



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2022 – 06:11 PM JST

PDB ID : 7EJI  
Title : Crystal structure of KRED F147L/L153Q/Y190P/L199A/M205F/M206F variant and methyl methacrylate complex  
Authors : Cui, J.; Huang, X.; Wang, B.; Zhao, H.; Zhou, J.  
Deposited on : 2021-04-02  
Resolution : 1.56 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.

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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) : 1.13  
EDS : 2.28.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

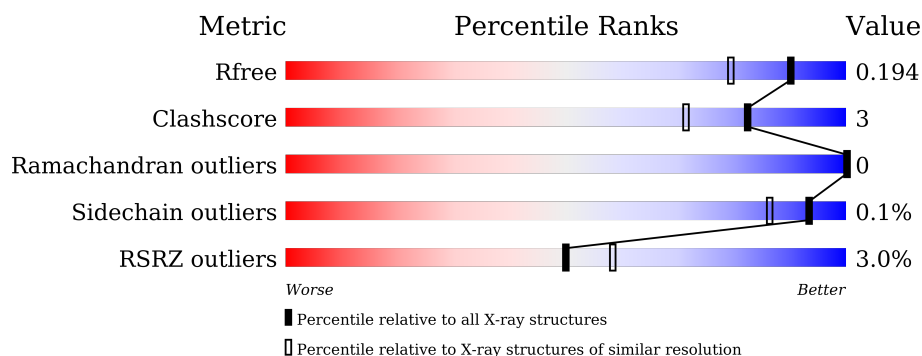
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 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))
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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  $\leq 5\%$ . 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	253	<div> <div></div> <div>96%</div> <div>.</div> </div>
1	B	253	<div> <div>4%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	C	253	<div> <div>%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
1	D	253	<div> <div>7%</div> <div>92%</div> <div>8%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	J69	D	305	-	X	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8485 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 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	3	0
			1899	1188	324	380	7			
1	B	251	Total	C	N	O	S	0	2	0
			1883	1179	322	376	6			
1	C	251	Total	C	N	O	S	0	2	0
			1880	1177	321	376	6			
1	D	252	Total	C	N	O	S	0	0	0
			1876	1176	320	373	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q6WVP7
A	147	LEU	PHE	engineered mutation	UNP Q6WVP7
A	153	GLN	LEU	engineered mutation	UNP Q6WVP7
A	190	PRO	TYR	engineered mutation	UNP Q6WVP7
A	199	ALA	LEU	engineered mutation	UNP Q6WVP7
A	205	PHE	MET	engineered mutation	UNP Q6WVP7
A	206	PHE	MET	engineered mutation	UNP Q6WVP7
B	0	GLY	-	expression tag	UNP Q6WVP7
B	147	LEU	PHE	engineered mutation	UNP Q6WVP7
B	153	GLN	LEU	engineered mutation	UNP Q6WVP7
B	190	PRO	TYR	engineered mutation	UNP Q6WVP7
B	199	ALA	LEU	engineered mutation	UNP Q6WVP7
B	205	PHE	MET	engineered mutation	UNP Q6WVP7
B	206	PHE	MET	engineered mutation	UNP Q6WVP7
C	0	GLY	-	expression tag	UNP Q6WVP7
C	147	LEU	PHE	engineered mutation	UNP Q6WVP7
C	153	GLN	LEU	engineered mutation	UNP Q6WVP7
C	190	PRO	TYR	engineered mutation	UNP Q6WVP7
C	199	ALA	LEU	engineered mutation	UNP Q6WVP7
C	205	PHE	MET	engineered mutation	UNP Q6WVP7
C	206	PHE	MET	engineered mutation	UNP Q6WVP7

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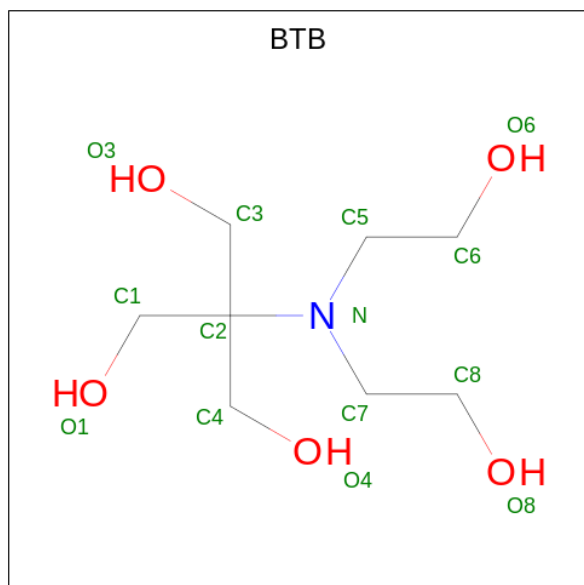
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP Q6WVP7
D	147	LEU	PHE	engineered mutation	UNP Q6WVP7
D	153	GLN	LEU	engineered mutation	UNP Q6WVP7
D	190	PRO	TYR	engineered mutation	UNP Q6WVP7
D	199	ALA	LEU	engineered mutation	UNP Q6WVP7
D	205	PHE	MET	engineered mutation	UNP Q6WVP7
D	206	PHE	MET	engineered mutation	UNP Q6WVP7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

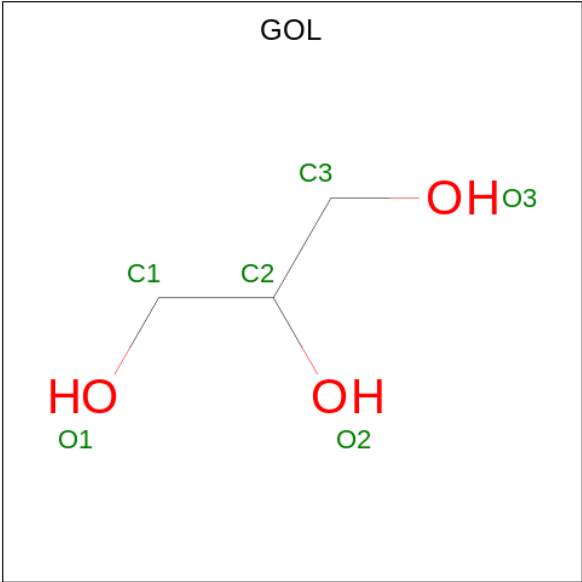
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



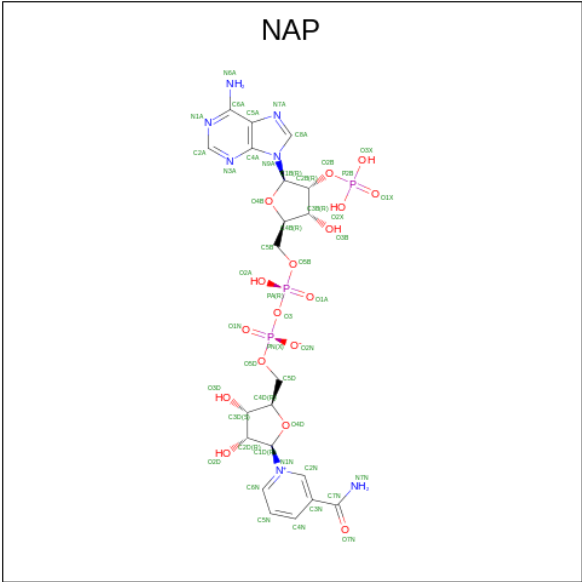
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



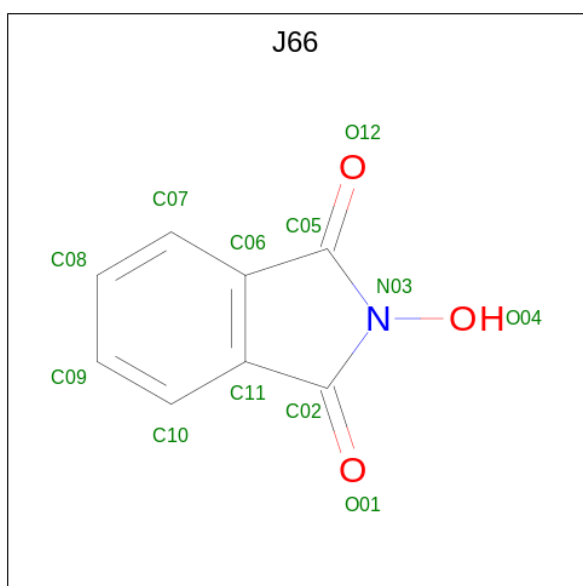
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 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>) (labeled as "Ligand of Interest" by depositor).



