Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 11:23 PM EST

PDB ID	:	1S14
Title	:	Crystal structure of Escherichia coli Topoisomerase IV ParE 24kDa subunit
Authors	:	Wei, Y.; Gross, C.H.
Deposited on	:	2004-01-05
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

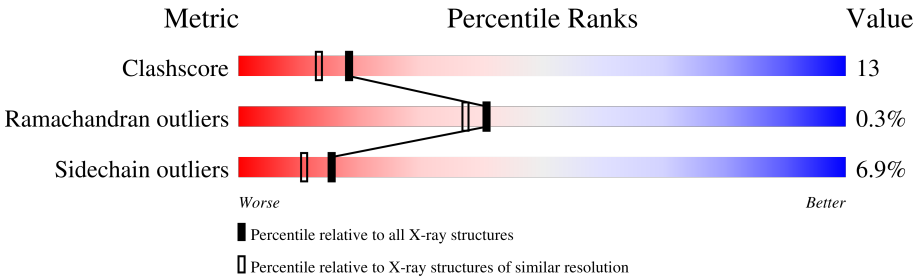
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	64% 19% • 13%
1	B	194	65% 23% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3337 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 Topoisomerase IV subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1318	819	235	259	5			
1	B	178	Total	C	N	O	S	0	0	0
			1405	873	254	272	6			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P20083
A	?	-	LEU	deletion	UNP P20083
A	?	-	HIS	deletion	UNP P20083
A	?	-	ALA	deletion	UNP P20083
A	?	-	GLY	deletion	UNP P20083
A	?	-	GLY	deletion	UNP P20083
A	?	-	LYS	deletion	UNP P20083
A	?	-	PHE	deletion	UNP P20083
A	?	-	SER	deletion	UNP P20083
A	?	-	ASN	deletion	UNP P20083
A	?	-	LYS	deletion	UNP P20083
A	?	-	ASN	deletion	UNP P20083
A	?	-	TYR	deletion	UNP P20083
A	?	-	GLN	deletion	UNP P20083
A	?	-	PHE	deletion	UNP P20083
A	?	-	SER	deletion	UNP P20083
A	?	-	GLY	deletion	UNP P20083
A	?	-	GLY	deletion	UNP P20083
A	?	-	LEU	deletion	UNP P20083
A	?	-	HIS	deletion	UNP P20083
A	?	-	GLY	deletion	UNP P20083
A	?	-	VAL	deletion	UNP P20083
A	?	-	GLY	deletion	UNP P20083
B	?	-	ARG	deletion	UNP P20083
B	?	-	LEU	deletion	UNP P20083

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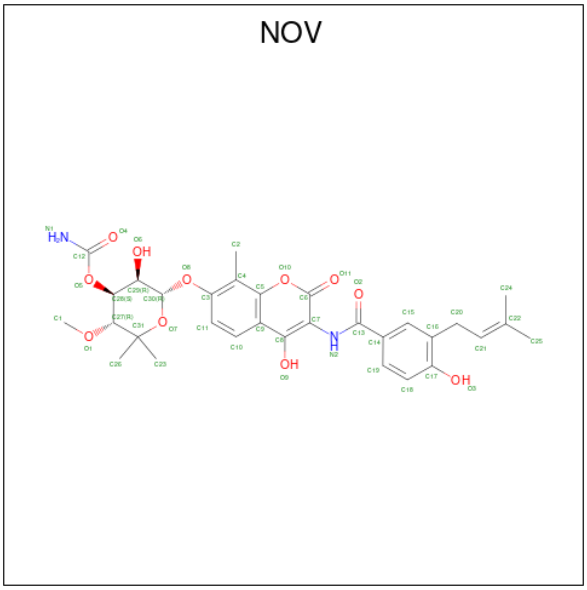
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP P20083
B	?	-	ALA	deletion	UNP P20083
B	?	-	GLY	deletion	UNP P20083
B	?	-	GLY	deletion	UNP P20083
B	?	-	LYS	deletion	UNP P20083
B	?	-	PHE	deletion	UNP P20083
B	?	-	SER	deletion	UNP P20083
B	?	-	ASN	deletion	UNP P20083
B	?	-	LYS	deletion	UNP P20083
B	?	-	ASN	deletion	UNP P20083
B	?	-	TYR	deletion	UNP P20083
B	?	-	GLN	deletion	UNP P20083
B	?	-	PHE	deletion	UNP P20083
B	?	-	SER	deletion	UNP P20083
B	?	-	GLY	deletion	UNP P20083
B	?	-	GLY	deletion	UNP P20083
B	?	-	LEU	deletion	UNP P20083
B	?	-	HIS	deletion	UNP P20083
B	?	-	GLY	deletion	UNP P20083
B	?	-	VAL	deletion	UNP P20083
B	?	-	GLY	deletion	UNP P20083

