



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2022 – 06:46 am GMT

PDB ID : 7OK7  
Title : Crystal structure of the UNC119B ARL3 complex  
Authors : Yelland, T.; Ismail, S.  
Deposited on : 2021-05-17  
Resolution : 3.15 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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

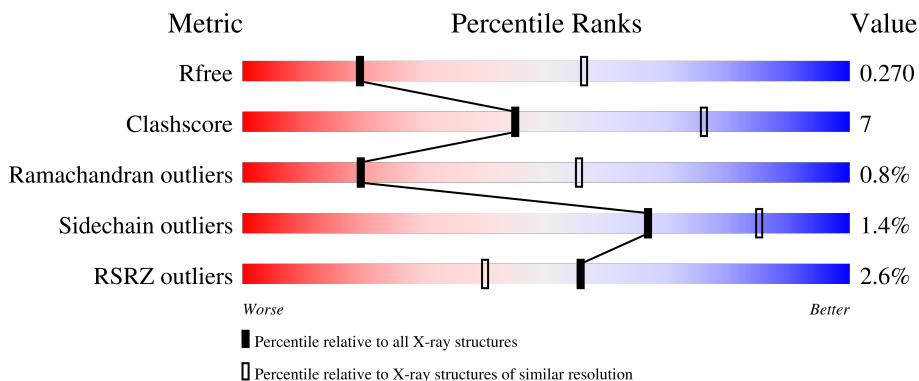
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	183	
1	B	183	
1	C	183	
1	D	183	
1	E	183	

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Mol	Chain	Length	Quality of chain
1	F	183	<p>9% 84% 11% . .</p>
2	G	183	<p>% 82% 13% . .</p>
2	H	183	<p>74% 19% . 6%</p>
2	I	183	<p>3% 79% 14% 7%</p>
2	J	183	<p>2% 70% 23% . 5%</p>
2	K	183	<p>11% 67% 21% . 10%</p>
2	L	183	<p>5% 70% 18% 11%</p>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17127 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 ADP-ribosylation factor-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	174	1374	867	239	264	4	0	0	0
1	B	177	1377	868	238	267	4	0	0	0
1	C	183	1453	920	252	277	4	0	1	0
1	D	177	1385	874	239	268	4	0	0	0
1	E	174	1367	862	236	265	4	0	0	0
1	F	180	1386	878	235	269	4	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	-	expression tag	UNP Q9WUL7
A	184	HIS	-	expression tag	UNP Q9WUL7
A	185	HIS	-	expression tag	UNP Q9WUL7
B	183	GLU	-	expression tag	UNP Q9WUL7
B	184	HIS	-	expression tag	UNP Q9WUL7
B	185	HIS	-	expression tag	UNP Q9WUL7
C	183	GLU	-	expression tag	UNP Q9WUL7
C	184	HIS	-	expression tag	UNP Q9WUL7
C	185	HIS	-	expression tag	UNP Q9WUL7
D	183	GLU	-	expression tag	UNP Q9WUL7
D	184	HIS	-	expression tag	UNP Q9WUL7
D	185	HIS	-	expression tag	UNP Q9WUL7
E	183	GLU	-	expression tag	UNP Q9WUL7
E	184	HIS	-	expression tag	UNP Q9WUL7
E	185	HIS	-	expression tag	UNP Q9WUL7
F	183	GLU	-	expression tag	UNP Q9WUL7
F	184	HIS	-	expression tag	UNP Q9WUL7

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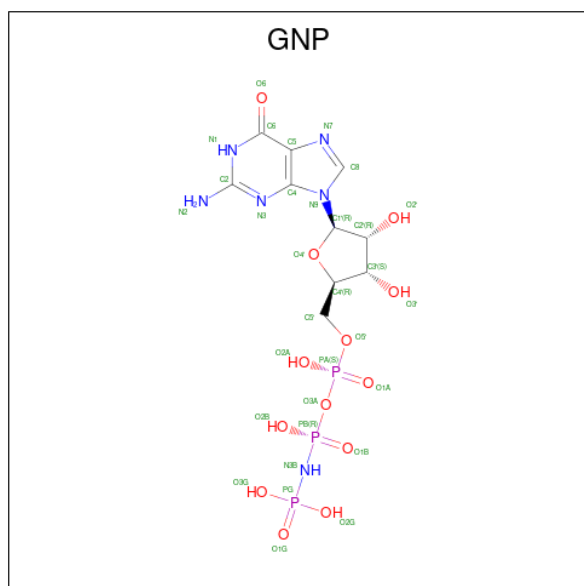
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Chain	Residue	Modelled	Actual	Comment	Reference
F	185	HIS	-	expression tag	UNP Q9WUL7

- Molecule 2 is a protein called Protein unc-119 homolog B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	175	Total	C	N	O	S	0	0	0
			1466	935	249	275	7			
2	H	172	Total	C	N	O	S	0	0	0
			1440	921	246	266	7			
2	I	171	Total	C	N	O	S	0	0	0
			1410	904	239	260	7			
2	J	174	Total	C	N	O	S	0	0	0
			1450	926	247	270	7			
2	K	165	Total	C	N	O	S	0	0	0
			1367	883	228	249	7			
2	L	162	Total	C	N	O	S	0	0	0
			1371	883	235	247	6			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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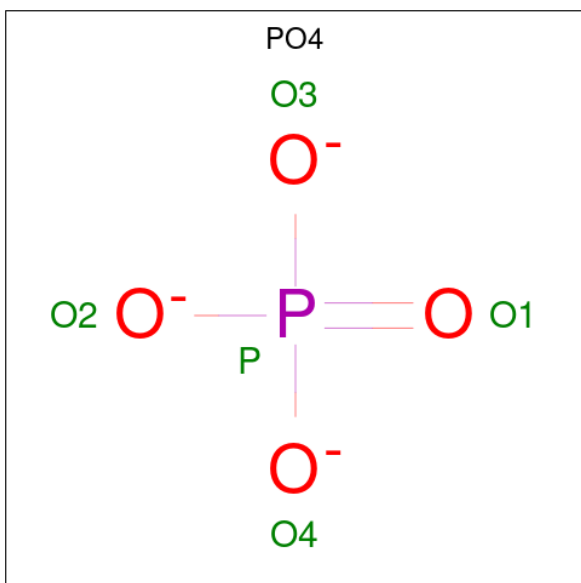
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

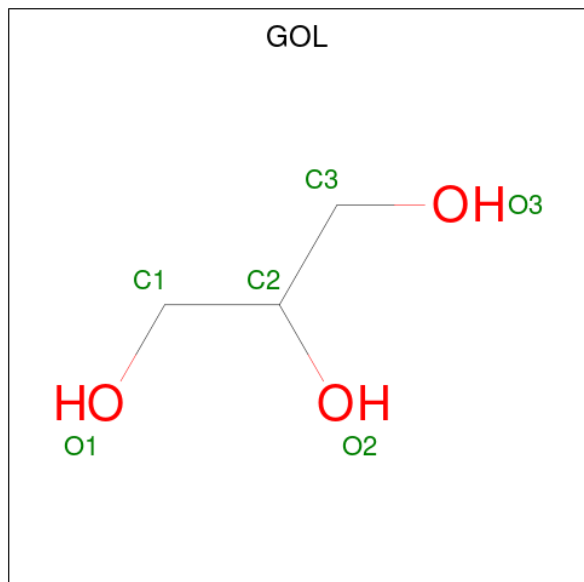
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O P 5 4 1	0	0
5	G	1	Total O P 5 4 1	0	0
5	I	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	K	1	Total O P 5 4 1	0	0
5	L	1	Total O P 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 6 3 3	0	0
6	H	1	Total C O 6 3 3	0	0
6	I	1	Total C O 6 3 3	0	0
6	J	1	Total C O 6 3 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0

- Molecule 8 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	5	Total O 5 5	0	0
8	C	2	Total O 2 2	0	0
8	E	1	Total O 1 1	0	0
8	G	2	Total O 2 2	0	0
8	H	2	Total O 2 2	0	0
8	I	1	Total O 1 1	0	0
8	J	1	Total O 1 1	0	0
8	K	5	Total O 5 5	0	0
8	L	2	Total O 2 2	0	0



### 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 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: ADP-ribosylation factor-like protein 3

Chain A: 




- Molecule 1: ADP-ribosylation factor-like protein 3

Chain B: 




- Molecule 1: ADP-ribosylation factor-like protein 3

Chain C: 




- Molecule 1: ADP-ribosylation factor-like protein 3

Chain D: 

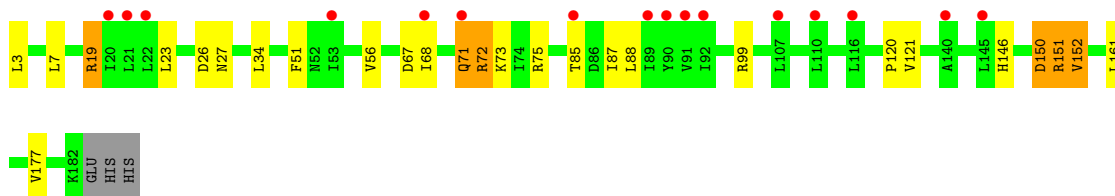
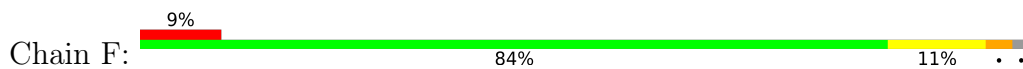


