



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 06:33 AM EST

PDB ID : 1VBJ  
Title : The crystal structure of prostaglandin F synthase from *Trypanosoma brucei*  
Authors : Inoue, T.  
Deposited on : 2004-02-27  
Resolution : 2.10 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](mailto: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)  
Xtrriage (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

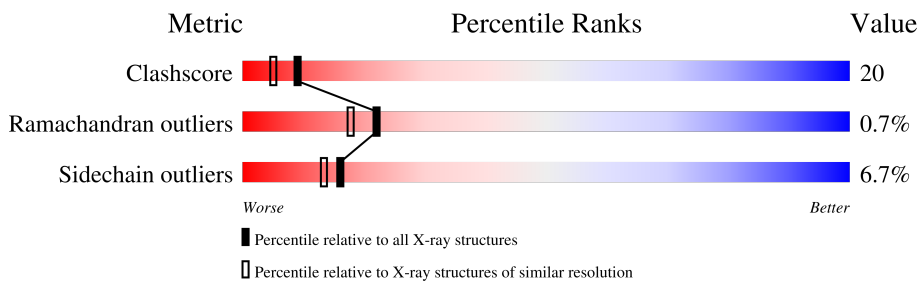
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $\geq 3$ , 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	281	69% 28% .
1	B	281	60% 35% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	A	4001	-	X	-	-
3	CIT	B	4002	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5094 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 prostaglandin F synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	Total	C	N	O	S	0	0	0
			2218	1418	376	411	13			
1	B	279	Total	C	N	O	S	0	0	0
			2208	1413	374	408	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	cloning artifact	UNP Q9GV41
A	-3	SER	-	cloning artifact	UNP Q9GV41
A	-2	PRO	-	cloning artifact	UNP Q9GV41
A	-1	GLU	-	cloning artifact	UNP Q9GV41
A	0	PHE	-	cloning artifact	UNP Q9GV41
B	-4	GLY	-	cloning artifact	UNP Q9GV41
B	-3	SER	-	cloning artifact	UNP Q9GV41
B	-2	PRO	-	cloning artifact	UNP Q9GV41
B	-1	GLU	-	cloning artifact	UNP Q9GV41
B	0	PHE	-	cloning artifact	UNP Q9GV41

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



- Molecule 4 is water.

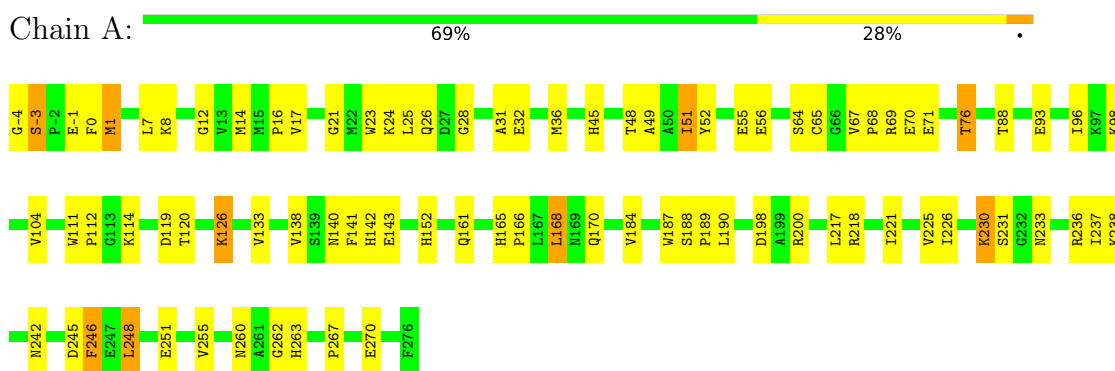
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	290	Total 290	O 290	0	0
4	B	256	Total 256	O 256	0	0

### 3 Residue-property plots [i](#)

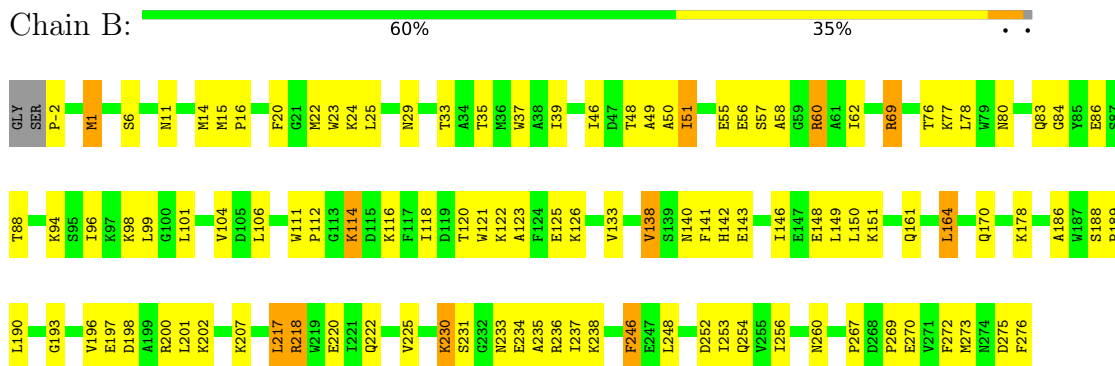
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: prostaglandin F synthase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.21Å 113.21Å 136.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.62 – 2.10	Depositor
% Data completeness (in resolution range)	89.0 (32.62-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.208 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: CIT, NAP