- Molecule 2 is NOVOBIOCIN (three-letter code: NOV) (formula: $C_{31}H_{36}N_2O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	31	2	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			44	31	2	11		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	237	Total	O	0	0
			237	237		
3	B	289	Total	O	0	0
			289	289		

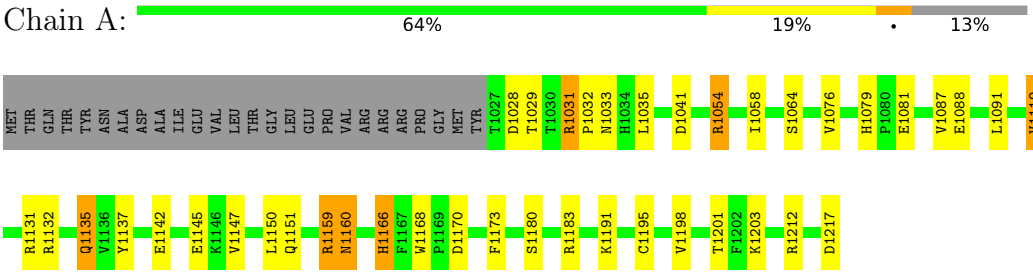
3 Residue-property plots (i)

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. 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.

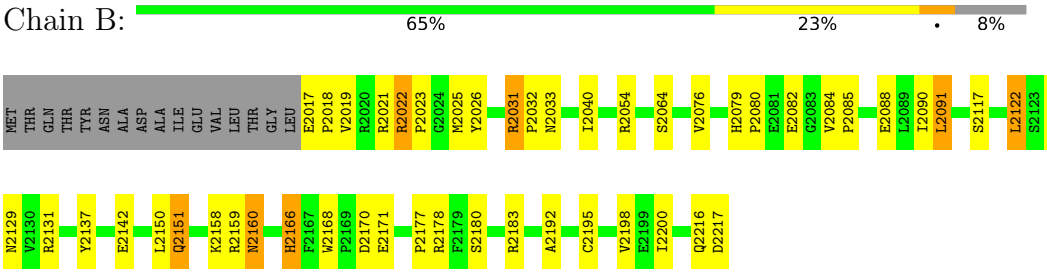
• Molecule 1: Topoisomerase IV subunit B

Chain A:



• Molecule 1: Topoisomerase IV subunit B

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	74.90Å 74.90Å 138.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.219 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3337	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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: NOV

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	0.32	0/1342	0.57	0/1823
1	B	0.30	0/1432	0.54	0/1944
All	All	0.31	0/2774	0.56	0/3767

There are no bond length outliers.

There are no bond angle outliers.

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	1318	0	1282	38	0
1	B	1405	0	1371	36	0
2	A	44	0	35	0	0
2	B	44	0	35	1	0
3	A	237	0	0	2	1
3	B	289	0	0	2	0
All	All	3337	0	2723	74	1

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 13.