- Molecule 1: ADP-ribosylation factor-like protein 3

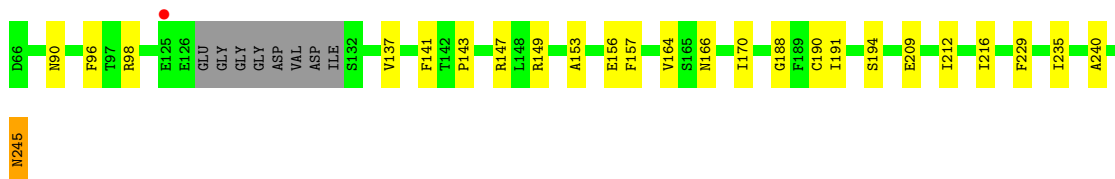
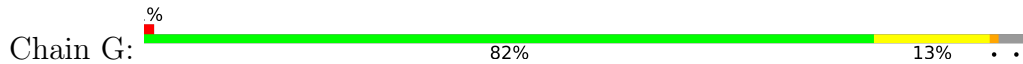
Chain E: 



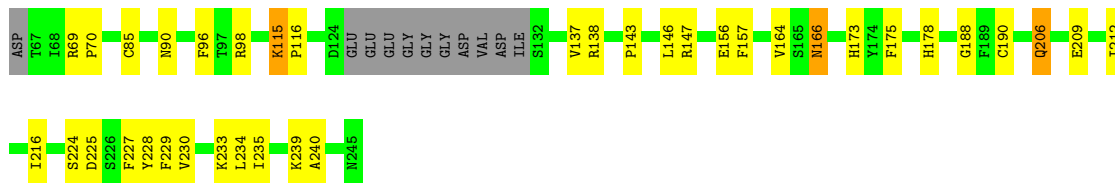
- Molecule 1: ADP-ribosylation factor-like protein 3



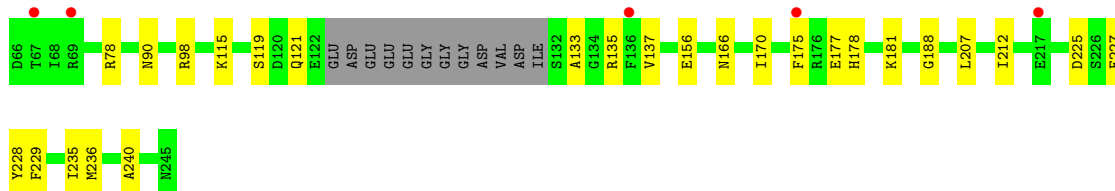
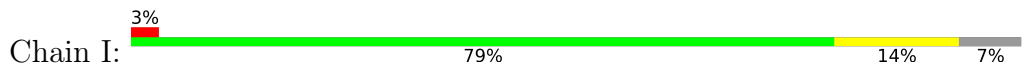
- Molecule 2: Protein unc-119 homolog B



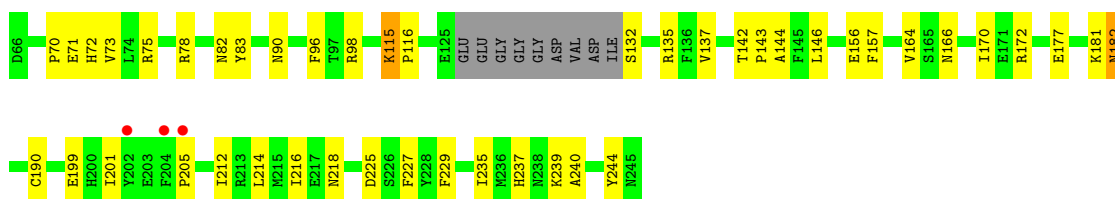
- Molecule 2: Protein unc-119 homolog B



- Molecule 2: Protein unc-119 homolog B

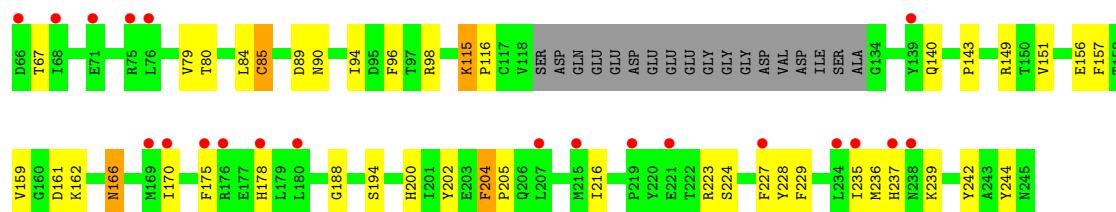


- Molecule 2: Protein unc-119 homolog B



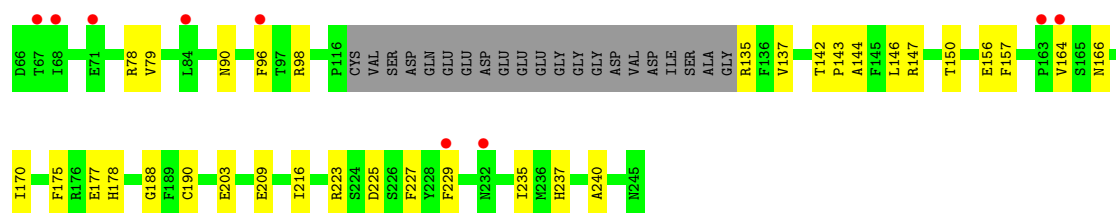
- Molecule 2: Protein unc-119 homolog B

Chain K: 11% 67% 21% 10%



- Molecule 2: Protein unc-119 homolog B

Chain L: 5% 70% 18% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.27Å 152.19Å 171.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.82 – 3.15 74.82 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (74.82-3.15) 99.9 (74.82-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.13Å)	Xtrriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, $R_{free}$	0.221 , 0.270 0.221 , 0.270	Depositor DCC
$R_{free}$ test set	2574 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.7	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: GNP, EDO, MG, PO4, GOL

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	0.25	0/1396	0.47	0/1890
1	B	0.25	0/1399	0.46	0/1898
1	C	0.25	0/1477	0.48	0/1999
1	D	0.25	0/1407	0.47	0/1907
1	E	0.24	0/1389	0.44	0/1882
1	F	0.24	0/1408	0.47	0/1913
2	G	0.26	0/1502	0.47	0/2029
2	H	0.27	0/1476	0.52	0/1994
2	I	0.26	0/1446	0.48	0/1958
2	J	0.27	0/1486	0.51	0/2009
2	K	0.26	0/1403	0.50	0/1899
2	L	0.26	0/1407	0.47	0/1901
All	All	0.25	0/17196	0.48	0/23279

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 [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	1374	0	1374	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1377	0	1354	13	0
1	C	1453	0	1451	18	0
1	D	1385	0	1377	16	0
1	E	1367	0	1359	12	0
1	F	1386	0	1364	20	0
2	G	1466	0	1399	13	0
2	H	1440	0	1383	27	0
2	I	1410	0	1336	17	0
2	J	1450	0	1380	28	0
2	K	1367	0	1307	25	0
2	L	1371	0	1327	18	0
3	A	32	0	13	3	0
3	B	32	0	13	2	0
3	C	32	0	13	1	0
3	D	32	0	13	3	0
3	E	32	0	13	1	0
3	F	32	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	C	5	0	0	0	0
5	G	5	0	0	0	0
5	I	5	0	0	0	0
5	J	5	0	0	0	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
6	G	6	0	8	1	0
6	H	6	0	8	0	0
6	I	6	0	8	1	0
6	J	6	0	8	1	0
7	G	4	0	6	0	0
7	H	4	0	6	0	0
8	A	5	0	0	0	0
8	C	2	0	0	0	0
8	E	1	0	0	0	0
8	G	2	0	0	0	0
8	H	2	0	0	0	0
8	I	1	0	0	0	0
8	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	K	5	0	0	0	0
8	L	2	0	0	0	0
All	All	17127	0	16533	219	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 7.