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	0.36	0/2270	0.61	0/3064
1	B	0.33	0/2260	0.59	0/3050
All	All	0.34	0/4530	0.60	0/6114

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	2218	0	2198	69	0
1	B	2208	0	2190	114	0
2	A	48	0	25	2	0
2	B	48	0	25	4	0
3	A	13	0	5	1	0
3	B	13	0	5	1	0
4	A	290	0	0	4	0
4	B	256	0	0	7	0
All	All	5094	0	4448	181	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 20.



All (181) 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:84:GLY:H	1:B:120:THR:HG22	1.23	1.02
1:B:48:THR:HG22	1:B:49:ALA:H	1.35	0.91
1:B:207:LYS:HG3	4:B:4045:HOH:O	1.75	0.87
1:B:118:ILE:H	1:B:118:ILE:HD12	1.37	0.86
1:B:84:GLY:N	1:B:120:THR:HG22	1.90	0.86
1:A:0:PHE:O	1:A:1:MET:HG2	1.79	0.83
1:B:233:ASN:O	1:B:237:ILE:HG12	1.82	0.79
1:B:116:LYS:O	1:B:120:THR:HG23	1.82	0.79
1:A:111:TRP:CH2	1:A:267:PRO:HG2	2.18	0.78
1:B:231:SER:HB3	1:B:237:ILE:HD13	1.62	0.78
1:B:22:MET:SD	1:B:46:ILE:HD11	2.24	0.78
1:A:48:THR:HG22	1:A:49:ALA:H	1.48	0.78
1:A:23:TRP:O	1:A:24:LYS:HG2	1.84	0.77
1:B:198:ASP:HB3	1:B:201:LEU:HD23	1.65	0.77
1:A:51:ILE:HD13	1:A:51:ILE:O	1.84	0.77
1:B:51:ILE:O	1:B:51:ILE:HD13	1.86	0.74
1:B:178:LYS:HE2	4:B:4163:HOH:O	1.86	0.74
1:A:21:GLY:O	1:A:230:LYS:HB2	1.87	0.73
1:A:55:GLU:OE2	1:A:76:THR:HG21	1.89	0.73
1:B:60:ARG:HB3	1:B:60:ARG:HH11	1.54	0.72
1:B:88:THR:HG21	1:B:120:THR:HB	1.70	0.72
1:A:230:LYS:HD2	1:A:231:SER:N	2.04	0.72
1:B:111:TRP:CH2	1:B:267:PRO:HG2	2.26	0.71
1:A:231:SER:HB3	1:A:237:ILE:HD13	1.74	0.69
1:B:69:ARG:HD2	1:B:101:LEU:HD22	1.73	0.69
1:B:233:ASN:HD22	1:B:236:ARG:HG3	1.58	0.69
1:B:148:GLU:HA	1:B:151:LYS:HE3	1.75	0.68
1:A:168:LEU:HD22	4:A:4061:HOH:O	1.93	0.67
1:A:233:ASN:HD22	1:A:236:ARG:H	1.40	0.67
1:A:104:VAL:O	1:A:133:VAL:HA	1.96	0.66
1:A:143:GLU:CG	1:B:260:ASN:HB3	2.26	0.66
1:A:233:ASN:O	1:A:237:ILE:HG12	1.96	0.65
1:A:8:LYS:HA	1:A:14:MET:HE1	1.78	0.64
1:A:96:ILE:HD13	1:A:104:VAL:HG23	1.81	0.63
1:B:76:THR:HG22	1:B:77:LYS:N	2.13	0.63
1:B:6:SER:HB2	1:B:15:MET:O	1.99	0.62
1:B:254:GLN:HG3	4:B:4133:HOH:O	1.98	0.62
1:B:222:GLN:NE2	1:B:253:ILE:HD11	2.15	0.62
1:B:114:LYS:HG2	1:B:273:MET:SD	2.40	0.62
2:B:3002:NAP:H4N	3:B:4002:CIT:H41	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:HB3	1:B:237:ILE:CD1	2.31	0.61
1:A:126:LYS:HD2	4:A:4049:HOH:O	2.00	0.61
1:B:233:ASN:HB3	1:B:236:ARG:HD2	1.82	0.60
1:B:83:GLN:HB3	1:B:120:THR:HG21	1.83	0.60
1:B:50:ALA:HA	1:B:55:GLU:OE1	2.02	0.59
1:B:233:ASN:HD21	1:B:235:ALA:HB3	1.68	0.59
1:A:8:LYS:HG3	1:A:14:MET:HE3	1.85	0.58
1:B:25:LEU:HD13	1:B:230:LYS:HE3	1.84	0.58
1:B:233:ASN:ND2	1:B:235:ALA:HB3	2.19	0.58
1:B:6:SER:OG	1:B:14:MET:HG3	2.03	0.57
1:B:193:GLY:O	1:B:196:VAL:HG22	2.04	0.57
1:B:188:SER:N	1:B:189:PRO:CD	2.68	0.57
1:A:140:ASN:HD21	1:A:187:TRP:HE1	1.54	0.56
1:B:146:ILE:O	1:B:150:LEU:HG	2.05	0.56
1:B:20:PHE:CE1	1:B:237:ILE:HD12	2.41	0.56