All (74) 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:2033:ASN:HD21	1:B:2180:SER:H	1.00	0.94
1:A:1033:ASN:HD21	1:A:1180:SER:H	1.13	0.93
1:A:1201:THR:HG22	1:A:1212:ARG:HG2	1.51	0.92
1:A:1054:ARG:HH11	1:A:1054:ARG:HB3	1.35	0.92
1:A:1131:ARG:HH21	1:A:1160:ASN:HD21	1.29	0.80
1:A:1035:LEU:HD11	1:A:1119:VAL:HA	1.64	0.79
1:B:2022:ARG:HG3	1:B:2025:MET:HG3	1.68	0.74
1:B:2076:VAL:HB	1:B:2150:LEU:HD21	1.70	0.74
1:B:2033:ASN:HD21	1:B:2180:SER:N	1.83	0.69
1:A:1054:ARG:HB3	1:A:1054:ARG:NH1	2.08	0.69
1:B:2079:HIS:HB3	1:B:2082:GLU:HB2	1.77	0.67
1:B:2033:ASN:ND2	1:B:2180:SER:H	1.84	0.65
1:B:2021:ARG:HG3	1:B:2022:ARG:HD2	1.80	0.64
1:A:1079:HIS:HE1	1:A:1081:GLU:HB2	1.62	0.64
1:A:1201:THR:CG2	1:A:1212:ARG:HG2	2.27	0.62
1:A:1091:LEU:HD21	1:A:1128:VAL:CG2	2.32	0.59
1:B:2131:ARG:HH21	1:B:2160:ASN:HD21	1.49	0.58
1:A:1058:ILE:HG12	1:A:1203:LYS:HB3	1.84	0.58
1:B:2090:ILE:HD11	2:B:2300:NOV:C24	2.34	0.58
1:A:1160:ASN:C	1:A:1160:ASN:HD22	2.05	0.58
1:A:1076:VAL:HB	1:A:1150:LEU:HD21	1.85	0.57
1:B:2091:LEU:HD11	1:B:2128:VAL:HG21	1.87	0.57
1:B:2171:GLU:HB3	1:B:2177:PRO:HB3	1.87	0.56
1:A:1159:ARG:HH11	1:A:1159:ARG:HB2	1.71	0.55
1:A:1135:GLN:HB2	1:A:1137:TYR:CE1	2.42	0.55
1:A:1079:HIS:CE1	1:A:1081:GLU:HB2	2.43	0.54
1:A:1054:ARG:HH11	1:A:1054:ARG:CB	2.14	0.52
1:B:2171:GLU:H	1:B:2171:GLU:CD	2.13	0.51
1:A:1064:SER:OG	1:A:1166:HIS:HE1	1.94	0.51
1:B:2084:VAL:HB	1:B:2088:GLU:OE2	2.11	0.51
1:A:1091:LEU:HD21	1:A:1128:VAL:HG23	1.93	0.51
1:B:2064:SER:HB3	1:B:2168:TRP:CD1	2.46	0.50
1:A:1091:LEU:HD11	1:A:1128:VAL:HG21	1.93	0.50
1:B:2019:VAL:HA	1:B:2026:TYR:CE2	2.46	0.50
1:B:2040:ILE:HA	3:B:454:HOH:O	2.11	0.49
1:A:1159:ARG:HH11	1:A:1159:ARG:CB	2.26	0.49
1:B:2192:ALA:HB2	1:B:2200:ILE:HD12	1.94	0.49
