	-2.36	115.77	120.77
2	D	1403	NDP	O3-PN-O1N	-2.35	103.64	110.70
2	B	1401	NDP	O2A-PA-O1A	2.33	123.30	112.44
2	B	1401	NDP	C4B-O4B-C1B	-2.31	104.38	109.47
3	C	1406	PYQ	C7-C6-C5	-2.30	101.43	103.67
2	C	1402	NDP	C3N-C2N-N1N	-2.30	119.83	123.20
2	B	1401	NDP	O2B-C2B-C1B	2.29	118.11	110.05
3	B	1405	PYQ	O10-C9-N8	-2.29	119.26	122.47
3	D	1407	PYQ	C7-C6-C5	-2.26	101.47	103.67
2	A	1400	NDP	O2A-PA-O1A	2.25	122.92	112.44
3	A	1404	PYQ	C7-C6-C5	-2.25	101.47	103.67
2	C	1402	NDP	C5A-C4A-N9A	-2.24	103.37	105.81
3	C	1406	PYQ	O10-C9-N8	-2.24	119.33	122.47
2	C	1402	NDP	C2B-C1B-N9A	-2.22	110.11	113.75
2	C	1402	NDP	C2A-N1A-C6A	2.20	122.34	118.73
2	B	1401	NDP	O2X-P2B-O2B	2.19	114.36	105.85
2	B	1401	NDP	C6N-N1N-C2N	2.18	121.65	119.32
2	C	1402	NDP	O2A-PA-O1A	2.18	122.57	112.44
2	B	1401	NDP	C5A-C4A-N9A	-2.18	103.44	105.81
2	C	1402	NDP	C1D-N1N-C6N	-2.14	116.24	120.77
2	A	1400	NDP	C2B-C1B-N9A	-2.14	110.24	113.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1403	NDP	O3B-C3B-C2B	-2.09	105.32	111.19
2	B	1401	NDP	O3-PN-O1N	-2.09	104.43	110.70
2	A	1400	NDP	C5A-C4A-N9A	-2.08	103.55	105.81
2	D	1403	NDP	C3N-C2N-N1N	-2.06	120.18	123.20
2	D	1403	NDP	C5A-C4A-N9A	-2.05	103.57	105.81
2	C	1402	NDP	O3B-C3B-C2B	-2.05	105.46	111.19
3	A	1404	PYQ	C12-C2-C3	-2.04	116.06	119.47
2	D	1403	NDP	C2A-N1A-C6A	2.01	122.03	118.73
2	B	1401	NDP	O3B-C3B-C2B	-2.01	105.57	111.19
2	A	1400	NDP	C1D-N1N-C6N	-2.00	116.54	120.77

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1400	NDP	C5B-O5B-PA-O1A
2	A	1400	NDP	C5B-O5B-PA-O2A
2	A	1400	NDP	O4B-C4B-C5B-O5B
2	C	1402	NDP	C5B-O5B-PA-O1A
2	C	1402	NDP	C5B-O5B-PA-O2A
2	C	1402	NDP	O4B-C4B-C5B-O5B
2	D	1403	NDP	C5B-O5B-PA-O1A
2	D	1403	NDP	C5B-O5B-PA-O2A
2	D	1403	NDP	O4B-C4B-C5B-O5B
2	A	1400	NDP	C3B-C4B-C5B-O5B
2	D	1403	NDP	C3B-C4B-C5B-O5B
2	B	1401	NDP	O4B-C4B-C5B-O5B
2	C	1402	NDP	C3B-C4B-C5B-O5B
2	B	1401	NDP	C3B-C4B-C5B-O5B
2	A	1400	NDP	PN-O3-PA-O1A
2	C	1402	NDP	PN-O3-PA-O1A
2	A	1400	NDP	C5B-O5B-PA-O3
2	C	1402	NDP	C5B-O5B-PA-O3
2	D	1403	NDP	C5B-O5B-PA-O3
2	D	1403	NDP	PN-O3-PA-O1A
2	B	1401	NDP	O4D-C1D-N1N-C6N
2	D	1403	NDP	O4D-C1D-N1N-C6N
2	A	1400	NDP	O4D-C1D-N1N-C6N
2	C	1402	NDP	O4D-C1D-N1N-C6N
2	B	1401	NDP	PN-O3-PA-O1A
2	D	1403	NDP	PN-O3-PA-O2A
2	A	1400	NDP	PN-O3-PA-O2A

Continued on next page...