1:B:218:ARG:HH21	1:B:218:ARG:HG2	1.71	0.56
1:B:48:THR:HG22	1:B:49:ALA:N	2.14	0.55
1:B:55:GLU:OE2	1:B:76:THR:HG21	2.07	0.55
1:B:35:THR:O	1:B:39:ILE:HG13	2.07	0.55
1:B:151:LYS:HB2	1:B:151:LYS:NZ	2.21	0.55
1:A:8:LYS:HG3	1:A:14:MET:CE	2.36	0.55
1:A:56:GLU:HG3	1:A:98:LYS:HB3	1.88	0.55
1:B:6:SER:HB3	1:B:16:PRO:HA	1.87	0.55
1:B:76:THR:HG22	1:B:77:LYS:H	1.70	0.55
1:B:78:LEU:HD21	1:B:88:THR:HG22	1.88	0.55
1:B:233:ASN:HD22	1:B:236:ARG:H	1.55	0.55
1:A:246:PHE:H	1:A:246:PHE:HD2	1.53	0.54
1:B:60:ARG:HH11	1:B:60:ARG:CB	2.20	0.54
1:B:99:LEU:O	1:B:101:LEU:HG	2.07	0.54
1:A:65:CYS:SG	1:A:67:VAL:HG12	2.47	0.54
1:B:20:PHE:HE1	1:B:237:ILE:HD12	1.72	0.54
1:B:78:LEU:CD2	1:B:88:THR:HG22	2.38	0.54
1:B:96:ILE:HD13	1:B:104:VAL:HG23	1.89	0.54
1:A:231:SER:HB3	1:A:237:ILE:CD1	2.36	0.53
1:A:161:GLN:NE2	2:A:3001:NAP:H2N	2.22	0.53
1:B:142:HIS:CD2	1:B:270:GLU:HG2	2.44	0.53
1:A:188:SER:N	1:A:189:PRO:CD	2.72	0.53
1:B:56:GLU:O	1:B:60:ARG:HG3	2.09	0.52
1:A:263:HIS:HD2	4:B:4015:HOH:O	1.91	0.52
1:B:6:SER:HB2	1:B:15:MET:C	2.30	0.52
1:A:0:PHE:O	1:A:1:MET:CG	2.56	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:O	1:B:133:VAL:HA	2.09	0.52
1:B:198:ASP:O	1:B:202:LYS:HG3	2.08	0.52
1:B:118:ILE:HD12	1:B:118:ILE:N	2.15	0.51
1:B:161:GLN:NE2	2:B:3002:NAP:H2N	2.25	0.51
1:B:23:TRP:O	1:B:24:LYS:HB2	2.09	0.51
1:B:233:ASN:ND2	1:B:236:ARG:HG3	2.24	0.51
1:B:121:TRP:O	1:B:125:GLU:HG3	2.11	0.51
1:A:17:VAL:HB	1:A:221:ILE:HD12	1.92	0.51
1:A:-4:GLY:O	1:A:-3:SER:HB3	2.11	0.50
1:A:230:LYS:HD2	1:A:230:LYS:C	2.31	0.50
1:B:140:ASN:O	1:B:269:PRO:HB3	2.11	0.50
1:A:36:MET:HE1	1:A:64:SER:HB2	1.94	0.50
1:B:246:PHE:N	1:B:246:PHE:CD2	2.80	0.50
1:A:114:LYS:C	1:A:114:LYS:HD3	2.31	0.50
1:A:70:GLU:HG2	4:A:4110:HOH:O	2.11	0.49
1:A:231:SER:O	1:A:237:ILE:HD11	2.12	0.49
1:A:7:LEU:C	1:A:7:LEU:HD12	2.33	0.49
1:A:12:GLY:O	1:A:14:MET:HE2	2.12	0.49
1:B:190:LEU:HD21	1:B:217:LEU:CD1	2.43	0.49
1:A:25:LEU:HB3	1:A:31:ALA:HA	1.95	0.48
1:B:77:LYS:HE2	2:B:3002:NAP:H71N	1.79	0.48
1:A:142:HIS:CE1	1:A:270:GLU:HG2	2.48	0.48
1:A:48:THR:HG22	1:A:49:ALA:N	2.24	0.48
1:B:138:VAL:HG21	1:B:141:PHE:CE1	2.49	0.48
1:B:190:LEU:HD21	1:B:217:LEU:HD13	1.95	0.48
1:B:1:MET:HA	1:B:1:MET:CE	2.44	0.47
1:B:84:GLY:O	1:B:88:THR:HG23	2.14	0.47
1:B:246:PHE:H	1:B:246:PHE:HD2	1.62	0.47
1:B:246:PHE:N	1:B:246:PHE:HD2	2.12	0.47
1:A:140:ASN:ND2	1:A:187:TRP:HE1	2.12	0.47
1:B:252:ASP:O	1:B:256:ILE:HG13	2.15	0.47
1:A:8:LYS:HE2	1:A:14:MET:HE3	1.97	0.47
1:B:83:GLN:OE1	1:B:276:PHE:HE2	1.97	0.47
1:B:25:LEU:CD1	1:B:230:LYS:HE3	2.45	0.47
1:B:233:ASN:CB	1:B:236:ARG:HD2	2.45	0.47
1:A:198:ASP:OD2	1:A:200:ARG:HB2	2.15	0.47
1:B:57:SER:HA	1:B:60:ARG:CD	2.44	0.47
1:B:58:ALA:O	1:B:62:ILE:HG13	2.15	0.47
1:B:198:ASP:CB	1:B:201:LEU:HD23	2.42	0.47
1:B:218:ARG:HD2	1:B:222:GLN:OE1	2.15	0.47