1:A:1160:ASN:C	1:A:1160:ASN:ND2	2.67	0.48
1:B:2031:ARG:HB2	1:B:2032:PRO:HD2	1.95	0.48
1:B:2017:GLU:N	1:B:2018:PRO:HD2	2.28	0.48
1:B:2195:CYS:O	1:B:2198:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2217:ASP:OD2	1:B:2217:ASP:C	2.52	0.48
1:A:1058:ILE:HB	3:A:339:HOH:O	2.15	0.47
1:A:1142:GLU:HB2	1:A:1147:VAL:HG11	1.96	0.47
1:B:2031:ARG:NH2	1:B:2183:ARG:CZ	2.77	0.47
1:A:1091:LEU:HD21	1:A:1128:VAL:HG21	1.95	0.46
1:B:2151:GLN:O	1:B:2151:GLN:HG2	2.12	0.46
1:B:2085:PRO:HG2	1:B:2088:GLU:HB2	1.98	0.45
1:A:1217:ASP:C	1:A:1217:ASP:OD2	2.54	0.45
1:A:1031:ARG:HB2	1:A:1032:PRO:HD2	1.98	0.45
1:A:1064:SER:HB3	1:A:1168:TRP:CD1	2.52	0.45
1:A:1201:THR:HG23	3:A:77:HOH:O	2.16	0.45
1:B:2085:PRO:HD2	1:B:2088:GLU:OE2	2.18	0.44
1:B:2124:LYS:HG3	1:B:2170:ASP:HA	1.99	0.44
1:B:2064:SER:OG	1:B:2166:HIS:HE1	2.01	0.44
1:A:1131:ARG:HH21	1:A:1160:ASN:ND2	2.07	0.43
1:B:2124:LYS:HD3	1:B:2171:GLU:OE2	2.19	0.43
1:A:1041:ASP:OD1	1:A:1191:LYS:HE3	2.19	0.43
1:B:2178:ARG:HB2	1:B:2178:ARG:NH1	2.34	0.43
1:A:1170:ASP:HB3	1:A:1173:PHE:CD2	2.54	0.43
1:B:2178:ARG:HB2	1:B:2178:ARG:HH11	1.84	0.42
1:A:1131:ARG:HD2	1:A:1160:ASN:ND2	2.35	0.42
1:B:2023:PRO:HB3	1:B:2122:LEU:HD11	2.01	0.42
1:A:1028:ASP:OD1	1:A:1029:THR:N	2.53	0.42
1:B:2084:VAL:HB	1:B:2085:PRO:HD2	2.00	0.41
1:A:1195:CYS:O	1:A:1198:VAL:HG12	2.20	0.41
1:B:2125:ARG:NH1	1:B:2142:GLU:OE1	2.53	0.41
1:B:2129:ASN:HA	1:B:2137:TYR:O	2.21	0.41
1:B:2159:ARG:HH21	1:B:2159:ARG:HG3	1.85	0.41
1:A:1033:ASN:HD21	1:A:1180:SER:N	1.97	0.41
1:A:1087:VAL:HG13	1:A:1088:GLU:N	2.36	0.41
1:B:2054:ARG:HG2	3:B:42:HOH:O	2.21	0.41
1:A:1031:ARG:NH2	1:A:1183:ARG:CZ	2.85	0.40
1:A:1033:ASN:ND2	1:A:1180:SER:H	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:192:HOH:O	3:A:192:HOH:O[4_556]	1.97	0.23