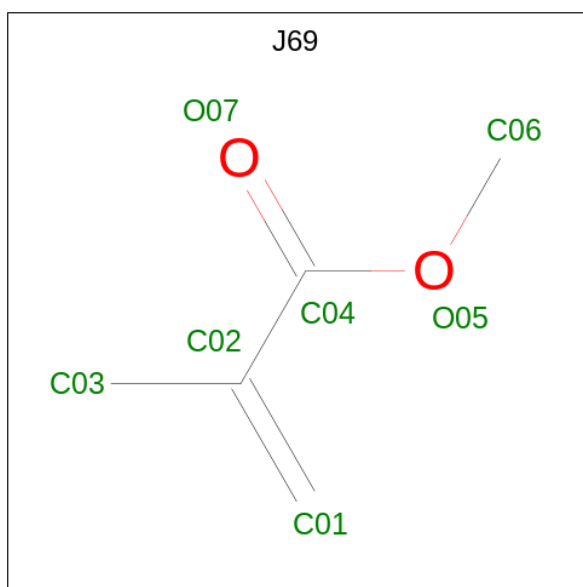
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is 2-oxidanylisindole-1,3-dione (three-letter code: J66) (formula:  $C_8H_5NO_3$ ).



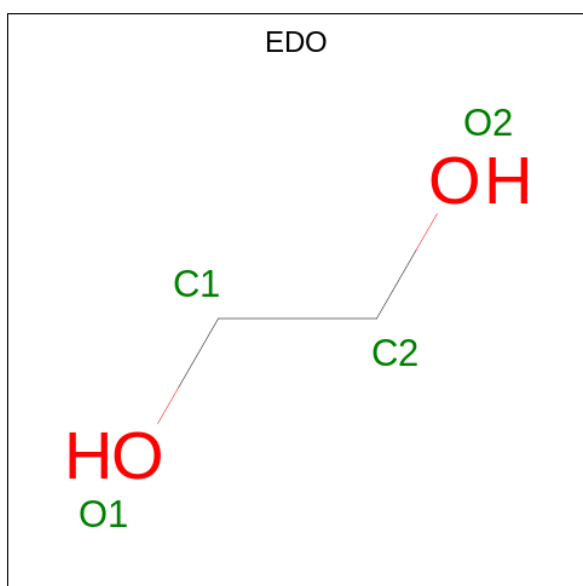
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	8	1	3		
6	C	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 7 is methyl 2-methylprop-2-enoate (three-letter code: J69) (formula:  $C_5H_8O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	5	2		
7	D	1	Total	C	O	0	0
			7	5	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

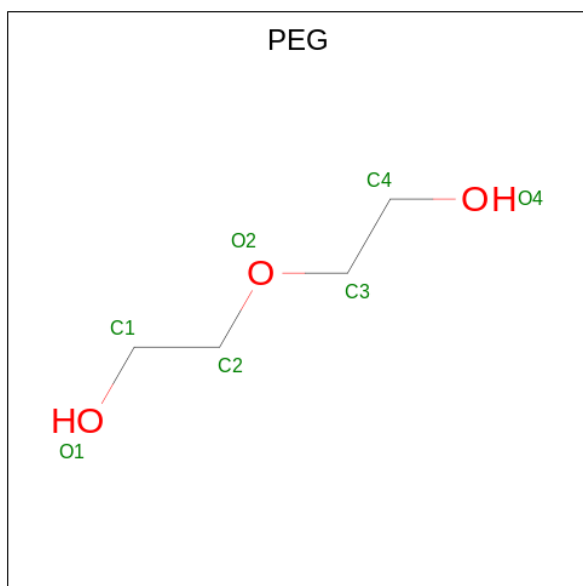
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

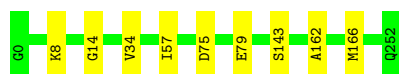
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	194	Total	O	0	0
			194	194		
10	B	160	Total	O	0	0
			160	160		
10	C	150	Total	O	0	0
			150	150		
10	D	140	Total	O	0	0
			140	140		

### 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: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase

Chain A:  96%



- Molecule 1: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase

Chain B:  93% 6%



- Molecule 1: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase

Chain C:  95%



- Molecule 1: 3-alpha-(Or 20-beta)-hydroxysteroid dehydrogenase

Chain D:  92% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.04Å 55.78Å 128.85Å 90.00° 103.67° 90.00°	Depositor
Resolution (Å)	50.69 – 1.56 62.26 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.69-1.56) 99.6 (62.26-1.52)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.185 , 0.213 0.185 , 0.194	Depositor DCC
$R_{free}$ test set	6939 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: J69, NAP, MG, GOL, PEG, BTB, J66, EDO

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	0/1929	0.58	1/2609 (0.0%)
1	B	0.34	0/1913	0.56	1/2588 (0.0%)
1	C	0.34	0/1910	0.54	0/2584
1	D	0.32	0/1906	0.51	0/2578
All	All	0.34	0/7658	0.55	2/10359 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	166	MET	CG-SD-CE	-5.25	91.81	100.20

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	1899	0	1881	6	0
1	B	1883	0	1863	9	0
1	C	1880	0	1860	9	0
1	D	1876	0	1864	11	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	14	0	19	4	0
3	C	14	0	19	1	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
4	D	12	0	16	0	0
5	A	48	0	25	1	0
5	B	48	0	25	1	0
5	C	48	0	25	0	0
5	D	48	0	25	1	0
6	A	12	0	0	1	0
6	C	12	0	0	1	0
7	B	7	0	0	2	0
7	D	7	0	0	3	0
8	C	4	0	6	2	0
8	D	8	0	12	1	0
9	C	7	0	10	0	0
10	A	194	0	0	0	0
10	B	160	0	0	0	0
10	C	150	0	0	0	0
10	D	140	0	0	1	0
All	All	8485	0	7666	39	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 (39) 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:33:LYS:HD2	1:C:56:VAL:HA	1.79	0.64
3:A:302:BTB:O1	1:D:116:ASP:OD1	2.24	0.55
7:D:305:J69:C03	7:D:305:J69:C06	2.86	0.54
1:C:178:ASP:HA	8:C:303:EDO:H21	1.89	0.54
5:B:302:NAP:C5N	7:B:303:J69:C01	2.86	0.53
1:D:3:ASP:HB3	1:D:30:GLU:O	2.08	0.53
1:A:75:ASP:O	1:A:79:GLU:HG3	2.10	0.52
1:A:162:ALA:HB2	1:D:162:ALA:HB2	1.90	0.52
3:A:302:BTB:O8	3:A:302:BTB:H12	2.10	0.52
5:D:304:NAP:C5N	7:D:305:J69:C01	2.88	0.51
1:B:143:SER:OG	7:B:303:J69:C01	2.62	0.48
1:C:78:GLU:OE2	1:C:128:ARG:NH1	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:BTB:H42	3:A:302:BTB:H51	1.70	0.47
1:D:16:THR:HG22	1:D:36:ILE:HD12	1.97	0.47
1:A:143:SER:OG	6:A:305:J66:O04	2.26	0.46
1:B:142:SER:HA	1:B:160:LYS:HD2	1.97	0.46
1:D:13:THR:HA	1:D:37:THR:OG1	2.17	0.45
1:B:162:ALA:HB2	1:C:162:ALA:HB2	2.00	0.44
1:C:55:ASP:OD1	1:C:55:ASP:N	2.48	0.43
1:C:180:ASP:H	8:C:303:EDO:C2	2.32	0.43
1:B:169:SER:HB2	1:C:157:ASN:OD1	2.18	0.43
1:D:93:ILE:HD11	1:D:110:LEU:HA	2.01	0.43
1:D:143:SER:OG	7:D:305:J69:C01	2.67	0.42
8:D:301:EDO:H22	10:D:404:HOH:O	2.19	0.42
1:B:157:ASN:OD1	1:C:169:SER:HB2	2.19	0.42
1:B:3:ASP:HB3	1:B:30:GLU:O	2.20	0.42
3:A:302:BTB:H32	3:A:302:BTB:H72	1.82	0.42
1:A:8:LYS:NZ	4:A:303:GOL:H32	2.35	0.41
1:B:85:THR:O	1:B:136:ALA:HA	2.21	0.41
1:A:14:GLY:HA2	5:A:304:NAP:H1B	2.02	0.41
1:D:142:SER:HA	1:D:160:LYS:HD2	2.02	0.41
1:D:54:THR:HA	1:D:57:ILE:O	2.21	0.41
1:D:211:LYS:HD3	1:D:211:LYS:HA	1.87	0.41
1:B:78:GLU:HA	1:B:82:GLY:O	2.21	0.41
1:D:85:THR:O	1:D:136:ALA:HA	2.20	0.41
1:C:196:VAL:HG22	6:C:306:J66:C08	2.51	0.40
1:A:34:VAL:O	1:A:57:ILE:HA	2.21	0.40
1:B:13:THR:HA	1:B:37:THR:OG1	2.21	0.40
3:C:302:BTB:H11	3:C:302:BTB:H71	1.90	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	254/253 (100%)	248 (98%)	6 (2%)	0	100	100
1	B	251/253 (99%)	243 (97%)	8 (3%)	0	100	100
1	C	251/253 (99%)	243 (97%)	8 (3%)	0	100	100
1	D	250/253 (99%)	244 (98%)	6 (2%)	0	100	100
All	All	1006/1012 (99%)	978 (97%)	28 (3%)	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	200/197 (102%)	200 (100%)	0	100	100
1	B	198/197 (100%)	198 (100%)	0	100	100
1	C	198/197 (100%)	198 (100%)	0	100	100
1	D	197/197 (100%)	196 (100%)	1 (0%)	88	78
All	All	793/788 (101%)	792 (100%)	1 (0%)	93	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	42	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	208	GLN