Continued from previous page...

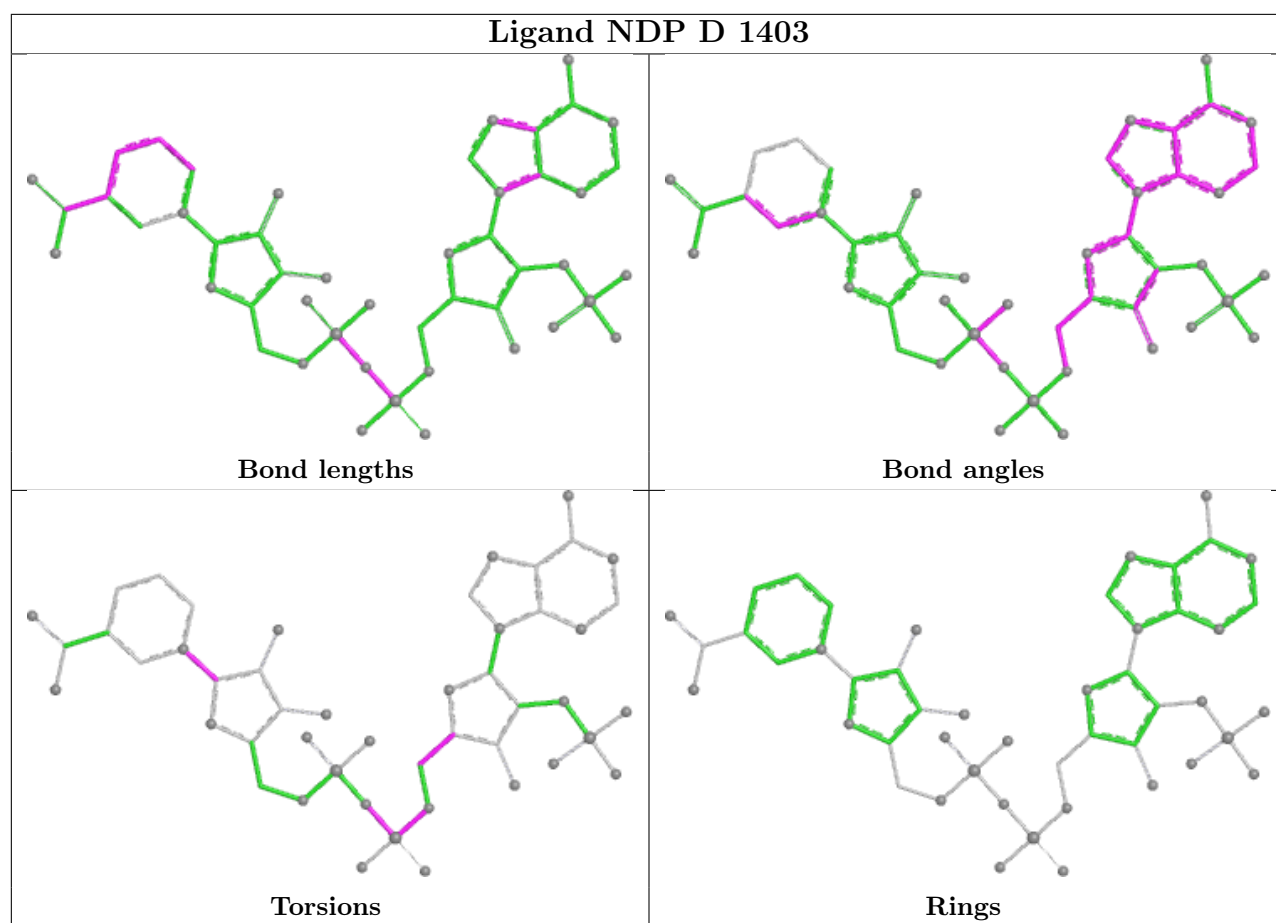
Mol	Chain	Res	Type	Atoms