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	166/194 (86%)	162 (98%)	4 (2%)	0	100 100
1	B	176/194 (91%)	171 (97%)	4 (2%)	1 (1%)	25 19
All	All	342/388 (88%)	333 (97%)	8 (2%)	1 (0%)	41 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2080	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	148/170 (87%)	137 (93%)	11 (7%)	13 9
1	B	157/170 (92%)	147 (94%)	10 (6%)	17 13
All	All	305/340 (90%)	284 (93%)	21 (7%)	15 11

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1031	ARG
1	A	1054	ARG
1	A	1119	VAL
1	A	1122	LEU
1	A	1132	ARG

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Mol	Chain	Res	Type
1	A	1135	GLN
1	A	1145	GLU
1	A	1151	GLN
1	A	1159	ARG
1	A	1160	ASN
1	A	1166	HIS
1	B	2022	ARG
1	B	2031	ARG
1	B	2091	LEU
1	B	2117	SER
1	B	2122	LEU
1	B	2151	GLN
1	B	2158	LYS
1	B	2160	ASN
1	B	2166	HIS
1	B	2216	GLN

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

Mol	Chain	Res	Type
1	A	1033	ASN
1	A	1138	ASN
1	A	1148	GLN
1	A	1160	ASN
1	A	1166	HIS
1	A	1207	ASN
1	B	2033	ASN
1	B	2148	GLN
1	B	2160	ASN
1	B	2166	HIS
1	B	2207	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	NOV	B	2300	-	47,47,47	3.04	20 (42%)	66,70,70	2.24	17 (25%)
2	NOV	A	1300	-	47,47,47	3.04	21 (44%)	66,70,70	1.99	16 (24%)

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	NOV	B	2300	-	-	3/23/46/46	0/4/4/4
2	NOV	A	1300	-	-	4/23/46/46	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	NOV	O7-C31	7.06	1.53	1.45
2	B	2300	NOV	C15-C14	6.15	1.48	1.39
2	B	2300	NOV	O5-C12	6.08	1.49	1.35
2	A	1300	NOV	C15-C14	5.83	1.48	1.39
2	A	1300	NOV	O6-C29	-5.82	1.29	1.43
2	B	2300	NOV	C5-C4	5.74	1.49	1.39
2	B	2300	NOV	C10-C9	5.52	1.48	1.39
2	A	1300	NOV	O5-C12	5.37	1.47	1.35
2	A	1300	NOV	C5-C4	5.33	1.48	1.39
2	B	2300	NOV	C9-C5	5.32	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2300	NOV	C17-C16	5.27	1.47	1.40
2	A	1300	NOV	C17-C16	4.98	1.47	1.40
2	A	1300	NOV	C10-C9	4.96	1.47	1.39
2	B	2300	NOV	O6-C29	-4.94	1.31	1.43
2	B	2300	NOV	C19-C14	4.86	1.47	1.39
2	B	2300	NOV	C19-C18	4.81	1.47	1.38
2	A	1300	NOV	C18-C17	4.75	1.48	1.39
2	A	1300	NOV	C19-C18	4.73	1.47	1.38
2	A	1300	NOV	C9-C5	4.69	1.50	1.40
2	A	1300	NOV	C15-C16	4.53	1.47	1.39
2	B	2300	NOV	C15-C16	4.44	1.47	1.39
2	B	2300	NOV	C18-C17	4.40	1.47	1.39
2	B	2300	NOV	C11-C3	4.29	1.48	1.39
2	B	2300	NOV	C11-C10	4.27	1.46	1.38
2	A	1300	NOV	C19-C14	4.19	1.46	1.39
2	A	1300	NOV	C11-C3	4.15	1.48	1.39
2	B	2300	NOV	O7-C31	3.99	1.50	1.45
2	A	1300	NOV	O10-C6	-3.83	1.32	1.38
2	A	1300	NOV	C11-C10	3.69	1.45	1.38
2	B	2300	NOV	C3-C4	3.68	1.45	1.40
2	B	2300	NOV	C7-C8	3.49	1.40	1.37
2	A	1300	NOV	C3-C4	3.14	1.44	1.40
2	B	2300	NOV	O10-C6	-3.07	1.33	1.38
2	B	2300	NOV	C7-C6	2.82	1.53	1.45
2	A	1300	NOV	C7-C6	2.80	1.53	1.45
2	A	1300	NOV	O5-C28	2.32	1.48	1.44
2	B	2300	NOV	O9-C8	2.24	1.39	1.33
2	A	1300	NOV	C23-C31	2.19	1.56	1.52
2	A	1300	NOV	O9-C8	2.14	1.39	1.33
2	A	1300	NOV	C7-C8	2.09	1.39	1.37
2	B	2300	NOV	O4-C12	-2.05	1.19	1.21