All (219) 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)
2:I:98:ARG:HB3	2:I:156:GLU:HB3	1.55	0.87
1:F:27:ASN:H	3:F:201:GNP:HNB3	1.27	0.82
2:K:79:VAL:HG11	2:K:223:ARG:HD2	1.63	0.81
2:K:204:PHE:HD1	2:K:205:PRO:HD2	1.48	0.78
2:H:98:ARG:HB3	2:H:156:GLU:HB3	1.64	0.78
2:L:98:ARG:HB3	2:L:156:GLU:HB3	1.66	0.77
2:G:98:ARG:HB3	2:G:156:GLU:HB3	1.67	0.74
1:C:27:ASN:H	3:C:201:GNP:HNB3	1.35	0.74
2:J:98:ARG:HB3	2:J:156:GLU:HB3	1.70	0.73
2:L:79:VAL:HG11	2:L:223:ARG:HD2	1.70	0.73
2:K:98:ARG:HB3	2:K:156:GLU:HB3	1.70	0.71
1:A:27:ASN:H	3:A:201:GNP:HNB3	1.38	0.70
2:L:142:THR:HG22	2:L:144:ALA:H	1.57	0.70
1:C:87:ILE:HD11	1:C:177:VAL:HA	1.74	0.70
2:K:80:THR:HG21	2:K:84:LEU:HD11	1.75	0.69
2:J:70:PRO:HA	2:J:73:VAL:HG12	1.74	0.68
2:I:207:LEU:HD13	2:I:212:ILE:CG1	2.26	0.66
2:I:133:ALA:HB1	2:I:135:ARG:HE	1.61	0.66
1:D:87:ILE:HD11	1:D:177:VAL:HA	1.77	0.66
2:H:230:VAL:N	2:H:235:ILE:HD11	2.11	0.65
1:F:120:PRO:HA	1:F:151:ARG:O	1.97	0.64
2:G:147:ARG:NH2	2:G:209:GLU:OE2	2.31	0.64
1:B:7:LEU:O	1:B:9:LYS:N	2.32	0.63
2:L:164:VAL:HB	2:L:190:CYS:HB2	1.80	0.63
1:A:57:GLN:HG2	1:A:62:LYS:HG2	1.80	0.62
2:L:147:ARG:NH1	2:L:209:GLU:OE2	2.33	0.62
1:F:23:LEU:HD21	1:F:68:ILE:HD11	1.82	0.61
2:K:115:LYS:HB3	2:K:116:PRO:CD	2.29	0.61
2:J:83:TYR:HE2	2:J:132:SER:HB3	1.65	0.61
1:B:37:LEU:HD11	1:B:170:MET:HE3	1.82	0.61
1:C:57:GLN:HE21	1:C:62:LYS:HE3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:GLN:HG2	1:D:62:LYS:HG2	1.81	0.61
1:C:37:LEU:HB3	1:F:3:LEU:HG	1.81	0.61
1:B:141:GLU:HG2	1:C:181:LYS:HD3	1.82	0.61
1:C:56:VAL:HG12	1:F:7:LEU:HD22	1.83	0.60
2:L:143:PRO:HB3	2:L:216:ILE:HD12	1.82	0.60
2:J:78:ARG:HB3	2:J:177:GLU:HG2	1.83	0.60
2:H:90:ASN:HA	2:H:235:ILE:HG22	1.83	0.60
2:H:143:PRO:HB3	2:H:216:ILE:HD12	1.84	0.59
1:C:83:GLU:HG3	1:C:115:LYS:HD3	1.84	0.59
2:H:115:LYS:CB	2:H:116:PRO:HD3	2.32	0.59
1:C:57:GLN:HG2	1:C:62:LYS:HG2	1.84	0.59
1:F:71:GLN:O	1:F:73:LYS:N	2.32	0.59
2:L:175:PHE:O	2:L:178:HIS:HB2	2.03	0.59
2:I:166:ASN:HA	2:I:188:GLY:HA2	1.85	0.58
2:H:147:ARG:NH2	2:H:209:GLU:OE2	2.36	0.58
1:E:19:ARG:NH2	1:E:83:GLU:O	2.37	0.57
2:H:90:ASN:HA	2:H:235:ILE:CG2	2.35	0.57
2:G:164:VAL:HB	2:G:190:CYS:HB2	1.86	0.57
1:D:27:ASN:H	3:D:201:GNP:HNB3	1.53	0.57
2:H:166:ASN:HA	2:H:188:GLY:HA2	1.86	0.56
2:G:143:PRO:HB3	2:G:216:ILE:HD12	1.87	0.56
1:A:35:LYS:HD2	1:A:45:ILE:HD11	1.87	0.56
1:D:140:ALA:HA	1:D:145:LEU:HD12	1.88	0.56
2:J:71:GLU:OE1	2:J:75:ARG:NH1	2.38	0.56
3:E:201:GNP:H8	3:E:201:GNP:H5'2	1.88	0.55
2:G:166:ASN:HA	2:G:188:GLY:HA2	1.88	0.55
2:I:119:SER:HB3	2:I:121:GLN:HG2	1.87	0.55
2:H:69:ARG:HH12	2:H:233:LYS:HG3	1.70	0.55
1:E:9:LYS:C	1:E:11:LYS:H	2.09	0.55
2:J:142:THR:HG23	2:J:144:ALA:H	1.71	0.55
1:C:7:LEU:HD22	1:F:56:VAL:HG12	1.88	0.54
1:B:102:GLU:O	1:B:105:GLN:HG3	2.08	0.54
2:K:166:ASN:HA	2:K:188:GLY:HA2	1.87	0.54
2:H:69:ARG:NH1	2:H:233:LYS:HG3	2.22	0.54
1:E:40:GLU:OE2	1:E:54:LYS:NZ	2.36	0.54
2:I:90:ASN:HA	2:I:235:ILE:HG23	1.89	0.54
2:J:143:PRO:HB3	2:J:216:ILE:HD12	1.90	0.53
2:L:170:ILE:HD12	2:L:229:PHE:CE1	2.44	0.53
3:F:201:GNP:H5'2	3:F:201:GNP:H8	1.90	0.53
2:K:85:CYS:SG	2:K:89:ASP:HB2	2.48	0.53
2:L:98:ARG:NH1	2:L:156:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TRP:HA	1:C:175:LYS:HE3	1.91	0.53
2:J:172:ARG:NH1	2:J:182:ASN:OD1	2.41	0.53
2:K:200:HIS:CD2	2:K:202:TYR:HD1	2.26	0.53
2:J:137:VAL:O	2:J:240:ALA:HA	2.08	0.53
2:K:90:ASN:HA	2:K:235:ILE:HG23	1.90	0.53
1:E:87:ILE:HG12	1:E:173:VAL:HG13	1.90	0.53
1:F:72:ARG:HA	1:F:75:ARG:HG3	1.91	0.53
2:H:164:VAL:HB	2:H:190:CYS:HB2	1.89	0.53
2:L:166:ASN:HA	2:L:188:GLY:HA2	1.90	0.52
1:E:9:LYS:O	1:E:11:LYS:N	2.42	0.52
2:K:143:PRO:HB3	2:K:216:ILE:HD12	1.90	0.52
2:I:207:LEU:HD12	2:I:207:LEU:O	2.09	0.52
1:B:72:ARG:HE	1:D:138:GLU:HG3	1.75	0.52
1:F:146:HIS:O	1:F:146:HIS:ND1	2.37	0.52
2:J:225:ASP:HB3	2:J:227:PHE:CE2	2.45	0.52
1:A:27:ASN:HA	3:A:201:GNP:H5'1	1.92	0.51
2:K:149:ARG:H	2:K:204:PHE:HD2	1.57	0.51
2:L:90:ASN:HA	2:L:235:ILE:HG23	1.93	0.51
1:E:83:GLU:HG3	1:E:115:LYS:HD3	1.91	0.51
2:I:175:PHE:O	2:I:178:HIS:HB2	2.10	0.51
1:A:87:ILE:HG12	1:A:173:VAL:HG13	1.93	0.50
2:J:83:TYR:CE2	2:J:132:SER:HB3	2.46	0.50
2:L:225:ASP:HB3	2:L:227:PHE:CE2	2.46	0.50
2:K:170:ILE:HD12	2:K:229:PHE:CE1	2.47	0.49
1:C:26:ASP:CG	1:C:99:ARG:HH22	2.15	0.49
1:F:51:PHE:HB3	1:F:68:ILE:HG22	1.93	0.49
1:E:26:ASP:CG	1:E:99:ARG:HH22	2.16	0.49
1:E:120:PRO:HB3	1:E:152:VAL:HG23	1.95	0.49
1:D:102:GLU:O	1:D:105:GLN:HG3	2.12	0.49
1:F:88:LEU:O	1:F:121:VAL:HA	2.12	0.49
2:H:146:LEU:C	2:H:147:ARG:HD2	2.33	0.49
2:L:150:THR:HG22	2:L:203:GLU:HG2	1.95	0.48
2:K:237:HIS:CE1	2:K:239:LYS:HE2	2.49	0.48
2:J:72:HIS:O	2:J:72:HIS:ND1	2.46	0.48
1:B:30:LYS:N	3:B:201:GNP:O2B	2.42	0.48
1:D:111:LEU:HD22	1:D:151:ARG:NE	2.29	0.48
2:H:212:ILE:O	2:H:216:ILE:HG12	2.14	0.48
2:L:96:PHE:CD1	2:L:157:PHE:HB3	2.49	0.48
1:E:57:GLN:HG2	1:E:62:LYS:HG2	1.95	0.48
2:H:96:PHE:CD1	2:H:157:PHE:HB3	2.49	0.48
2:K:115:LYS:HD2	2:K:116:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HB2	1:A:145:LEU:HG	1.97	0.47
2:G:170:ILE:HD12	2:G:229:PHE:CE1	2.49	0.47
2:H:227:PHE:HD1	2:H:234:LEU:HD11	1.79	0.47
1:A:13:ALA:N	1:A:14:PRO:HD3	2.30	0.47
2:K:175:PHE:O	2:K:178:HIS:HB2	2.14	0.47
1:B:79:ARG:NH1	1:B:113:GLU:OE1	2.48	0.47
2:J:115:LYS:CB	2:J:116:PRO:HD3	2.44	0.47
2:K:224:SER:HB3	2:K:242:TYR:HE1	1.80	0.47
2:J:72:HIS:O	2:J:72:HIS:CG	2.67	0.47
1:E:88:LEU:O	1:E:121:VAL:HA	2.14	0.47
2:H:239:LYS:HB3	2:H:239:LYS:HE2	1.58	0.47
2:J:214:LEU:O	2:J:218:ASN:ND2	2.47	0.47
2:H:225:ASP:HB3	2:H:227:PHE:CE2	2.50	0.47
2:J:96:PHE:CD1	2:J:157:PHE:HB3	2.50	0.47
2:K:151:VAL:HB	2:K:202:TYR:CE2	2.50	0.47
2:H:115:LYS:HB2	2:H:116:PRO:HD3	1.95	0.47
1:B:140:ALA:HA	1:B:145:LEU:HD12	1.97	0.46
2:I:170:ILE:HD12	2:I:229:PHE:CE1	2.50	0.46