2	B	1401	NDP	PN-O3-PA-O2A
2	C	1402	NDP	PN-O3-PA-O2A

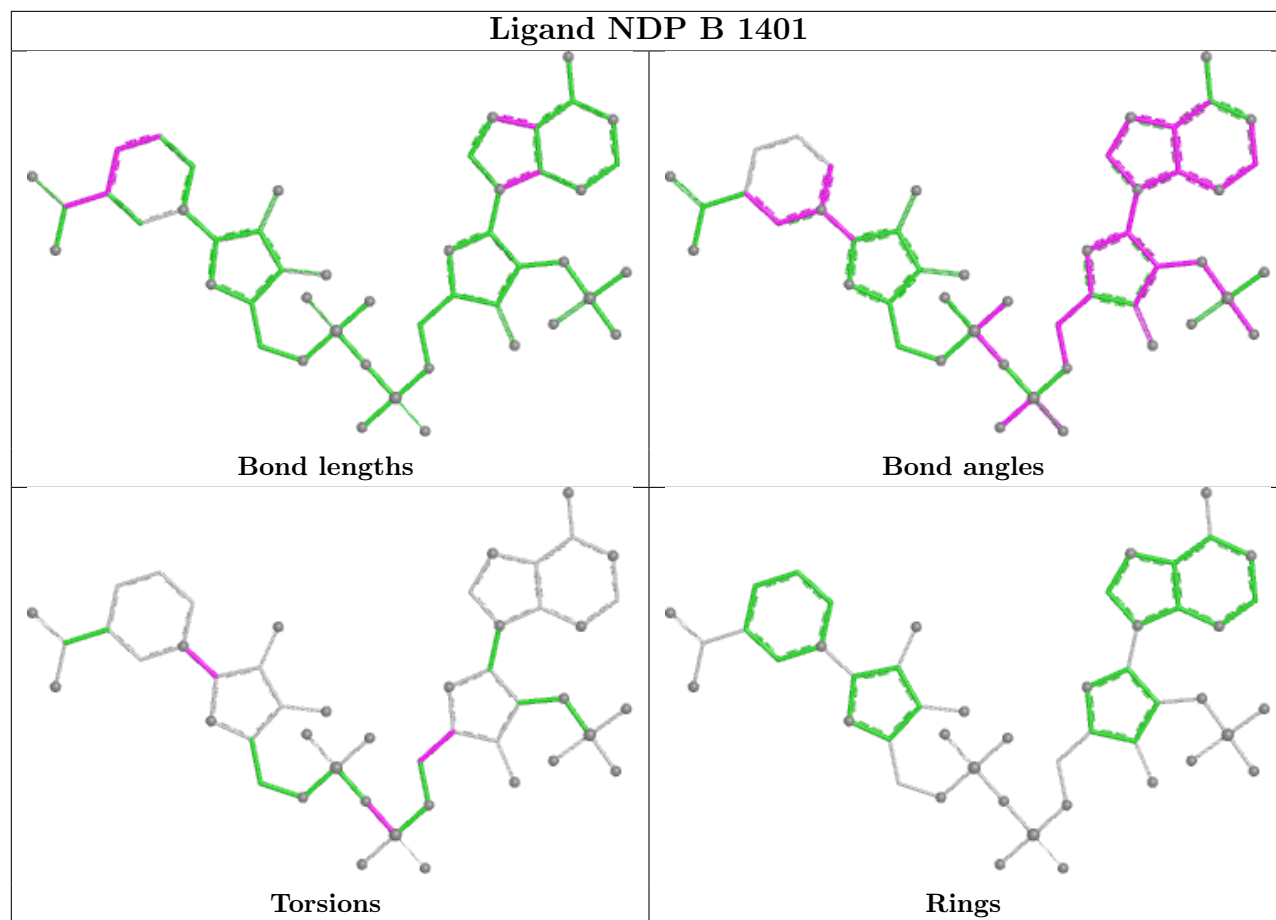
There are no ring outliers.