### 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](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

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	$\# Z  > 2$
5	NAP	B	302	-	45,52,52	0.83	1 (2%)	56,80,80	1.14	4 (7%)
5	NAP	C	305	-	45,52,52	0.84	2 (4%)	56,80,80	1.20	4 (7%)
5	NAP	D	304	-	45,52,52	0.79	1 (2%)	56,80,80	1.15	3 (5%)
3	BTB	C	302	-	13,13,13	0.75	0	7,16,16	0.37	0
4	GOL	B	301	-	5,5,5	0.31	0	5,5,5	0.45	0
4	GOL	D	303[B]	-	5,5,5	0.36	0	5,5,5	0.28	0
7	J69	D	305	-	6,6,6	2.08	4 (66%)	7,7,7	4.79	3 (42%)
9	PEG	C	304	-	6,6,6	0.15	0	5,5,5	0.16	0
4	GOL	D	303[A]	-	5,5,5	0.34	0	5,5,5	0.33	0
8	EDO	D	301	-	3,3,3	0.07	0	2,2,2	0.21	0
8	EDO	C	303	-	3,3,3	0.08	0	2,2,2	0.33	0
7	J69	B	303	-	6,6,6	2.08	3 (50%)	7,7,7	2.75	1 (14%)
4	GOL	A	303	-	5,5,5	0.32	0	5,5,5	0.32	0
3	BTB	A	302	-	13,13,13	0.77	1 (7%)	7,16,16	0.24	0
5	NAP	A	304	-	45,52,52	0.85	1 (2%)	56,80,80	1.29	5 (8%)
6	J66	A	305	-	11,13,13	1.62	3 (27%)	15,19,19	2.64	3 (20%)
6	J66	C	306	-	11,13,13	1.66	3 (27%)	15,19,19	2.76	3 (20%)
8	EDO	D	302	-	3,3,3	0.10	0	2,2,2	0.18	0

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
5	NAP	B	302	-	-	5/31/67/67	0/5/5/5
5	NAP	C	305	-	-	6/31/67/67	0/5/5/5
5	NAP	D	304	-	-	5/31/67/67	0/5/5/5
3	BTB	C	302	-	-	0/21/21/21	-
4	GOL	B	301	-	-	4/4/4/4	-
4	GOL	D	303[B]	-	-	3/4/4/4	-
7	J69	D	305	-	-	2/6/6/6	-
9	PEG	C	304	-	-	0/4/4/4	-
4	GOL	D	303[A]	-	-	2/4/4/4	-
8	EDO	D	301	-	-	0/1/1/1	-
8	EDO	C	303	-	-	0/1/1/1	-
7	J69	B	303	-	-	0/6/6/6	-
4	GOL	A	303	-	-	4/4/4/4	-
3	BTB	A	302	-	-	8/21/21/21	-
5	NAP	A	304	-	-	6/31/67/67	0/5/5/5
6	J66	A	305	-	-	-	0/2/2/2
6	J66	C	306	-	-	-	0/2/2/2
8	EDO	D	302	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	306	J66	C11-C02	3.29	1.54	1.48
6	A	305	J66	C06-C05	3.28	1.54	1.48
6	C	306	J66	C06-C05	3.19	1.54	1.48
6	A	305	J66	C11-C02	3.06	1.53	1.48
7	B	303	J69	O05-C06	-2.90	1.38	1.45
7	D	305	J69	O05-C04	2.84	1.39	1.33
7	B	303	J69	O07-C04	-2.80	1.15	1.21
7	B	303	J69	O05-C04	2.41	1.38	1.33
5	D	304	NAP	C5A-C4A	2.39	1.47	1.40
7	D	305	J69	O07-C04	-2.36	1.16	1.21
7	D	305	J69	O05-C06	-2.31	1.39	1.45
5	C	305	NAP	C5A-C4A	2.25	1.46	1.40
5	A	304	NAP	O4B-C1B	2.24	1.44	1.41
6	A	305	J66	O01-C02	-2.12	1.18	1.22
5	B	302	NAP	C5A-C4A	2.08	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	BTB	C2-N	2.07	1.52	1.48
7	D	305	J69	C04-C02	2.07	1.54	1.49
5	C	305	NAP	C2A-N3A	2.05	1.35	1.32
6	C	306	J66	O01-C02	-2.02	1.18	1.22

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	305	J69	O05-C04-C02	11.42	126.47	111.77
7	B	303	J69	O05-C04-C02	6.87	120.61	111.77
6	C	306	J66	C05-N03-C02	-6.24	108.70	114.22
6	A	305	J66	C05-N03-C02	-6.05	108.87	114.22
6	C	306	J66	C11-C02-N03	5.86	107.59	103.78
6	C	306	J66	C06-C05-N03	5.75	107.52	103.78
6	A	305	J66	C11-C02-N03	5.65	107.45	103.78
6	A	305	J66	C06-C05-N03	5.45	107.33	103.78
7	D	305	J69	O05-C04-O07	-4.09	115.65	123.53
5	B	302	NAP	N3A-C2A-N1A	-3.54	123.15	128.68
5	A	304	NAP	N3A-C2A-N1A	-3.43	123.32	128.68
5	C	305	NAP	N3A-C2A-N1A	-3.40	123.37	128.68
5	D	304	NAP	N3A-C2A-N1A	-3.29	123.54	128.68
5	A	304	NAP	C4A-C5A-N7A	-3.10	106.17	109.40
5	C	305	NAP	C4A-C5A-N7A	-3.00	106.27	109.40
5	A	304	NAP	C1B-N9A-C4A	-2.88	121.59	126.64
5	A	304	NAP	C2A-N1A-C6A	2.63	123.26	118.75
5	B	302	NAP	C1B-N9A-C4A	-2.62	122.03	126.64
5	D	304	NAP	C2A-N1A-C6A	2.38	122.83	118.75
5	C	305	NAP	C1B-N9A-C4A	-2.36	122.49	126.64
5	A	304	NAP	O2A-PA-O1A	2.36	123.90	112.24
5	B	302	NAP	C2A-N1A-C6A	2.28	122.65	118.75
7	D	305	J69	C03-C02-C01	-2.23	116.57	123.05
5	D	304	NAP	C4A-C5A-N7A	-2.19	107.11	109.40
5	B	302	NAP	C4A-C5A-N7A	-2.14	107.17	109.40
5	C	305	NAP	C2A-N1A-C6A	2.09	122.32	118.75