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2300	NOV	O10-C5-C4	6.92	123.28	114.84
2	B	2300	NOV	O10-C5-C9	-5.81	114.34	121.27
2	A	1300	NOV	O10-C5-C4	5.66	121.74	114.84
2	B	2300	NOV	O9-C8-C9	5.58	125.27	115.53
2	A	1300	NOV	O9-C8-C9	5.47	125.08	115.53
2	B	2300	NOV	O9-C8-C7	-5.21	116.18	123.19
2	A	1300	NOV	O10-C5-C9	-5.20	115.06	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2300	NOV	O10-C6-C7	4.50	124.60	116.88
2	A	1300	NOV	O9-C8-C7	-4.41	117.26	123.19
2	A	1300	NOV	C5-C9-C8	4.31	123.67	116.83
2	B	2300	NOV	C6-C7-N2	4.24	121.06	112.39
2	B	2300	NOV	C5-C9-C8	4.13	123.39	116.83
2	A	1300	NOV	O2-C13-N2	-4.11	116.14	122.26
2	A	1300	NOV	C6-C7-N2	4.11	120.80	112.39
2	B	2300	NOV	C14-C13-N2	3.95	122.14	116.24
2	A	1300	NOV	O10-C6-C7	3.88	123.53	116.88
2	B	2300	NOV	O5-C12-N1	3.58	116.15	110.58
2	A	1300	NOV	C14-C13-N2	3.32	121.20	116.24
2	B	2300	NOV	O2-C13-N2	-3.27	117.39	122.26
2	B	2300	NOV	O8-C30-C29	-3.25	102.42	107.14
2	A	1300	NOV	O8-C30-C29	-3.13	102.59	107.14
2	B	2300	NOV	C30-C29-C28	-3.09	104.64	110.07
2	B	2300	NOV	C20-C16-C17	2.60	124.80	120.49
2	A	1300	NOV	C20-C16-C17	2.47	124.58	120.49
2	B	2300	NOV	C3-O8-C30	2.46	122.80	118.09
2	A	1300	NOV	O5-C12-N1	2.20	114.00	110.58
2	B	2300	NOV	C28-O5-C12	-2.17	114.02	117.12
2	A	1300	NOV	C9-C8-C7	-2.15	117.44	121.30
2	A	1300	NOV	C30-C29-C28	-2.13	106.33	110.07
2	B	2300	NOV	O4-C12-N1	-2.12	122.02	125.51
2	A	1300	NOV	O4-C12-N1	-2.10	122.04	125.51
2	A	1300	NOV	C25-C22-C24	2.08	119.19	114.60
2	B	2300	NOV	C20-C16-C15	-2.06	116.78	120.93

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1300	NOV	O2-C13-N2-C7
2	A	1300	NOV	C14-C13-N2-C7
2	B	2300	NOV	O2-C13-N2-C7
2	B	2300	NOV	C14-C13-N2-C7
2	B	2300	NOV	C6-C7-N2-C13
2	A	1300	NOV	O2-C13-C14-C19
2	A	1300	NOV	N2-C13-C14-C19