1:A:93:GLU:O	1:A:96:ILE:HG22	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:LYS:HD2	1:B:231:SER:N	2.30	0.46
1:A:238:LYS:NZ	1:A:238:LYS:HB3	2.30	0.46
1:B:114:LYS:HE3	1:B:114:LYS:HA	1.98	0.46
1:B:123:ALA:O	1:B:126:LYS:HB3	2.16	0.46
1:B:220:GLU:O	1:B:225:VAL:HG22	2.16	0.46
1:B:218:ARG:O	1:B:218:ARG:HD3	2.17	0.45
1:B:234:GLU:HG2	1:B:238:LYS:HE2	1.98	0.45
1:A:52:TYR:HE1	3:A:4001:CIT:O2	2.00	0.45
1:A:68:PRO:HG2	1:A:71:GLU:HG3	1.98	0.45
1:A:28:GLY:O	1:A:32:GLU:HB2	2.15	0.45
1:A:190:LEU:HB2	2:A:3001:NAP:H52A	1.99	0.45
1:B:23:TRP:CH2	1:B:24:LYS:HE3	2.51	0.45
1:B:57:SER:HA	1:B:60:ARG:HD3	1.99	0.45
1:A:260:ASN:HB3	1:B:143:GLU:CG	2.47	0.45
1:B:253:ILE:HD12	4:B:4132:HOH:O	2.17	0.44
1:A:143:GLU:HG3	1:B:260:ASN:HB3	1.97	0.44
1:A:168:LEU:HD23	1:A:262:GLY:HA2	1.99	0.44
1:B:1:MET:HA	1:B:1:MET:HE2	2.00	0.44
1:B:11:ASN:HB2	4:B:4026:HOH:O	2.16	0.44
1:A:225:VAL:HG12	1:A:226:ILE:N	2.33	0.44
1:B:80:ASN:OD1	1:B:111:TRP:HB2	2.18	0.43
1:B:37:TRP:CE3	1:B:234:GLU:HB2	2.53	0.43
1:B:164:LEU:HB3	1:B:186:ALA:CB	2.48	0.43
1:B:29:ASN:O	1:B:33:THR:HG23	2.18	0.43
1:B:118:ILE:H	1:B:118:ILE:CD1	2.15	0.43
1:A:152:HIS:HA	4:A:4202:HOH:O	2.17	0.43
1:A:251:GLU:O	1:A:255:VAL:HG23	2.18	0.43
1:A:65:CYS:SG	1:A:67:VAL:CG1	3.07	0.43
1:B:138:VAL:HG22	1:B:141:PHE:CE2	2.53	0.43
1:B:112:PRO:HG3	1:B:141:PHE:CD2	2.53	0.43
1:B:151:LYS:HB2	1:B:151:LYS:HZ2	1.84	0.43
1:A:55:GLU:OE2	1:A:76:THR:CG2	2.64	0.43
1:A:-3:SER:OG	1:A:-1:GLU:HB2	2.18	0.43
1:B:94:LYS:O	1:B:98:LYS:HG3	2.19	0.43
1:A:88:THR:OG1	1:A:120:THR:HG23	2.20	0.42
1:A:184:VAL:O	1:A:225:VAL:HG13	2.19	0.42
1:B:234:GLU:O	1:B:238:LYS:HG3	2.20	0.42
1:A:165:HIS:HB2	1:A:166:PRO:CD	2.49	0.42
1:B:-2:PRO:HB2	4:B:4144:HOH:O	2.19	0.42
1:A:246:PHE:CD2	1:A:246:PHE:N	2.88	0.42
1:B:138:VAL:HG22	1:B:141:PHE:CZ	2.55	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PRO:HB2	1:A:45:HIS:HB2	2.01	0.42
1:B:118:ILE:O	1:B:122:LYS:HG3	2.20	0.42
1:A:0:PHE:O	1:A:0:PHE:HD1	2.03	0.41
1:B:83:GLN:HB3	1:B:120:THR:CG2	2.49	0.41
1:B:104:VAL:HB	1:B:133:VAL:HG12	2.01	0.41
1:B:80:ASN:O	1:B:83:GLN:HG3	2.20	0.41
1:B:161:GLN:HE21	2:B:3002:NAP:H2N	1.85	0.41
1:A:104:VAL:HB	1:A:133:VAL:HG12	2.02	0.41
1:B:76:THR:CG2	1:B:77:LYS:N	2.81	0.41
1:B:198:ASP:OD2	1:B:200:ARG:HB2	2.20	0.41
1:A:218:ARG:CG	1:A:248:LEU:HD22	2.51	0.41
1:B:164:LEU:HB3	1:B:186:ALA:HB1	2.02	0.41
1:A:112:PRO:HG3	1:A:141:PHE:CD2	2.56	0.41
1:B:218:ARG:HG2	1:B:218:ARG:NH2	2.36	0.41
1:B:49:ALA:HA	1:B:76:THR:HG23	2.03	0.40
1:A:17:VAL:HB	1:A:221:ILE:CD1	2.51	0.40
1:A:165:HIS:HB2	1:A:166:PRO:HD2	2.03	0.40
1:B:197:GLU:OE2	1:B:197:GLU:HA	2.20	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	279/281 (99%)	265 (95%)	11 (4%)	3 (1%)	14 9
1	B	277/281 (99%)	257 (93%)	19 (7%)	1 (0%)	34 32
All	All	556/562 (99%)	522 (94%)	30 (5%)	4 (1%)	22 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	GLN
1	B	272	PHE
1	A	-3	SER