2:J:90:ASN:HA	2:J:235:ILE:HG13	1.98	0.46
2:H:115:LYS:HB3	2:H:116:PRO:HD3	1.98	0.46
2:I:137:VAL:O	2:I:240:ALA:HA	2.15	0.46
2:J:181:LYS:HE2	2:J:205:PRO:HD3	1.98	0.46
1:A:26:ASP:CG	1:A:99:ARG:HH22	2.19	0.45
1:C:88:LEU:O	1:C:121:VAL:HA	2.16	0.45
2:G:212:ILE:O	2:G:216:ILE:HG12	2.16	0.45
2:K:162:LYS:H	2:K:162:LYS:HD2	1.82	0.45
2:H:137:VAL:O	2:H:240:ALA:HA	2.16	0.45
1:B:26:ASP:CG	1:B:99:ARG:HH22	2.20	0.45
2:G:90:ASN:HA	2:G:235:ILE:HG23	1.99	0.44
2:I:133:ALA:HB1	2:I:135:ARG:NE	2.29	0.44
2:J:164:VAL:HB	2:J:190:CYS:HB2	1.98	0.44
1:F:27:ASN:N	3:F:201:GNP:HNB3	2.06	0.44
2:K:149:ARG:N	2:K:149:ARG:HD2	2.32	0.44
2:K:159:VAL:HG12	2:K:194:SER:H	1.82	0.44
1:C:87:ILE:HG12	1:C:173:VAL:HG13	1.99	0.44
2:H:173:HIS:CD2	2:H:224:SER:HB3	2.52	0.44
1:D:27:ASN:N	3:D:201:GNP:HNB3	2.15	0.44
1:E:119:VAL:O	1:E:151:ARG:HD3	2.17	0.44
2:J:170:ILE:HD12	2:J:229:PHE:CE1	2.53	0.44
2:J:212:ILE:O	2:J:216:ILE:HG12	2.17	0.44
2:K:94:ILE:HB	2:K:236:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:ARG:HD2	2:L:237:HIS:O	2.18	0.44
1:D:30:LYS:N	3:D:201:GNP:O2B	2.42	0.44
2:H:175:PHE:O	2:H:178:HIS:HB2	2.17	0.44
2:J:244:TYR:OH	6:J:301:GOL:H2	2.17	0.44
1:D:174:CYS:HA	1:D:177:VAL:HG13	2.00	0.43
2:G:141:PHE:O	2:G:245:ASN:N	2.51	0.43
2:H:70:PRO:HA	2:H:229:PHE:CZ	2.52	0.43
2:K:228:TYR:HD2	2:K:236:MET:HB3	1.82	0.43
2:L:146:LEU:HD12	2:L:216:ILE:HD11	2.00	0.43
1:A:7:LEU:O	1:A:7:LEU:HD23	2.18	0.43
2:G:137:VAL:O	2:G:240:ALA:HA	2.18	0.43
1:C:181:LYS:HE3	1:C:181:LYS:HB3	1.83	0.43
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.82	0.43
1:B:27:ASN:H	3:B:201:GNP:HNB3	1.65	0.43
1:C:119:VAL:O	1:C:151:ARG:HD3	2.19	0.43
1:F:23:LEU:HD12	1:F:88:LEU:HD11	2.01	0.43
2:K:96:PHE:CD1	2:K:157:PHE:HB3	2.54	0.43
1:B:72:ARG:NE	1:D:138:GLU:HG3	2.34	0.43
1:F:26:ASP:OD2	1:F:99:ARG:NH2	2.51	0.43
2:J:146:LEU:HD23	2:J:146:LEU:HA	1.92	0.43
1:D:88:LEU:O	1:D:121:VAL:HA	2.19	0.43
2:J:237:HIS:CE1	2:J:239:LYS:HE2	2.54	0.42
2:K:84:LEU:HD12	2:K:227:PHE:HE1	1.84	0.42
2:K:216:ILE:HD13	2:K:244:TYR:HB2	1.99	0.42
1:A:88:LEU:O	1:A:121:VAL:HA	2.19	0.42
1:F:87:ILE:HD11	1:F:177:VAL:HA	2.01	0.42
2:I:181:LYS:HZ1	6:I:301:GOL:H31	1.84	0.42
1:A:30:LYS:HB2	1:A:30:LYS:HE2	1.90	0.42
2:L:137:VAL:O	2:L:240:ALA:HA	2.20	0.42
2:L:78:ARG:HH11	2:L:177:GLU:HG3	1.83	0.42
2:I:181:LYS:HE2	2:I:181:LYS:HB3	1.81	0.42
2:G:153:ALA:HB3	6:G:301:GOL:H2	2.01	0.42
1:C:100[B]:PHE:HE1	1:C:139:ILE:HG23	1.84	0.42
1:D:26:ASP:CG	1:D:99:ARG:HH22	2.22	0.41
1:F:34:LEU:HD22	1:F:67:ASP:HB3	2.01	0.41
1:C:59:GLN:NE2	2:H:206:GLN:OE1	2.50	0.41
2:J:199:GLU:HG2	2:J:201:ILE:HG13	2.02	0.41
1:A:100:PHE:O	1:A:103:THR:HG22	2.20	0.41
1:D:26:ASP:HB3	1:D:71:GLN:HA	2.01	0.41
1:E:22:LEU:HA	1:E:89:ILE:O	2.20	0.41
2:I:207:LEU:CD1	2:I:212:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PRO:HB3	1:C:152:VAL:HG23	2.03	0.41
1:A:35:LYS:HD2	1:A:45:ILE:CD1	2.48	0.41
1:F:23:LEU:HA	1:F:23:LEU:HD23	1.88	0.41
1:D:87:ILE:HG12	1:D:173:VAL:HG13	2.01	0.41
2:G:96:PHE:CD1	2:G:157:PHE:HB3	2.56	0.41
2:G:191:ILE:HB	2:G:194:SER:HB3	2.03	0.41
2:J:142:THR:OG1	2:J:143:PRO:HD2	2.21	0.41
1:A:70:GLY:N	3:A:201:GNP:O2G	2.48	0.41
1:A:111:LEU:HD22	1:A:151:ARG:NE	2.36	0.41
1:B:34:LEU:HD22	1:B:67:ASP:HB3	2.03	0.41
1:F:19:ARG:HB3	1:F:85:THR:HA	2.02	0.41
1:F:150:ASP:O	1:F:152:VAL:N	2.54	0.41
1:A:92:ILE:CD1	1:A:143:LEU:HD11	2.51	0.41
1:A:146:HIS:HD1	1:A:153:TRP:HZ2	1.69	0.40
1:F:26:ASP:HB3	1:F:71:GLN:HA	2.04	0.40
2:H:206:GLN:H	2:H:206:GLN:HG2	1.69	0.40
2:H:228:TYR:O	2:H:235:ILE:HD12	2.21	0.40
2:I:78:ARG:HB3	2:I:177:GLU:HG2	2.02	0.40
2:J:146:LEU:HD12	2:J:216:ILE:HD11	2.03	0.40
2:H:85:CYS:HB3	2:H:234:LEU:HD23	2.04	0.40
2:I:225:ASP:HB3	2:I:227:PHE:CE2	2.56	0.40
1:B:58:SER:O	1:B:60:GLY:N	2.53	0.40
2:I:228:TYR:HD2	2:I:236:MET:HB3	1.87	0.40
2:J:73:VAL:HG11	2:J:229:PHE:CZ	2.57	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	172/183 (94%)	158 (92%)	12 (7%)	2 (1%)	<b>13</b> 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	175/183 (96%)	164 (94%)	10 (6%)	1 (1%)	25	62
1	C	182/183 (100%)	171 (94%)	11 (6%)	0	100	100
1	D	175/183 (96%)	166 (95%)	8 (5%)	1 (1%)	25	62
1	E	172/183 (94%)	160 (93%)	10 (6%)	2 (1%)	13	46
1	F	178/183 (97%)	166 (93%)	7 (4%)	5 (3%)	5	26
2	G	171/183 (93%)	162 (95%)	9 (5%)	0	100	100
2	H	168/183 (92%)	159 (95%)	8 (5%)	1 (1%)	25	62
2	I	167/183 (91%)	155 (93%)	11 (7%)	1 (1%)	25	62
2	J	170/183 (93%)	162 (95%)	7 (4%)	1 (1%)	25	62
2	K	161/183 (88%)	149 (92%)	10 (6%)	2 (1%)	13	46
2	L	158/183 (86%)	151 (96%)	7 (4%)	0	100	100
All	All	2049/2196 (93%)	1923 (94%)	110 (5%)	16 (1%)	19	55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	115	LYS
2	I	115	LYS
2	J	115	LYS
2	K	115	LYS
1	E	10	LEU
1	F	72	ARG
1	A	12	SER
1	B	59	GLN
1	E	14	PRO
1	F	71	GLN
1	F	150	ASP
1	F	151	ARG
1	F	152	VAL
2	K	67	THR
1	D	13	ALA
1	A	14	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	150/161 (93%)	148 (99%)	2 (1%)	69	86
1	B	148/161 (92%)	147 (99%)	1 (1%)	84	93
1	C	158/161 (98%)	156 (99%)	2 (1%)	69	86
1	D	151/161 (94%)	149 (99%)	2 (1%)	69	86
1	E	150/161 (93%)	148 (99%)	2 (1%)	69	86
1	F	149/161 (92%)	147 (99%)	2 (1%)	69	86
2	G	163/169 (96%)	161 (99%)	2 (1%)	71	87
2	H	160/169 (95%)	157 (98%)	3 (2%)	57	80
2	I	154/169 (91%)	154 (100%)	0	100	100
2	J	160/169 (95%)	156 (98%)	4 (2%)	47	75
2	K	150/169 (89%)	145 (97%)	5 (3%)	38	69
2	L	152/169 (90%)	152 (100%)	0	100	100
All	All	1845/1980 (93%)	1820 (99%)	25 (1%)	67	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	CYS
1	A	161	LEU
1	B	158	CYS
1	C	3	LEU
1	C	17	GLU
1	D	17	GLU
1	D	72	ARG
1	E	9	LYS
1	E	15	ASP
1	F	19	ARG
1	F	161	LEU
2	G	149	ARG
2	G	245	ASN
2	H	138	ARG
2	H	166	ASN
2	H	206	GLN
2	J	82	ASN
2	J	135	ARG
2	J	166	ASN