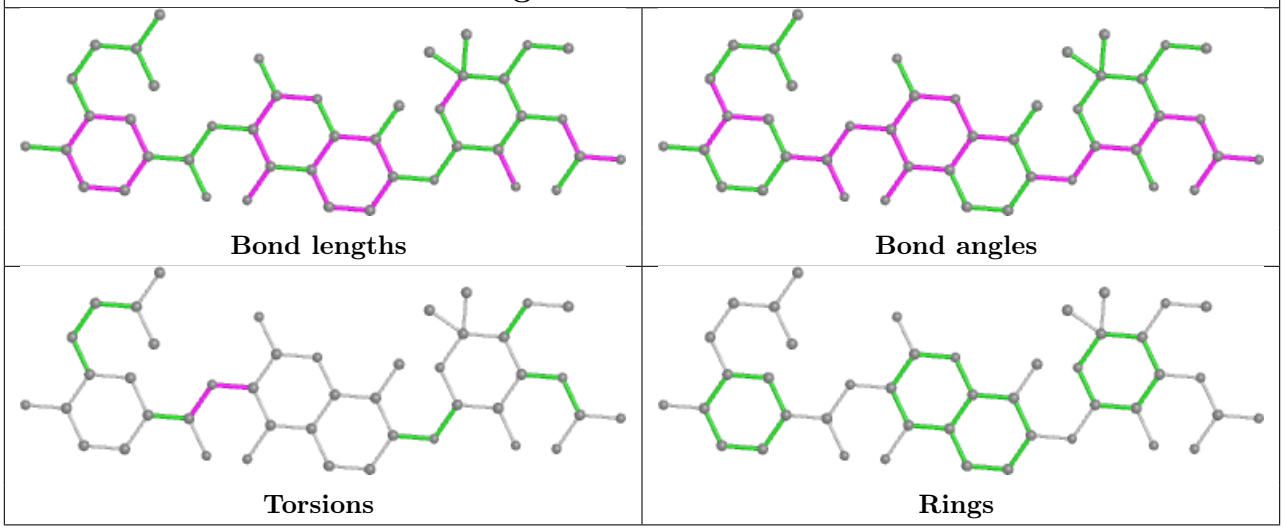
There are no ring outliers.

1 monomer is involved in 1 short contact:

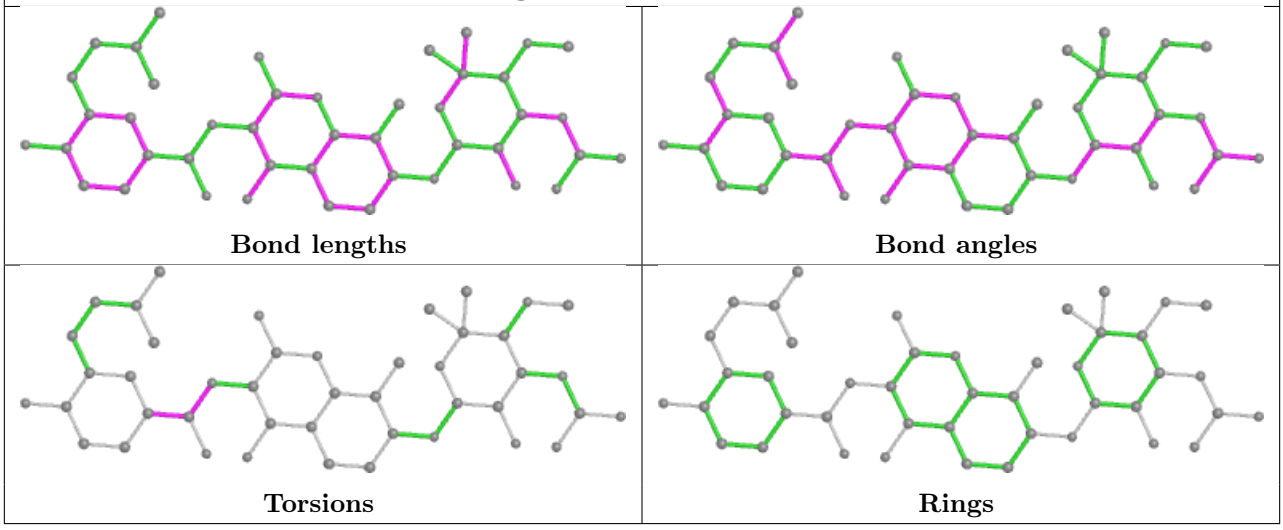
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2300	NOV	1	0

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 then 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 NOV B 2300



Ligand NOV A 1300



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.