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	BTB	C1-C2-N-C5
3	A	302	BTB	C3-C2-N-C5
3	A	302	BTB	C4-C2-N-C5

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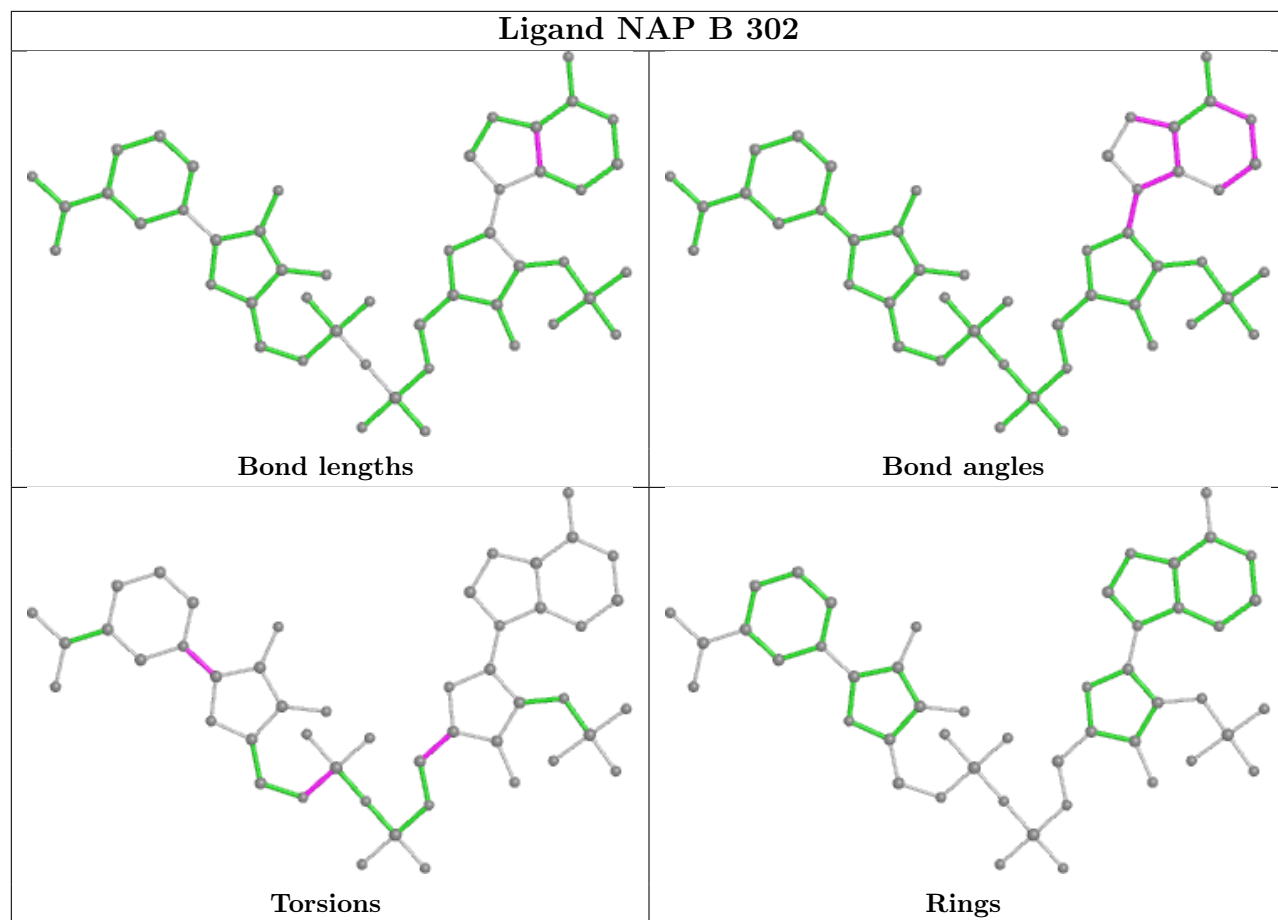
Mol	Chain	Res	Type	Atoms
4	B	301	GOL	O1-C1-C2-O2
4	B	301	GOL	O1-C1-C2-C3
4	D	303[A]	GOL	C1-C2-C3-O3
4	D	303[B]	GOL	O2-C2-C3-O3
5	A	304	NAP	C2B-O2B-P2B-O3X
5	A	304	NAP	C5D-O5D-PN-O2N
5	A	304	NAP	O4D-C1D-N1N-C2N
5	B	302	NAP	C5D-O5D-PN-O2N
5	B	302	NAP	O4D-C1D-N1N-C2N
5	C	305	NAP	C2B-O2B-P2B-O3X
5	C	305	NAP	C5D-O5D-PN-O2N
5	C	305	NAP	O4D-C1D-N1N-C2N
5	D	304	NAP	C5D-O5D-PN-O2N
5	D	304	NAP	O4D-C1D-N1N-C2N
7	D	305	J69	C02-C04-O05-C06
7	D	305	J69	O07-C04-O05-C06
4	B	301	GOL	O2-C2-C3-O3
4	A	303	GOL	C1-C2-C3-O3
4	B	301	GOL	C1-C2-C3-O3
4	D	303[B]	GOL	C1-C2-C3-O3
4	A	303	GOL	O2-C2-C3-O3
4	D	303[A]	GOL	O2-C2-C3-O3
4	D	303[B]	GOL	O1-C1-C2-C3
5	A	304	NAP	C5D-O5D-PN-O3
5	B	302	NAP	C5D-O5D-PN-O3
5	C	305	NAP	C5D-O5D-PN-O3
5	D	304	NAP	C5D-O5D-PN-O3
5	B	302	NAP	C5D-O5D-PN-O1N
5	C	305	NAP	C5D-O5D-PN-O1N
5	D	304	NAP	C5D-O5D-PN-O1N
3	A	302	BTB	O1-C1-C2-C3
3	A	302	BTB	O1-C1-C2-C4
3	A	302	BTB	O1-C1-C2-N
3	A	302	BTB	C1-C2-N-C7
3	A	302	BTB	C3-C2-N-C7
4	A	303	GOL	O1-C1-C2-O2
5	A	304	NAP	O4B-C4B-C5B-O5B
5	B	302	NAP	O4B-C4B-C5B-O5B
5	C	305	NAP	O4B-C4B-C5B-O5B
4	A	303	GOL	O1-C1-C2-C3
5	A	304	NAP	C5D-O5D-PN-O1N
5	D	304	NAP	O4B-C4B-C5B-O5B