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Mol	Chain	Res	Type
2	J	182	ASN
2	K	85	CYS
2	K	140	GLN
2	K	161	ASP
2	K	166	ASN
2	K	204	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
1	E	57	GLN
2	K	200	HIS

### 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](#)

Of 24 ligands modelled in this entry, 6 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
6	GOL	G	301	-	5,5,5	0.86	0	5,5,5	1.02	0
3	GNP	B	201	4	29,34,34	1.64	7 (24%)	33,54,54	2.17	7 (21%)
5	PO4	C	202	-	4,4,4	0.89	0	6,6,6	0.42	0
5	PO4	I	302	-	4,4,4	0.89	0	6,6,6	0.42	0
3	GNP	A	201	4	29,34,34	1.67	7 (24%)	33,54,54	2.15	7 (21%)
5	PO4	K	301	-	4,4,4	0.92	0	6,6,6	0.46	0
7	EDO	G	302	-	3,3,3	0.45	0	2,2,2	0.35	0
5	PO4	L	301	-	4,4,4	0.91	0	6,6,6	0.42	0
6	GOL	J	301	-	5,5,5	0.90	0	5,5,5	0.98	0
5	PO4	J	302	-	4,4,4	0.91	0	6,6,6	0.49	0
7	EDO	H	302	-	3,3,3	0.46	0	2,2,2	0.34	0
3	GNP	C	201	4	29,34,34	1.64	7 (24%)	33,54,54	2.11	7 (21%)
6	GOL	H	301	-	5,5,5	0.90	0	5,5,5	1.05	0
5	PO4	G	303	-	4,4,4	0.91	0	6,6,6	0.40	0
3	GNP	E	201	4	29,34,34	1.60	7 (24%)	33,54,54	2.16	7 (21%)
3	GNP	F	201	4	29,34,34	1.66	7 (24%)	33,54,54	2.10	5 (15%)
3	GNP	D	201	4	29,34,34	1.65	7 (24%)	33,54,54	2.11	6 (18%)
6	GOL	I	301	-	5,5,5	0.86	0	5,5,5	1.06	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
6	GOL	G	301	-	-	1/4/4/4	-
3	GNP	B	201	4	-	2/14/38/38	0/3/3/3
7	EDO	G	302	-	-	1/1/1/1	-
3	GNP	A	201	4	-	8/14/38/38	0/3/3/3
6	GOL	J	301	-	-	3/4/4/4	-
7	EDO	H	302	-	-	0/1/1/1	-
3	GNP	C	201	4	-	5/14/38/38	0/3/3/3
6	GOL	H	301	-	-	4/4/4/4	-
3	GNP	E	201	4	-	4/14/38/38	0/3/3/3
3	GNP	F	201	4	-	3/14/38/38	0/3/3/3
3	GNP	D	201	4	-	8/14/38/38	0/3/3/3
6	GOL	I	301	-	-	3/4/4/4	-

All (42) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	GNP	PB-O3A	4.91	1.65	1.59
3	A	201	GNP	PB-O3A	4.74	1.65	1.59
3	C	201	GNP	PB-O3A	4.64	1.64	1.59
3	D	201	GNP	PB-O3A	4.55	1.64	1.59
3	B	201	GNP	PB-O3A	4.43	1.64	1.59
3	E	201	GNP	PB-O3A	4.19	1.64	1.59
3	B	201	GNP	PG-N3B	3.28	1.71	1.63
3	A	201	GNP	PB-O1B	3.14	1.51	1.46
3	A	201	GNP	PG-N3B	3.13	1.71	1.63
3	E	201	GNP	C6-N1	3.13	1.38	1.33
3	F	201	GNP	PB-O1B	3.13	1.51	1.46
3	D	201	GNP	PB-O1B	3.13	1.51	1.46
3	D	201	GNP	C6-N1	3.12	1.38	1.33
3	C	201	GNP	C6-N1	3.12	1.38	1.33
3	C	201	GNP	PG-N3B	3.11	1.71	1.63
3	A	201	GNP	C6-N1	3.11	1.38	1.33
3	B	201	GNP	C6-N1	3.10	1.38	1.33
3	F	201	GNP	C6-N1	3.09	1.38	1.33
3	B	201	GNP	PB-O1B	3.08	1.51	1.46
3	D	201	GNP	PG-N3B	3.08	1.71	1.63
3	C	201	GNP	PB-O1B	3.02	1.50	1.46
3	F	201	GNP	PG-N3B	2.99	1.71	1.63
3	E	201	GNP	PB-O1B	2.98	1.50	1.46
3	E	201	GNP	PG-N3B	2.93	1.71	1.63
3	D	201	GNP	PG-O1G	2.85	1.50	1.46
3	B	201	GNP	PG-O1G	2.85	1.50	1.46
3	A	201	GNP	PG-O1G	2.83	1.50	1.46
3	E	201	GNP	PG-O1G	2.80	1.50	1.46
3	C	201	GNP	PG-O1G	2.78	1.50	1.46
3	F	201	GNP	PG-O1G	2.73	1.50	1.46
3	E	201	GNP	PB-O2B	-2.35	1.50	1.56
3	A	201	GNP	PB-O2B	-2.33	1.50	1.56
3	C	201	GNP	PB-O2B	-2.22	1.50	1.56
3	D	201	GNP	PB-O2B	-2.21	1.50	1.56
3	F	201	GNP	PB-O2B	-2.20	1.50	1.56
3	B	201	GNP	PB-O2B	-2.12	1.51	1.56
3	D	201	GNP	C5-C6	2.10	1.45	1.41
3	E	201	GNP	C5-C6	2.09	1.45	1.41
3	A	201	GNP	C5-C6	2.08	1.44	1.41
3	F	201	GNP	C5-C6	2.08	1.44	1.41
3	C	201	GNP	C5-C6	2.05	1.44	1.41
3	B	201	GNP	C5-C6	2.03	1.44	1.41

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	GNP	C5-C6-N1	-8.42	111.91	123.43
3	F	201	GNP	C5-C6-N1	-8.41	111.92	123.43
3	C	201	GNP	C5-C6-N1	-8.38	111.97	123.43
3	A	201	GNP	C5-C6-N1	-8.38	111.97	123.43
3	E	201	GNP	C5-C6-N1	-8.38	111.98	123.43
3	B	201	GNP	C5-C6-N1	-8.37	111.98	123.43
3	F	201	GNP	C2-N1-C6	5.86	125.24	115.93
3	A	201	GNP	C2-N1-C6	5.83	125.19	115.93
3	D	201	GNP	C2-N1-C6	5.83	125.19	115.93
3	E	201	GNP	C2-N1-C6	5.82	125.17	115.93
3	B	201	GNP	C2-N1-C6	5.81	125.16	115.93
3	C	201	GNP	C2-N1-C6	5.80	125.15	115.93
3	B	201	GNP	PB-O3A-PA	-3.56	120.06	132.62
3	A	201	GNP	O3G-PG-O1G	-3.14	105.56	113.45
3	D	201	GNP	PB-O3A-PA	-2.86	122.54	132.62
3	B	201	GNP	N3-C2-N1	-2.81	123.48	127.22
3	A	201	GNP	N3-C2-N1	-2.81	123.48	127.22
3	C	201	GNP	N3-C2-N1	-2.78	123.52	127.22
3	F	201	GNP	N3-C2-N1	-2.75	123.55	127.22
3	D	201	GNP	N3-C2-N1	-2.75	123.56	127.22
3	E	201	GNP	N3-C2-N1	-2.73	123.59	127.22
3	E	201	GNP	C4-C5-C6	-2.70	118.22	120.80
3	B	201	GNP	O3G-PG-O1G	-2.68	106.72	113.45
3	E	201	GNP	PB-O3A-PA	-2.67	123.22	132.62
3	C	201	GNP	C4-C5-C6	-2.67	118.25	120.80
3	A	201	GNP	PB-O3A-PA	-2.64	123.33	132.62
3	A	201	GNP	C4-C5-C6	-2.62	118.30	120.80
3	B	201	GNP	C4-C5-C6	-2.59	118.32	120.80
3	F	201	GNP	C4-C5-C6	-2.59	118.33	120.80
3	D	201	GNP	C4-C5-C6	-2.58	118.33	120.80
3	E	201	GNP	O1B-PB-N3B	-2.28	108.42	111.77
3	E	201	GNP	C2-N3-C4	-2.20	112.84	115.36
3	D	201	GNP	C2-N3-C4	-2.19	112.86	115.36
3	F	201	GNP	C2-N3-C4	-2.19	112.86	115.36
3	C	201	GNP	PB-O3A-PA	-2.17	124.96	132.62
3	B	201	GNP	C2-N3-C4	-2.12	112.93	115.36
3	C	201	GNP	C2-N3-C4	-2.12	112.94	115.36
3	A	201	GNP	C2-N3-C4	-2.10	112.96	115.36
3	C	201	GNP	O1B-PB-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (42) torsion outliers are listed below:

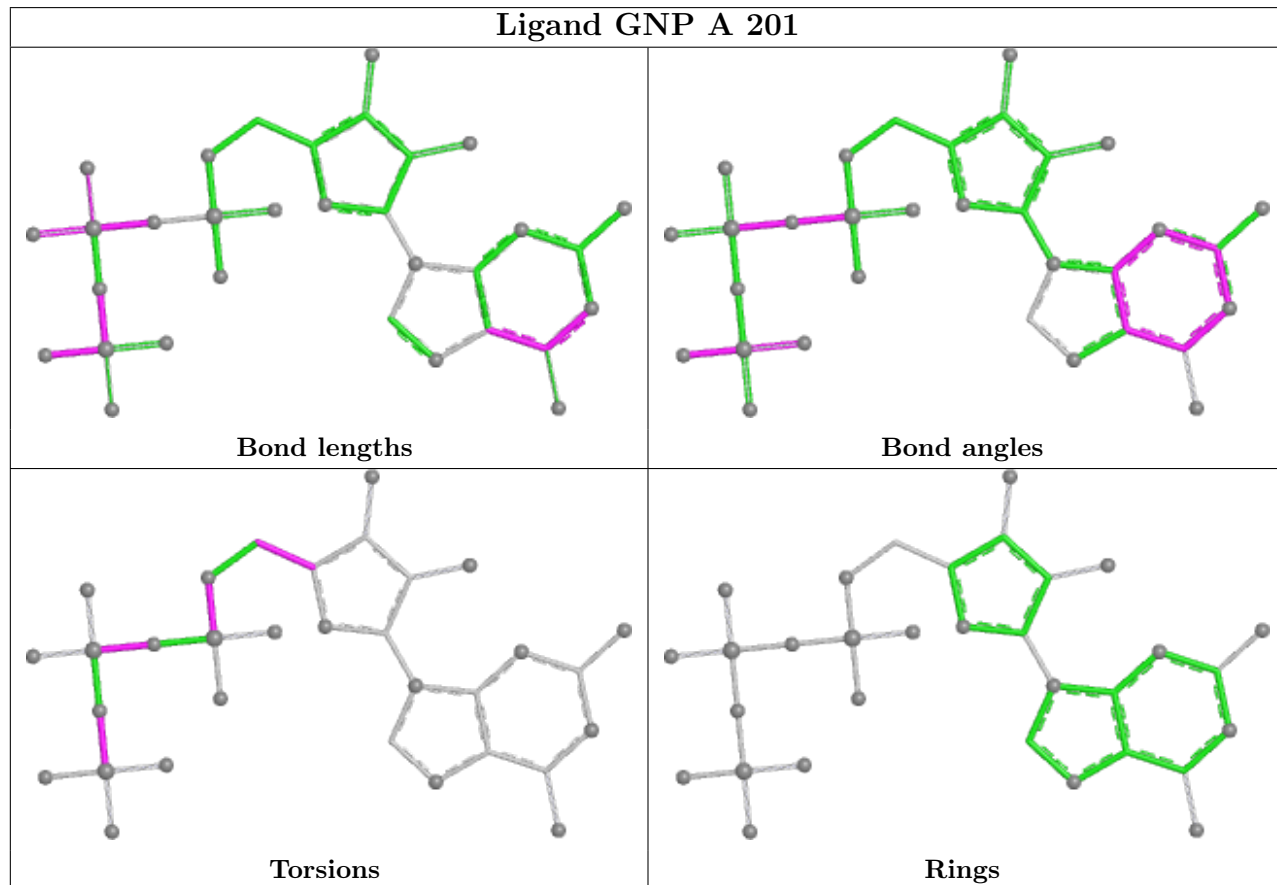
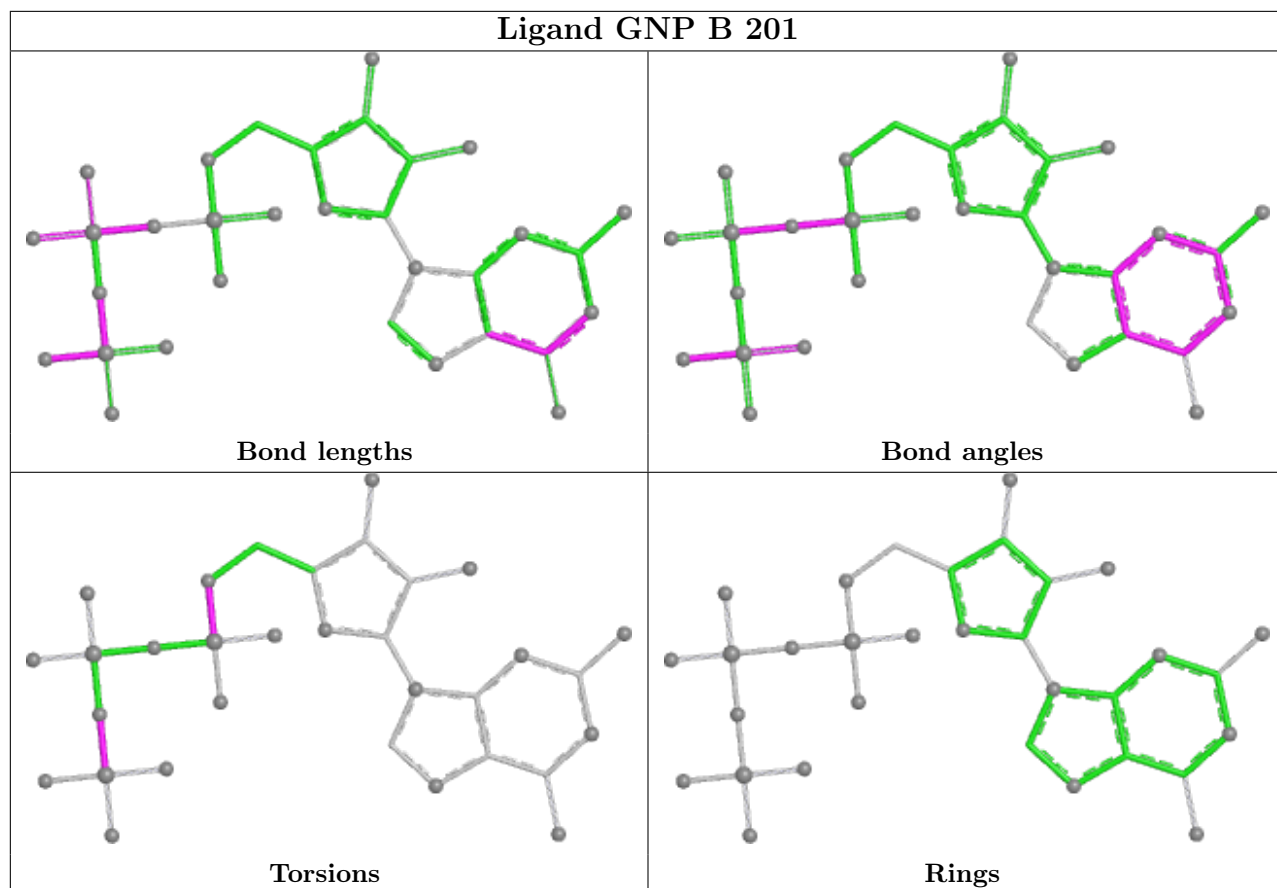
Mol	Chain	Res	Type	Atoms
3	A	201	GNP	PB-N3B-PG-O1G
3	A	201	GNP	PA-O3A-PB-O1B
3	A	201	GNP	PA-O3A-PB-O2B
3	B	201	GNP	PB-N3B-PG-O1G
3	C	201	GNP	PB-N3B-PG-O1G
3	C	201	GNP	PG-N3B-PB-O1B
3	C	201	GNP	PA-O3A-PB-O1B
3	D	201	GNP	PB-N3B-PG-O1G
3	D	201	GNP	PA-O3A-PB-O1B
3	D	201	GNP	PA-O3A-PB-O2B
3	D	201	GNP	C5'-O5'-PA-O3A
3	D	201	GNP	C5'-O5'-PA-O1A
3	D	201	GNP	C5'-O5'-PA-O2A
3	D	201	GNP	O4'-C4'-C5'-O5'
3	E	201	GNP	C5'-O5'-PA-O3A
3	E	201	GNP	C5'-O5'-PA-O2A
3	F	201	GNP	C5'-O5'-PA-O3A
3	F	201	GNP	C5'-O5'-PA-O1A
6	H	301	GOL	O1-C1-C2-C3
6	H	301	GOL	C1-C2-C3-O3
3	A	201	GNP	O4'-C4'-C5'-O5'
3	C	201	GNP	O4'-C4'-C5'-O5'
3	C	201	GNP	C3'-C4'-C5'-O5'
3	A	201	GNP	C3'-C4'-C5'-O5'
3	D	201	GNP	C3'-C4'-C5'-O5'
6	J	301	GOL	O1-C1-C2-C3
6	H	301	GOL	O1-C1-C2-O2
6	H	301	GOL	O2-C2-C3-O3
3	F	201	GNP	O4'-C4'-C5'-O5'
6	I	301	GOL	O2-C2-C3-O3
6	J	301	GOL	O1-C1-C2-O2
3	A	201	GNP	C5'-O5'-PA-O3A
3	E	201	GNP	C5'-O5'-PA-O1A
6	G	301	GOL	O1-C1-C2-C3
6	J	301	GOL	C1-C2-C3-O3
3	E	201	GNP	O4'-C4'-C5'-O5'
6	I	301	GOL	O1-C1-C2-C3
6	I	301	GOL	C1-C2-C3-O3
3	A	201	GNP	C5'-O5'-PA-O1A
3	A	201	GNP	C5'-O5'-PA-O2A
3	B	201	GNP	C5'-O5'-PA-O1A
7	G	302	EDO	O1-C1-C2-O2