### 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	233/233 (100%)	219 (94%)	14 (6%)	19	16
1	B	232/233 (100%)	215 (93%)	17 (7%)	14	11
All	All	465/466 (100%)	434 (93%)	31 (7%)	16	13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	69	ARG
1	A	76	THR
1	A	119	ASP
1	A	126	LYS
1	A	138	VAL
1	A	168	LEU
1	A	170	GLN
1	A	217	LEU
1	A	230	LYS
1	A	242	ASN
1	A	245	ASP
1	A	246	PHE
1	A	248	LEU
1	B	1	MET
1	B	51	ILE
1	B	60	ARG
1	B	69	ARG
1	B	86	GLU
1	B	106	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	114	LYS
1	B	138	VAL
1	B	149	LEU
1	B	164	LEU
1	B	170	GLN
1	B	217	LEU
1	B	218	ARG
1	B	230	LYS
1	B	246	PHE
1	B	248	LEU
1	B	275	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	160	ASN
1	A	161	GLN
1	A	170	GLN
1	A	192	GLN
1	A	233	ASN
1	A	263	HIS
1	A	274	ASN
1	B	5	GLN
1	B	26	GLN
1	B	140	ASN
1	B	152	HIS
1	B	161	GLN
1	B	170	GLN
1	B	192	GLN
1	B	233	ASN
1	B	242	ASN
1	B	263	HIS
1	B	274	ASN