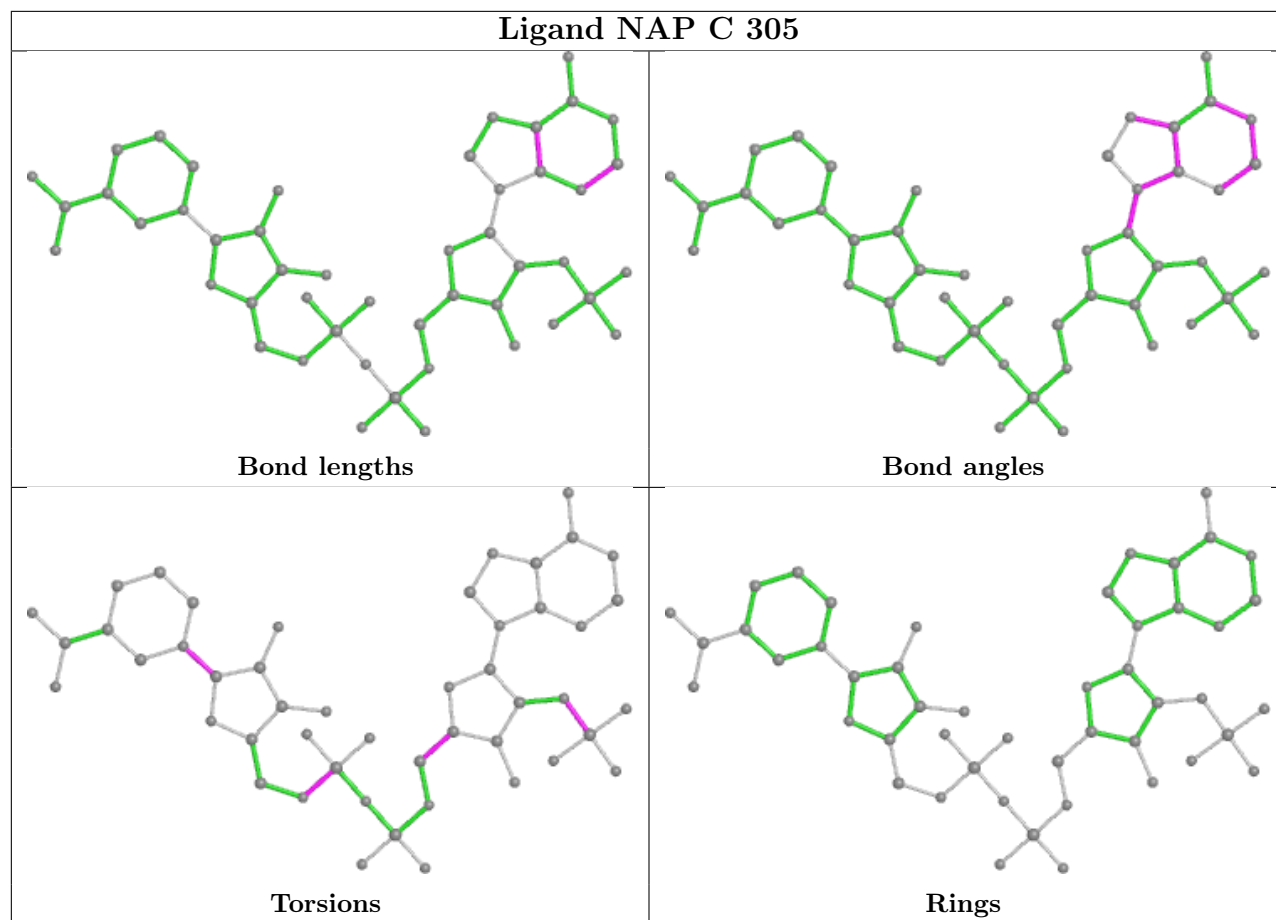
There are no ring outliers.

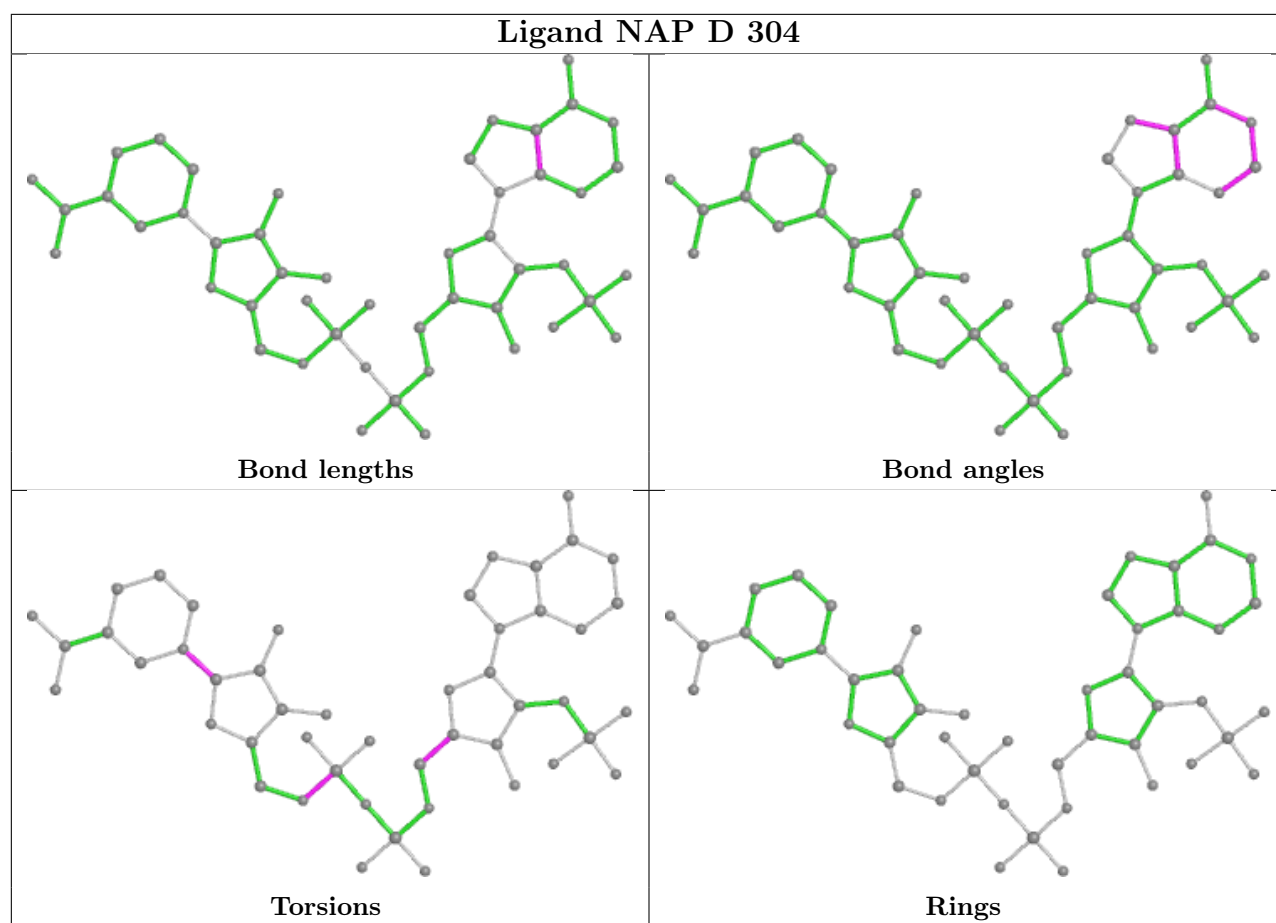
12 monomers are involved in 17 short contacts:

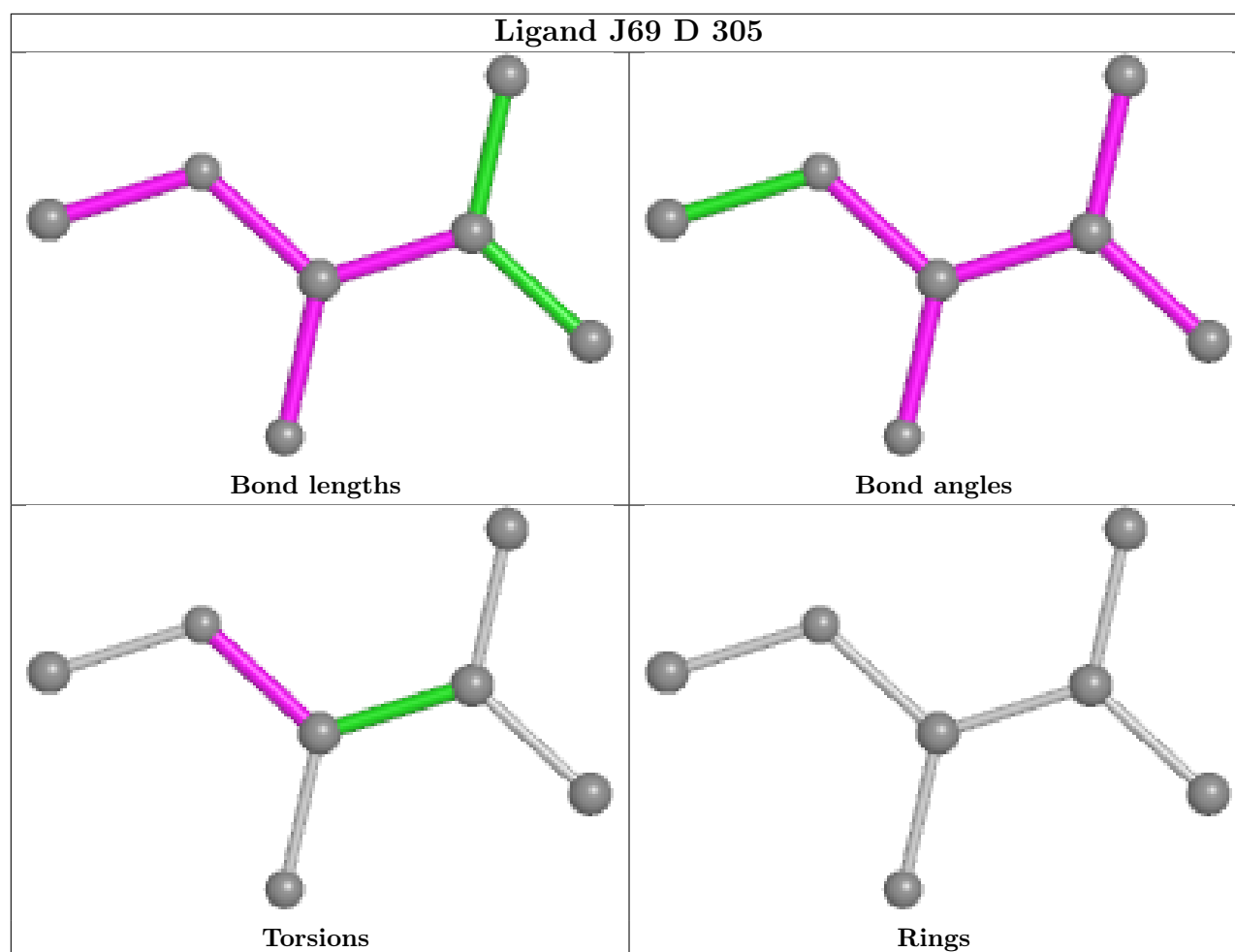
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	302	NAP	1	0
5	D	304	NAP	1	0
3	C	302	BTB	1	0
7	D	305	J69	3	0
8	D	301	EDO	1	0
8	C	303	EDO	2	0
7	B	303	J69	2	0
4	A	303	GOL	1	0
3	A	302	BTB	4	0
5	A	304	NAP	1	0
6	A	305	J66	1	0
6	C	306	J66	1	0

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.