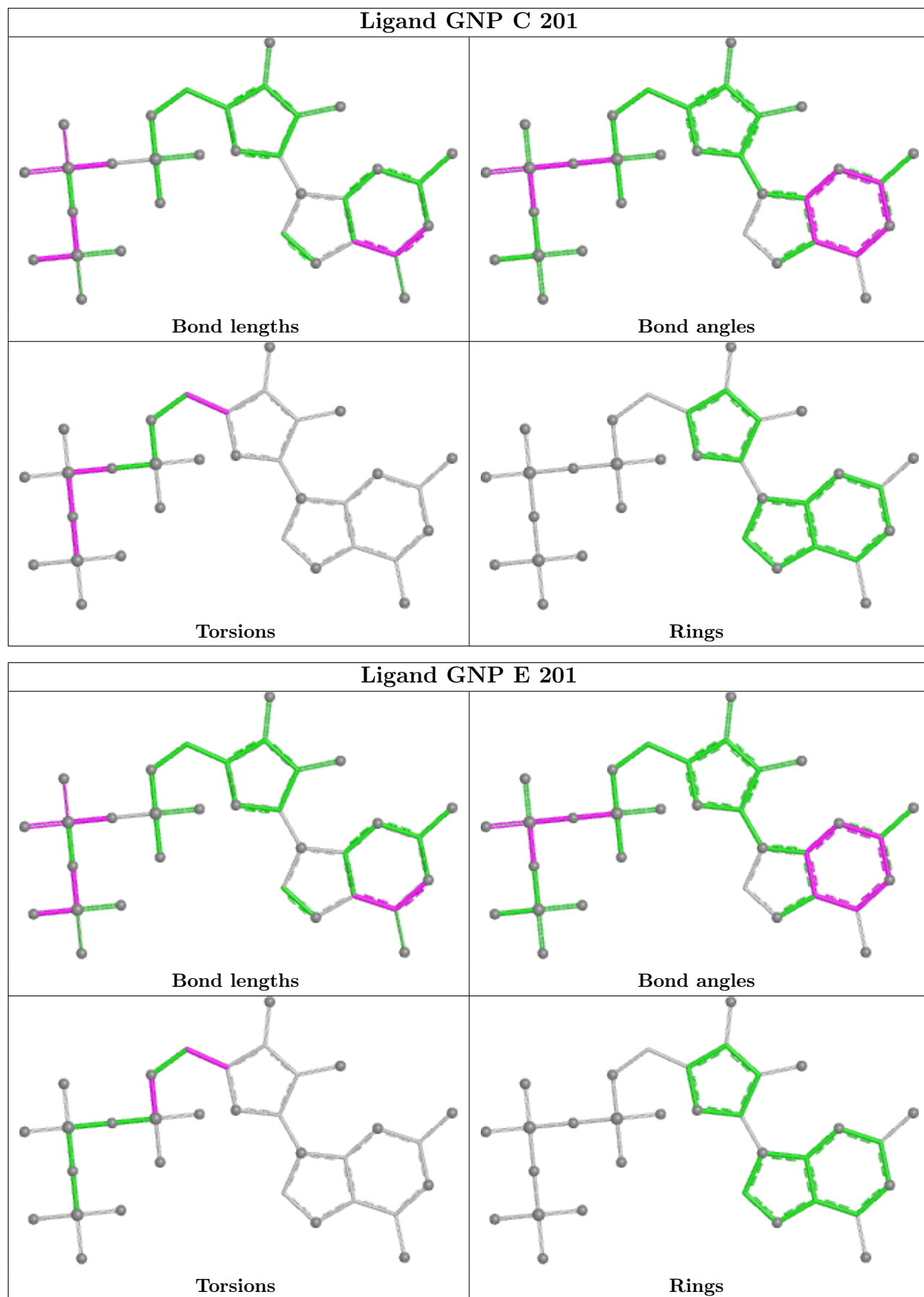
There are no ring outliers.

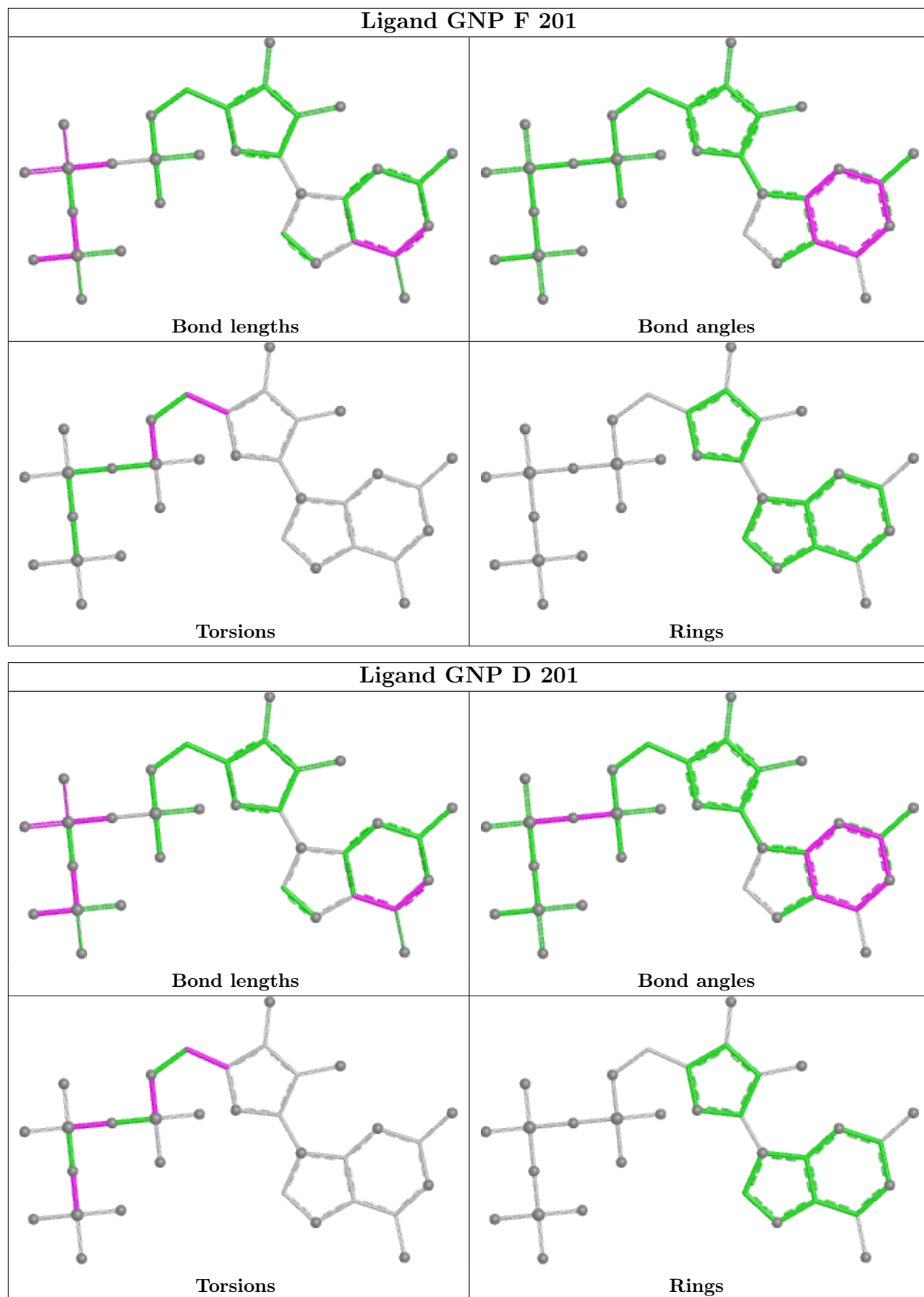
9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	301	GOL	1	0
3	B	201	GNP	2	0
3	A	201	GNP	3	0
6	J	301	GOL	1	0
3	C	201	GNP	1	0
3	E	201	GNP	1	0
3	F	201	GNP	3	0
3	D	201	GNP	3	0
6	I	301	GOL	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](#)