### 5.3.3 RNA

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	B	3002	-	45,52,52	2.06	13 (28%)	56,80,80	1.54	12 (21%)
3	CIT	A	4001	-	12,12,12	2.52	4 (33%)	17,17,17	3.50	9 (52%)
2	NAP	A	3001	-	45,52,52	2.07	13 (28%)	56,80,80	1.56	12 (21%)
3	CIT	B	4002	-	12,12,12	2.07	4 (33%)	17,17,17	3.24	9 (52%)

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	NAP	B	3002	-	-	6/31/67/67	0/5/5/5
3	CIT	A	4001	-	-	10/16/16/16	-
2	NAP	A	3001	-	-	6/31/67/67	0/5/5/5
3	CIT	B	4002	-	-	8/16/16/16	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4001	CIT	C3-C6	6.10	1.59	1.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	NAP	C2N-N1N	5.91	1.42	1.35
2	B	3002	NAP	C2N-N1N	5.69	1.41	1.35
3	A	4001	CIT	O2-C1	-4.79	1.14	1.30
3	B	4002	CIT	C3-C6	4.62	1.58	1.53
2	B	3002	NAP	C4N-C3N	4.62	1.47	1.39
2	A	3001	NAP	C4N-C3N	4.51	1.47	1.39
2	A	3001	NAP	O4D-C1D	4.34	1.47	1.41
2	A	3001	NAP	C2A-N3A	4.29	1.39	1.32
2	B	3002	NAP	C2A-N3A	4.28	1.39	1.32
2	B	3002	NAP	O4D-C1D	4.19	1.46	1.41
2	A	3001	NAP	C2A-N1A	4.09	1.41	1.33
2	B	3002	NAP	C6N-N1N	3.70	1.44	1.35
2	B	3002	NAP	C2A-N1A	3.66	1.40	1.33
2	A	3001	NAP	C6N-N1N	3.65	1.44	1.35
2	B	3002	NAP	C2D-C1D	-3.43	1.48	1.53
3	B	4002	CIT	O2-C1	-3.36	1.19	1.30
2	A	3001	NAP	P2B-O2B	3.14	1.65	1.59
3	B	4002	CIT	C4-C3	2.81	1.57	1.53
2	A	3001	NAP	C2D-C1D	-2.77	1.49	1.53
2	B	3002	NAP	PA-O1A	-2.68	1.41	1.50
2	B	3002	NAP	P2B-O2B	2.64	1.64	1.59
2	A	3001	NAP	PA-O1A	-2.50	1.42	1.50
2	A	3001	NAP	C4A-N3A	2.50	1.39	1.35
2	A	3001	NAP	C5B-C4B	2.40	1.59	1.51
3	A	4001	CIT	C4-C3	2.33	1.56	1.53
2	B	3002	NAP	C4A-N3A	2.32	1.38	1.35
3	A	4001	CIT	C4-C5	2.28	1.57	1.50
2	B	3002	NAP	C3D-C4D	2.20	1.58	1.53
3	B	4002	CIT	C4-C5	2.13	1.57	1.50
2	A	3001	NAP	C3D-C4D	2.10	1.58	1.53
2	B	3002	NAP	C3N-C7N	2.08	1.53	1.50
2	B	3002	NAP	C5B-C4B	2.07	1.58	1.51
2	A	3001	NAP	C5N-C4N	2.06	1.43	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4001	CIT	C2-C3-C6	7.68	126.62	110.11
3	B	4002	CIT	O5-C6-C3	7.05	132.23	122.25
3	A	4001	CIT	O5-C6-C3	6.98	132.14	122.25
3	A	4001	CIT	O7-C3-C6	-6.62	99.58	108.86
3	B	4002	CIT	O7-C3-C6	-6.19	100.17	108.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4002	CIT	C2-C3-C6	5.88	122.75	110.11
3	B	4002	CIT	O6-C6-C3	-4.55	105.14	113.05
2	B	3002	NAP	C5A-C6A-N6A	4.16	126.67	120.35
2	A	3001	NAP	C5A-C6A-N6A	4.15	126.66	120.35
3	A	4001	CIT	O6-C6-C3	-4.05	106.02	113.05
2	A	3001	NAP	N3A-C2A-N1A	-3.90	122.58	128.68
2	B	3002	NAP	N3A-C2A-N1A	-3.83	122.69	128.68
2	A	3001	NAP	O4B-C4B-C5B	-3.29	98.56	109.37
3	B	4002	CIT	C4-C3-C6	-3.16	103.31	110.11
2	B	3002	NAP	O4B-C4B-C5B	-3.07	99.26	109.37
2	B	3002	NAP	C3N-C7N-N7N	2.97	121.31	117.75
2	A	3001	NAP	C3N-C7N-N7N	2.91	121.25	117.75
2	A	3001	NAP	O7N-C7N-C3N	-2.75	116.34	119.63
2	A	3001	NAP	C2N-C3N-C4N	2.74	121.37	118.26
2	B	3002	NAP	O2A-PA-O1A	2.68	125.51	112.24
3	A	4001	CIT	O2-C1-C2	2.67	122.92	114.35
2	A	3001	NAP	C2B-C3B-C4B	2.67	107.79	101.99
2	B	3002	NAP	C3D-C2D-C1D	2.66	104.98	100.98
3	B	4002	CIT	O2-C1-C2	2.63	122.80	114.35
2	B	3002	NAP	C2N-C3N-C4N	2.59	121.19	118.26
2	A	3001	NAP	C1B-N9A-C4A	-2.58	122.11	126.64
2	A	3001	NAP	O2A-PA-O1A	2.58	124.99	112.24
2	A	3001	NAP	O3X-P2B-O2X	2.49	117.14	107.64
2	B	3002	NAP	O7N-C7N-C3N	-2.46	116.69	119.63
2	A	3001	NAP	O3B-C3B-C4B	-2.44	104.00	111.05
3	A	4001	CIT	C3-C4-C5	-2.43	107.94	113.81
2	B	3002	NAP	C2B-C3B-C4B	2.39	107.19	101.99
2	B	3002	NAP	O3X-P2B-O2X	2.35	116.60	107.64
3	A	4001	CIT	C3-C2-C1	2.24	119.23	113.81
3	B	4002	CIT	O1-C1-C2	-2.23	116.44	122.94
2	B	3002	NAP	O3B-C3B-C4B	-2.20	104.68	111.05
2	B	3002	NAP	C1B-N9A-C4A	-2.12	122.91	126.64
3	B	4002	CIT	O4-C5-C4	-2.11	107.58	114.35
3	A	4001	CIT	O7-C3-C4	-2.08	104.53	109.40
3	B	4002	CIT	O3-C5-C4	2.04	128.90	122.94
2	A	3001	NAP	C3D-C2D-C1D	2.01	104.01	100.98
3	A	4001	CIT	O7-C3-C2	-2.00	104.71	109.40