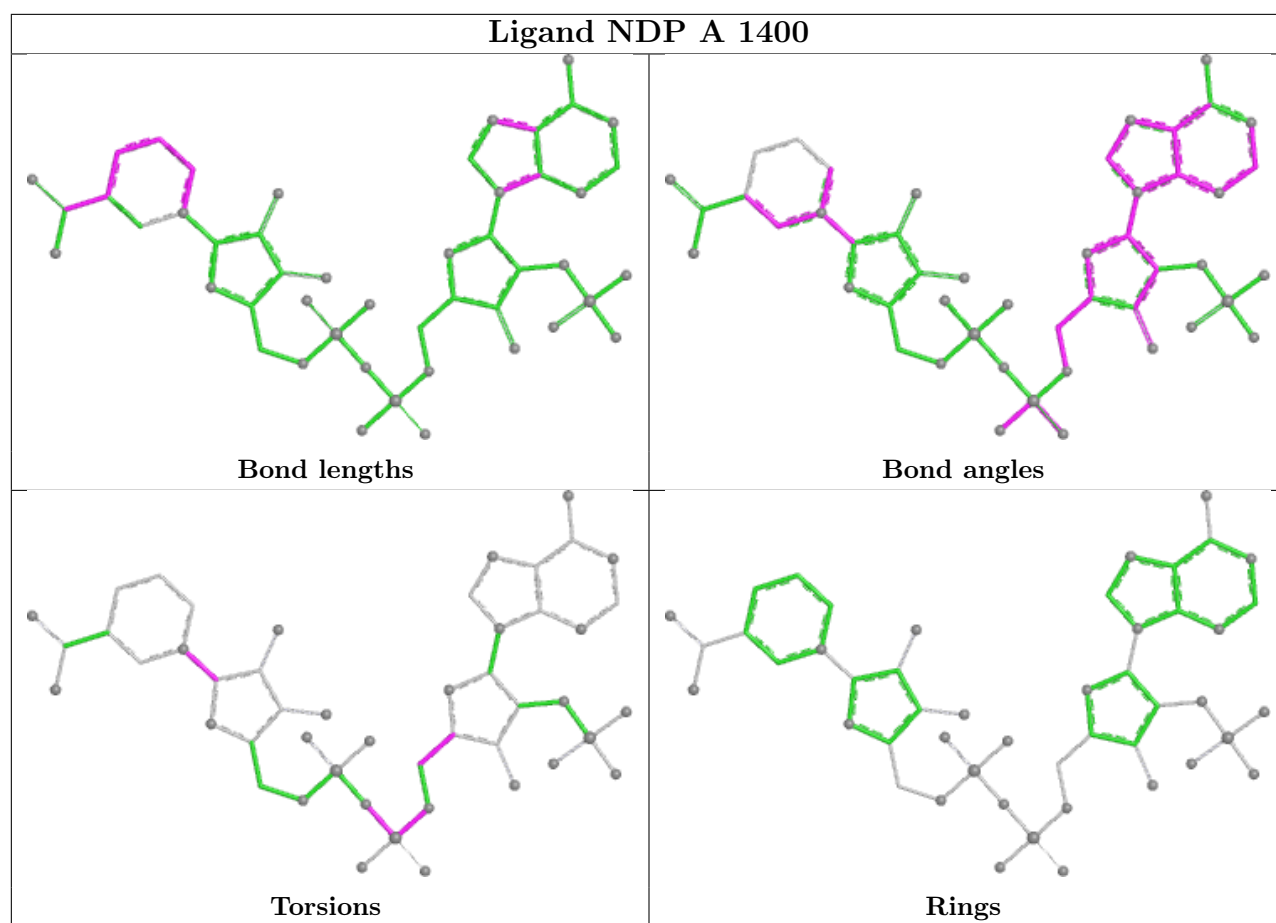
7 monomers are involved in 8 short contacts:

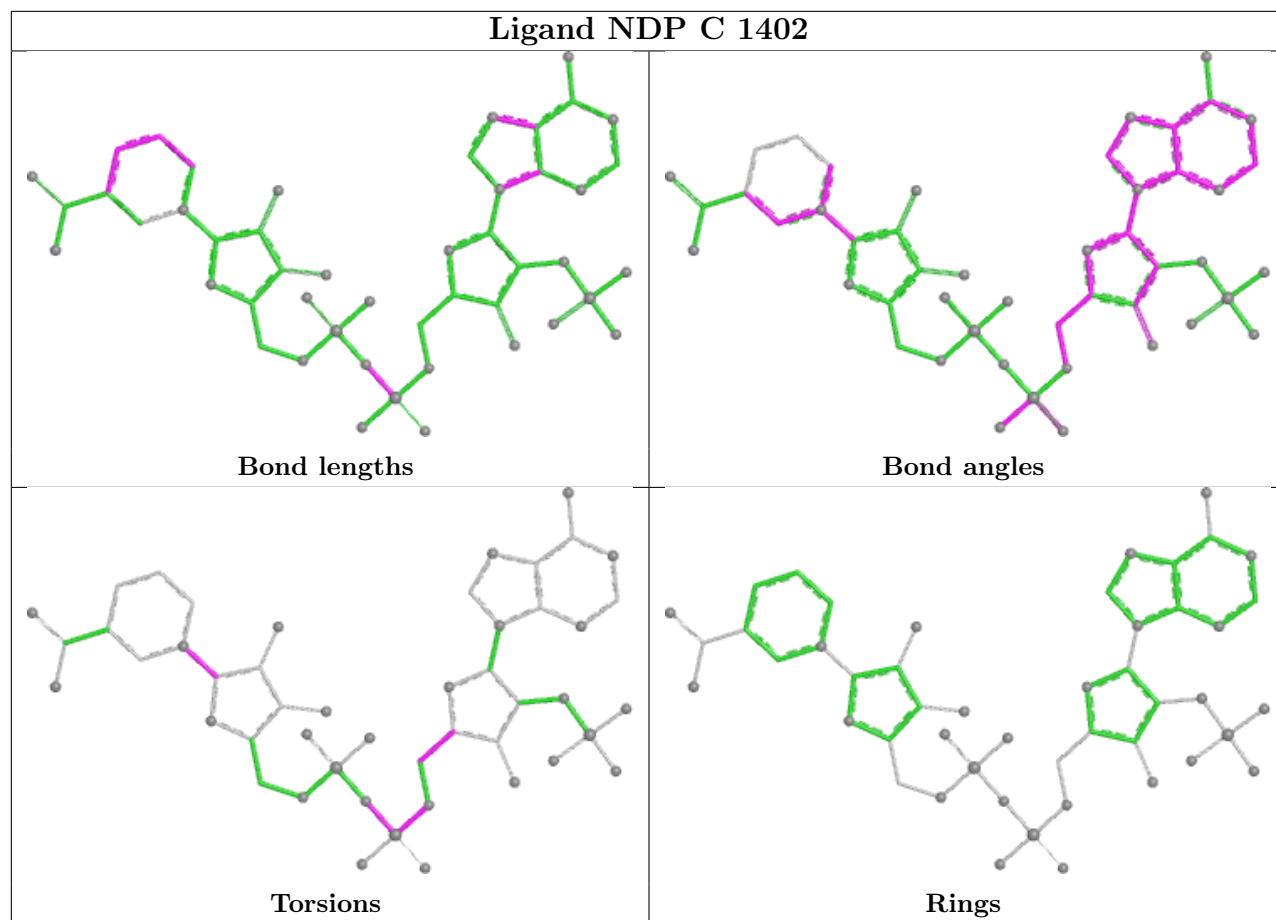
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1403	NDP	2	0
2	B	1401	NDP	1	0
3	C	1406	PYQ	1	0
2	A	1400	NDP	2	0
3	B	1405	PYQ	1	0
3	A	1404	PYQ	2	0
3	D	1407	PYQ	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.