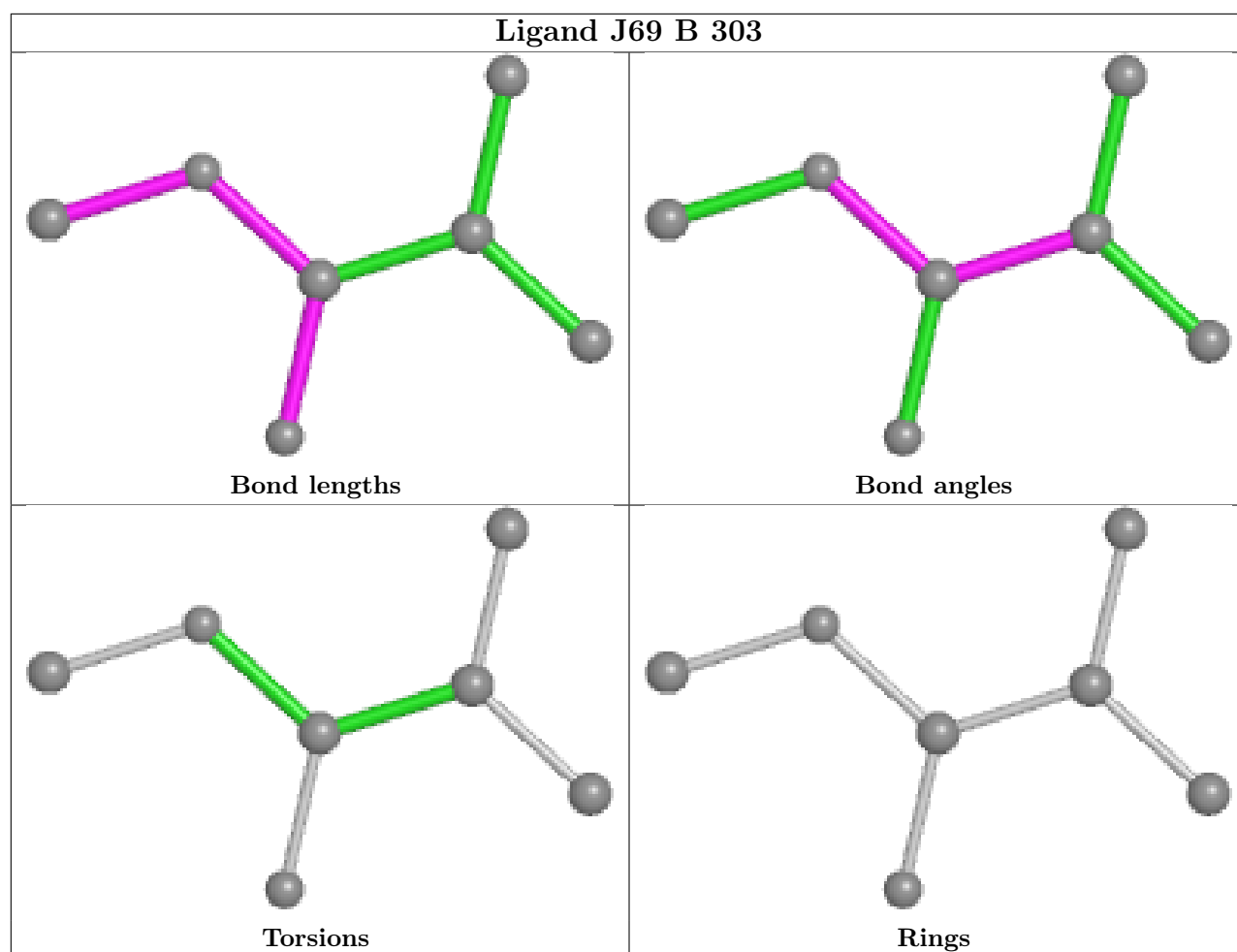


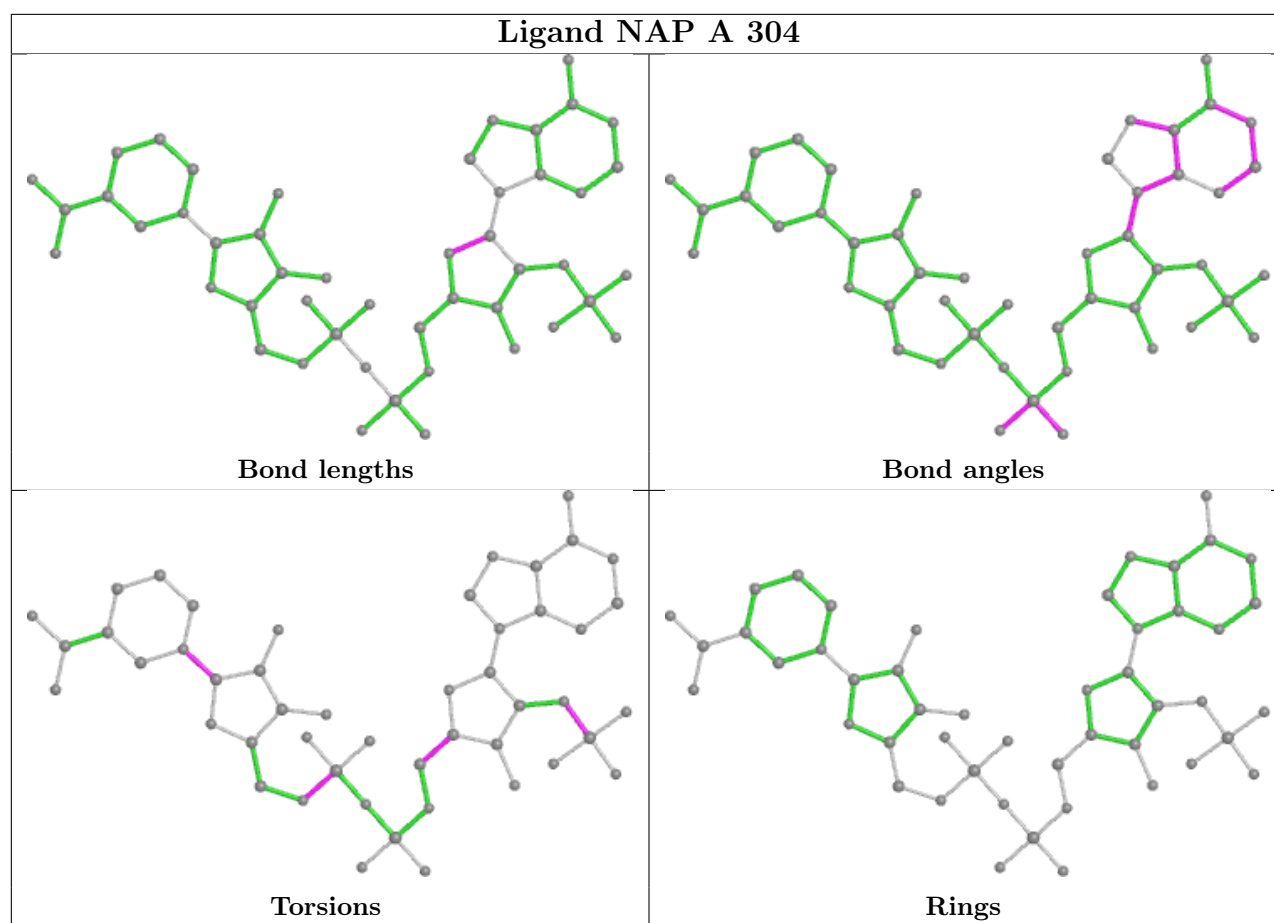












## 5.7 Other polymers [i](#)

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	253/253 (100%)	-0.23	0 100 100	15, 21, 35, 50	0
1	B	251/253 (99%)	-0.02	10 (3%) 38 44	16, 25, 43, 62	0
1	C	251/253 (99%)	-0.01	3 (1%) 79 83	16, 26, 44, 55	0
1	D	252/253 (99%)	0.23	17 (6%) 17 21	17, 31, 55, 71	0
All	All	1007/1012 (99%)	-0.01	30 (2%) 50 58	15, 25, 47, 71	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	199	ALA	5.8
1	D	195	LEU	5.4
1	D	202	ALA	5.1
1	D	196	VAL	4.8
1	D	43	VAL	4.7
1	B	199	ALA	4.6
1	D	200	GLU	3.8
1	B	196	VAL	3.7
1	B	200	GLU	3.6
1	D	194	PRO	3.4
1	C	79	GLU	3.1
1	B	195	LEU	3.0
1	D	198	ASP	3.0
1	C	206	PHE	3.0
1	D	42	ASP	2.9
1	C	2	THR	2.8
1	B	42	ASP	2.8
1	D	206	PHE	2.8
1	D	45	GLU	2.7
1	B	49	LYS	2.6
1	D	201	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.4
1	D	47	ALA	2.4
1	D	48	ALA	2.3
1	B	46	LYS	2.2
1	D	49	LYS	2.2
1	B	45	GLU	2.2
1	B	198	ASP	2.2
1	B	206	PHE	2.1
1	D	41	ALA	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EDO	D	301	4/4	0.63	0.21	47,48,49,53	0
3	BTB	A	302	14/14	0.72	0.16	26,33,39,42	14
8	EDO	C	303	4/4	0.76	0.26	36,38,38,39	0
4	GOL	B	301	6/6	0.80	0.22	40,42,51,60	0
7	J69	B	303	7/7	0.80	0.13	23,30,38,39	7
4	GOL	A	303	6/6	0.81	0.14	34,40,42,46	0
4	GOL	D	303[A]	6/6	0.81	0.16	34,40,42,43	6
4	GOL	D	303[B]	6/6	0.81	0.16	36,41,42,43	6
7	J69	D	305	7/7	0.84	0.15	26,39,43,46	7
3	BTB	C	302	14/14	0.85	0.12	28,34,40,40	0
6	J66	C	306	12/12	0.89	0.21	24,32,35,37	12
8	EDO	D	302	4/4	0.89	0.17	23,30,31,45	0
9	PEG	C	304	7/7	0.89	0.23	39,40,49,50	0
6	J66	A	305	12/12	0.90	0.17	24,28,33,34	12

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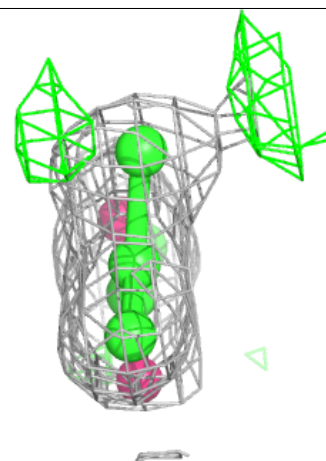
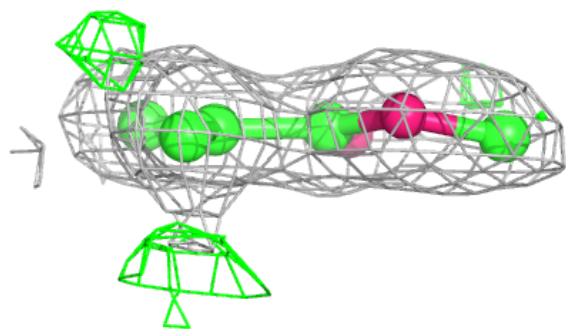
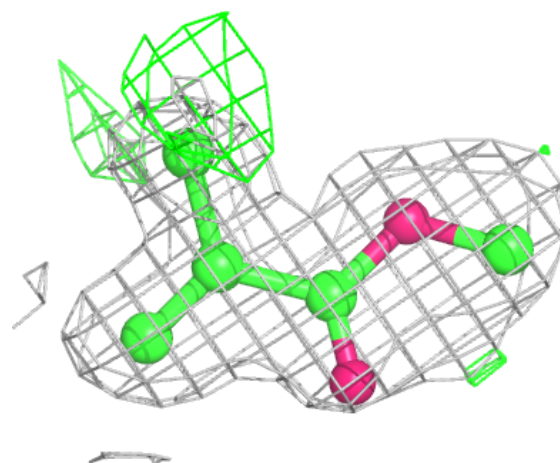
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAP	D	304	48/48	0.92	0.10	26,33,40,49	48
5	NAP	C	305	48/48	0.96	0.07	19,24,30,39	0
5	NAP	B	302	48/48	0.96	0.07	19,24,28,32	48
5	NAP	A	304	48/48	0.97	0.07	15,19,24,28	0
2	MG	A	301	1/1	0.99	0.05	18,18,18,18	0
2	MG	C	301	1/1	0.99	0.05	14,14,14,14	1

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.