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	NAP	O4D-C1D-N1N-C6N
2	B	3002	NAP	O4D-C1D-N1N-C6N
3	A	4001	CIT	C1-C2-C3-O7
3	A	4001	CIT	C1-C2-C3-C4
3	A	4001	CIT	C1-C2-C3-C6
3	A	4001	CIT	C2-C3-C6-O5
3	A	4001	CIT	C2-C3-C6-O6
3	A	4001	CIT	O7-C3-C6-O5
3	A	4001	CIT	O7-C3-C6-O6
3	B	4002	CIT	C6-C3-C4-C5
3	A	4001	CIT	O1-C1-C2-C3
3	A	4001	CIT	O2-C1-C2-C3
3	B	4002	CIT	O1-C1-C2-C3
3	B	4002	CIT	O2-C1-C2-C3
3	B	4002	CIT	C2-C3-C4-C5
3	A	4001	CIT	O7-C3-C4-C5
2	A	3001	NAP	C5B-O5B-PA-O2A
2	B	3002	NAP	C5B-O5B-PA-O2A
3	B	4002	CIT	C4-C3-C6-O6
2	B	3002	NAP	C4D-C5D-O5D-PN
3	B	4002	CIT	C4-C3-C6-O5
2	A	3001	NAP	C4D-C5D-O5D-PN
2	B	3002	NAP	O4B-C4B-C5B-O5B
2	B	3002	NAP	PN-O3-PA-O2A
3	B	4002	CIT	C2-C3-C6-O6
2	A	3001	NAP	O4B-C4B-C5B-O5B
2	A	3001	NAP	C5B-O5B-PA-O3
2	B	3002	NAP	C5B-O5B-PA-O3
2	A	3001	NAP	PN-O3-PA-O2A
3	B	4002	CIT	O7-C3-C4-C5

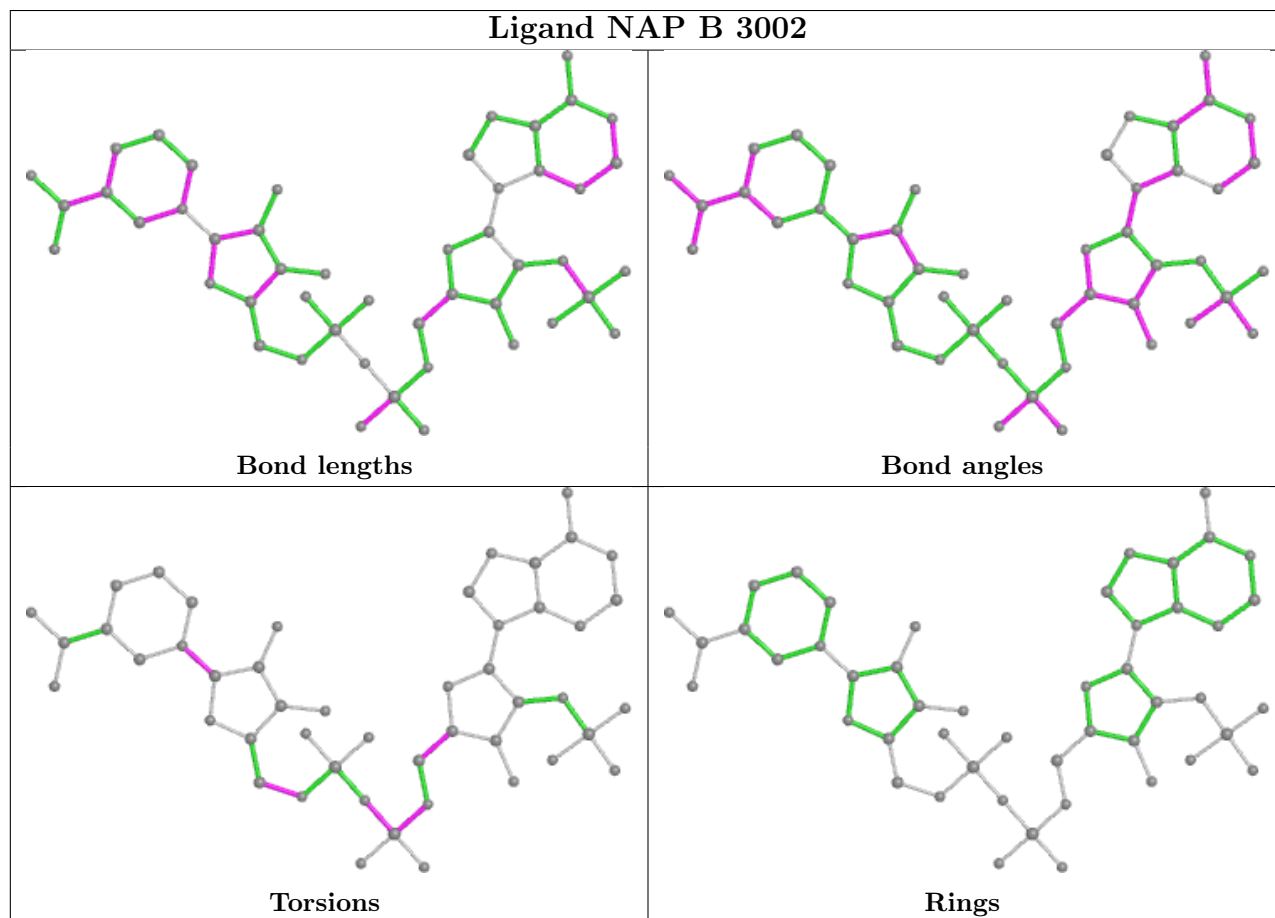
There are no ring outliers.

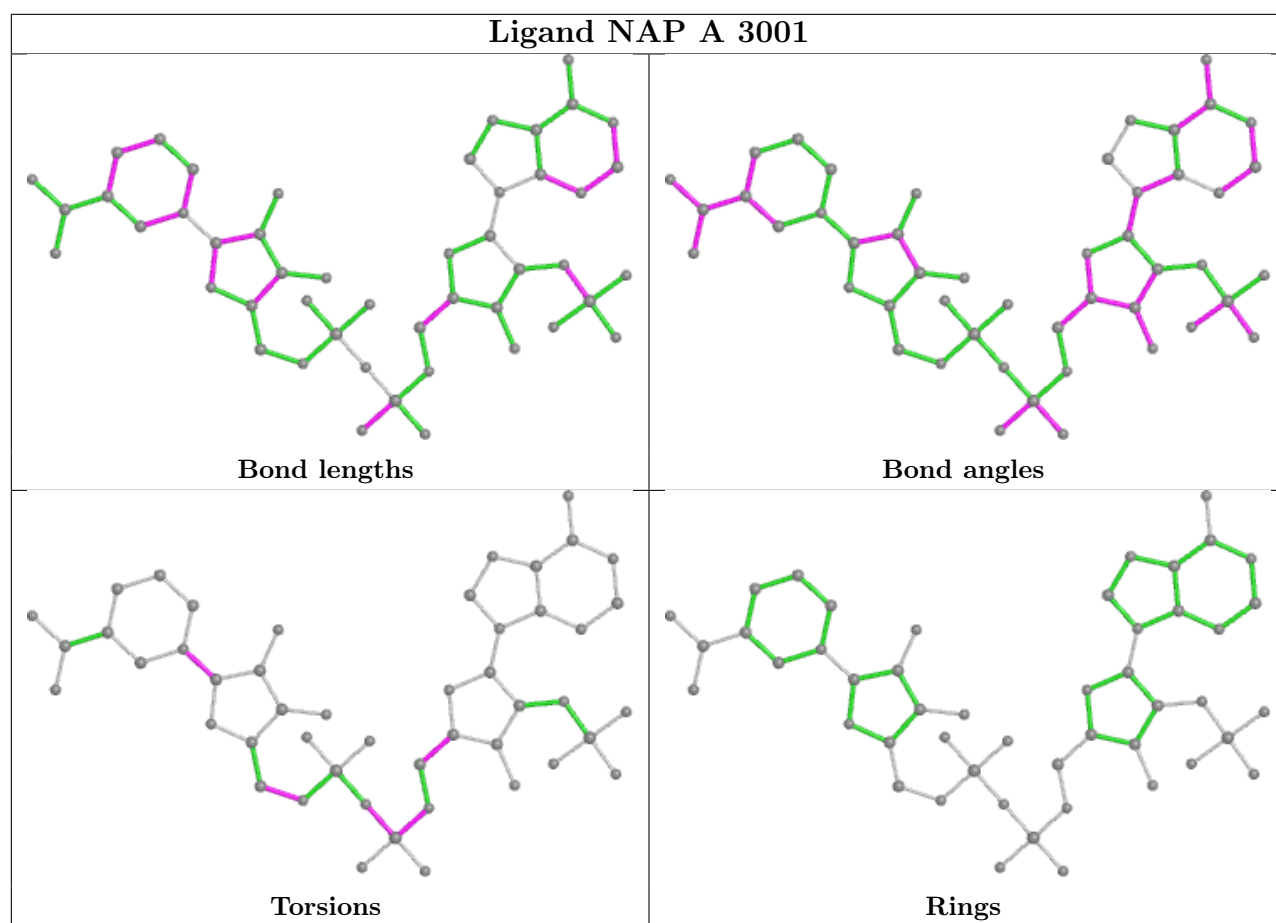
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	NAP	4	0
3	A	4001	CIT	1	0
2	A	3001	NAP	2	0
3	B	4002	CIT	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.





## 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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.