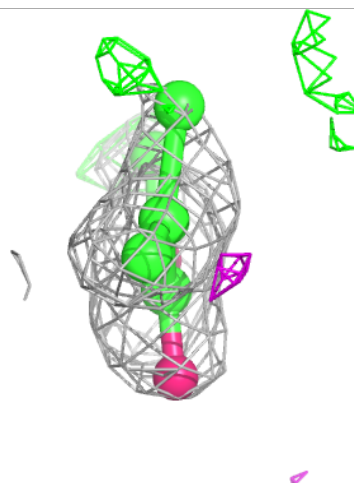
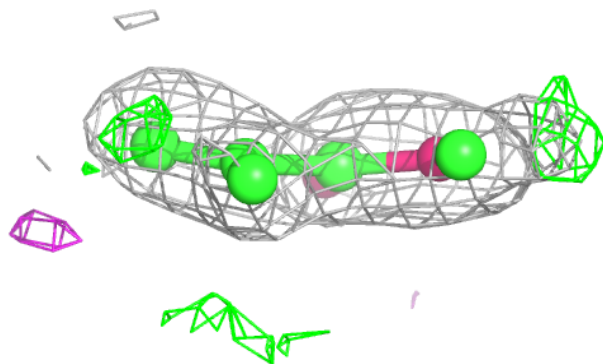
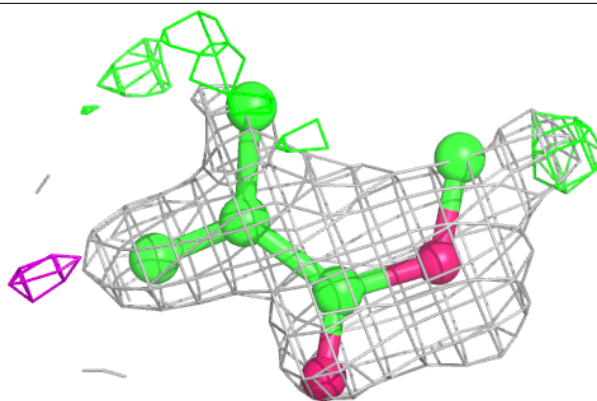
**Electron density around J69 B 303:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



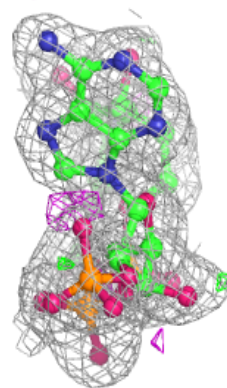
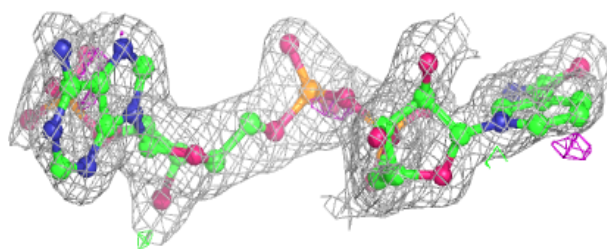
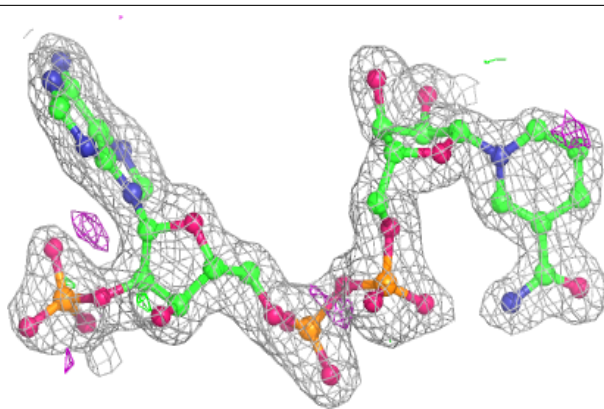
**Electron density around J69 D 305:**

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

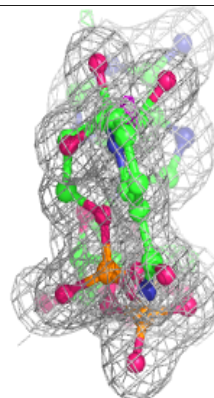
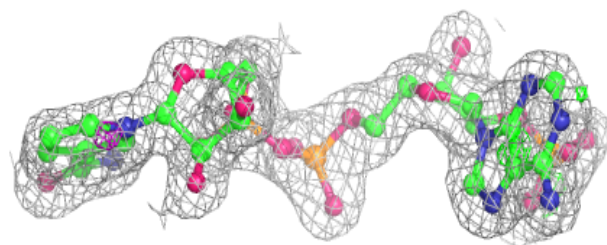
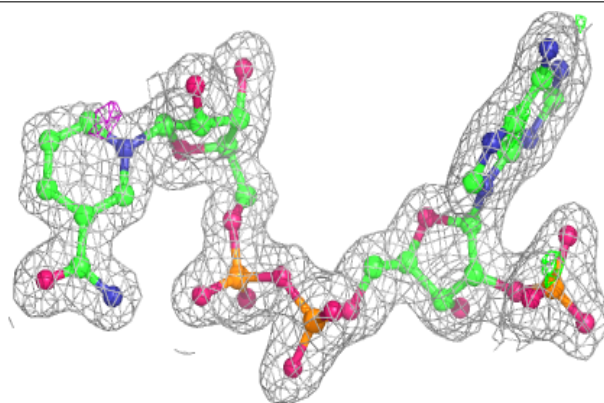


**Electron density around NAP D 304:**

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

**Electron density around NAP C 305:**

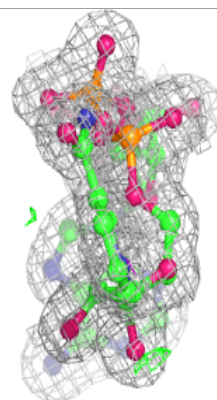
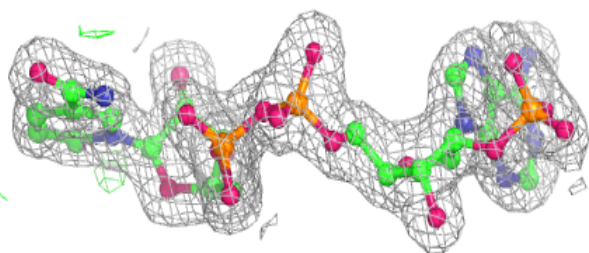
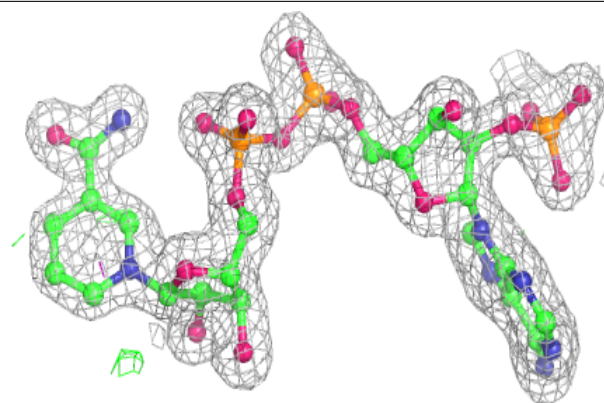
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



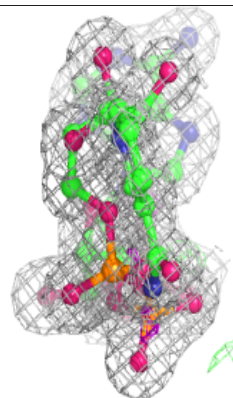
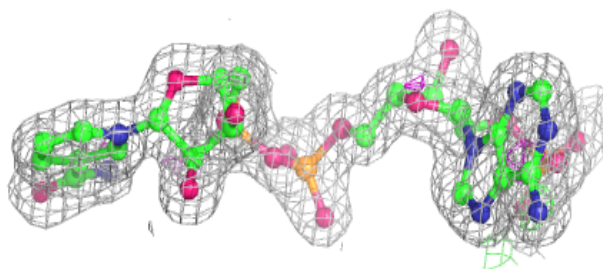
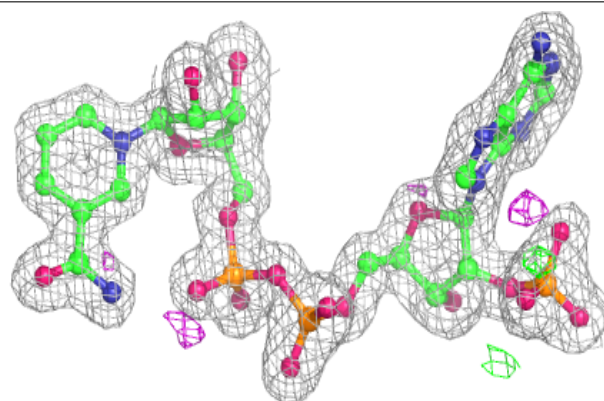


**Electron density around NAP B 302:**

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

**Electron density around NAP A 304:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.