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	174/183 (95%)	-0.01	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	40, 59, 108, 139	0
1	B	177/183 (96%)	0.08	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	44, 66, 104, 123	0
1	C	183/183 (100%)	0.04	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	48, 65, 95, 117	0
1	D	177/183 (96%)	0.10	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	49, 72, 105, 126	0
1	E	174/183 (95%)	-0.08	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	48, 74, 106, 127	0
1	F	180/183 (98%)	0.49	16 (8%) <span style="border: 1px solid red; padding: 2px;">9</span> <span style="border: 1px solid red; padding: 2px;">5</span>	57, 111, 148, 158	0
2	G	175/183 (95%)	0.17	1 (0%) <span style="border: 1px solid blue; padding: 2px;">89</span> <span style="border: 1px solid blue; padding: 2px;">84</span>	50, 76, 106, 142	0
2	H	172/183 (93%)	0.14	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	49, 74, 104, 123	0
2	I	171/183 (93%)	0.43	5 (2%) <span style="border: 1px solid lightgray; padding: 2px;">51</span> <span style="border: 1px solid lightgray; padding: 2px;">35</span>	45, 98, 141, 154	0
2	J	174/183 (95%)	0.39	3 (1%) <span style="border: 1px solid lightgray; padding: 2px;">70</span> <span style="border: 1px solid lightgray; padding: 2px;">57</span>	54, 89, 123, 144	0
2	K	165/183 (90%)	0.79	21 (12%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">2</span>	60, 117, 189, 197	0
2	L	162/183 (88%)	0.47	9 (5%) <span style="border: 1px solid red; padding: 2px;">24</span> <span style="border: 1px solid red; padding: 2px;">12</span>	70, 116, 156, 176	0
All	All	2084/2196 (94%)	0.25	55 (2%) <span style="border: 1px solid lightgray; padding: 2px;">56</span> <span style="border: 1px solid lightgray; padding: 2px;">40</span>	40, 80, 146, 197	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	66	ASP	5.0
2	L	68	ILE	4.2
2	I	175	PHE	4.0
2	L	67	THR	3.9
1	F	90	TYR	3.6
2	J	204	PHE	3.5
1	F	85	THR	3.4
1	F	110	LEU	3.3
2	L	164	VAL	3.3
1	F	116	LEU	3.2
1	F	145	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	K	139	TYR	3.1
1	F	21	LEU	3.1
1	F	107	LEU	3.1
2	K	221	GLU	3.0
2	K	237	HIS	3.0
1	F	20	ILE	2.7
2	G	125	GLU	2.7
2	I	217	GLU	2.7
2	K	68	ILE	2.7
2	L	84	LEU	2.6
2	K	75	ARG	2.5
1	F	22	LEU	2.5
2	K	71	GLU	2.5
2	K	176	ARG	2.5
2	K	235	ILE	2.5
2	K	215	MET	2.4
1	F	91	VAL	2.4
2	J	205	PRO	2.4
2	I	69	ARG	2.3
2	K	170	ILE	2.3
2	L	229	PHE	2.3
2	I	67	THR	2.3
1	F	71	GLN	2.3
2	K	238	ASN	2.3
2	L	232	ASN	2.3
2	K	169	MET	2.3
2	I	136	PHE	2.2
1	F	140	ALA	2.2
2	J	202	TYR	2.2
2	K	207	LEU	2.2
1	F	53	ILE	2.2
2	L	96	PHE	2.2
2	K	219	PRO	2.1
2	K	180	LEU	2.1
2	K	175	PHE	2.1
1	F	89	ILE	2.1
1	F	92	ILE	2.1
2	L	71	GLU	2.1
2	K	227	PHE	2.1
2	L	163	PRO	2.1
2	K	234	LEU	2.1
2	K	76	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	K	178	HIS	2.0
1	F	68	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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.

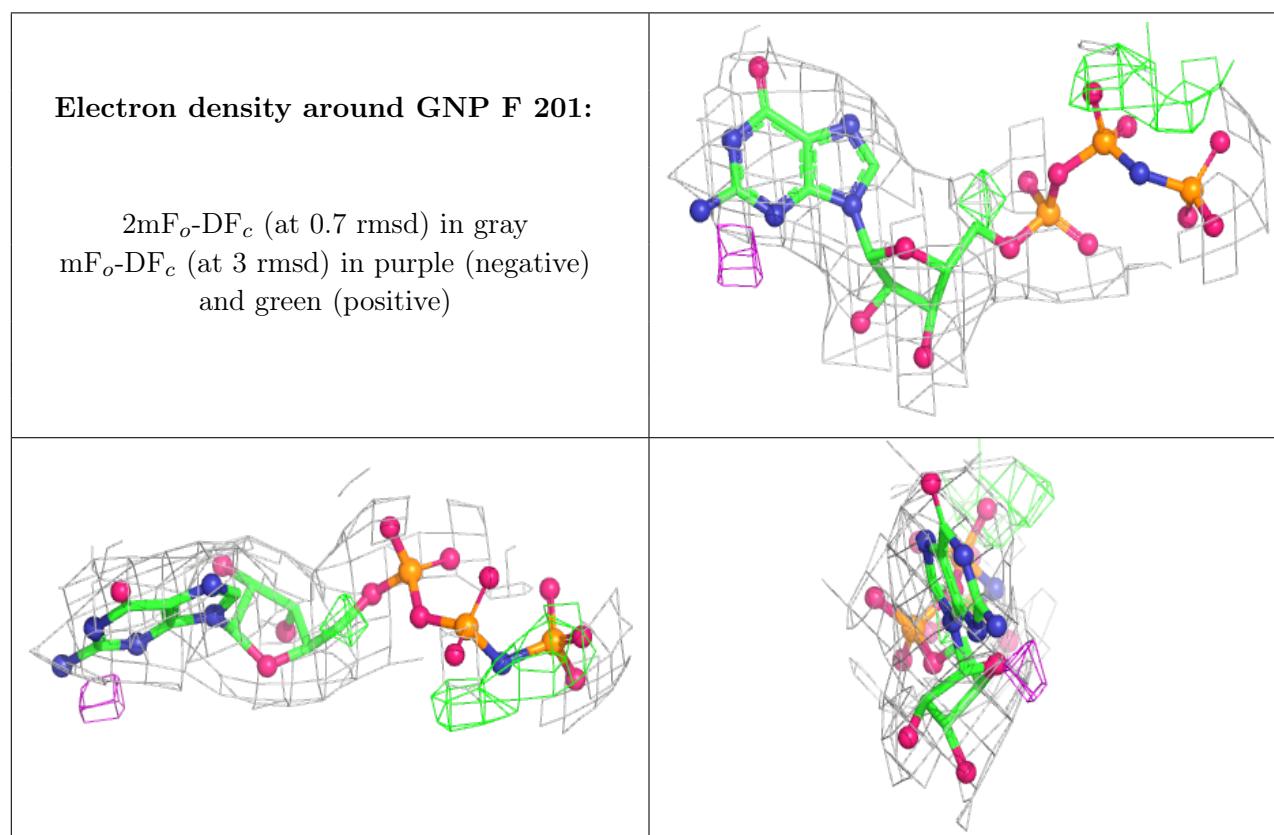
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	I	301	6/6	0.60	0.33	78,86,86,90	0
6	GOL	G	301	6/6	0.74	0.30	80,80,82,83	0
5	PO4	L	301	5/5	0.77	0.20	109,110,110,111	0
5	PO4	G	303	5/5	0.80	0.19	84,85,85,85	0
6	GOL	H	301	6/6	0.83	0.28	71,73,74,75	0
7	EDO	H	302	4/4	0.84	0.37	62,67,72,73	0
4	MG	A	202	1/1	0.86	0.25	48,48,48,48	0
5	PO4	C	202	5/5	0.87	0.17	86,87,87,88	0
5	PO4	I	302	5/5	0.88	0.17	82,82,83,83	0
6	GOL	J	301	6/6	0.89	0.30	88,90,94,97	0
5	PO4	K	301	5/5	0.92	0.16	85,86,87,90	0
7	EDO	G	302	4/4	0.93	0.32	73,74,75,76	0
5	PO4	J	302	5/5	0.94	0.16	76,77,78,79	0
4	MG	E	202	1/1	0.94	0.29	53,53,53,53	0
4	MG	C	203	1/1	0.94	0.15	45,45,45,45	0
3	GNP	F	201	32/32	0.95	0.17	79,86,107,111	0
3	GNP	B	201	32/32	0.96	0.19	43,51,58,61	0
3	GNP	D	201	32/32	0.96	0.20	43,50,63,65	0
4	MG	F	202	1/1	0.96	0.16	107,107,107,107	0
4	MG	B	202	1/1	0.97	0.21	61,61,61,61	0
3	GNP	E	201	32/32	0.97	0.21	54,58,62,65	0

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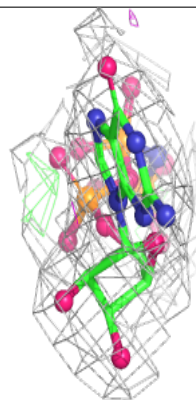
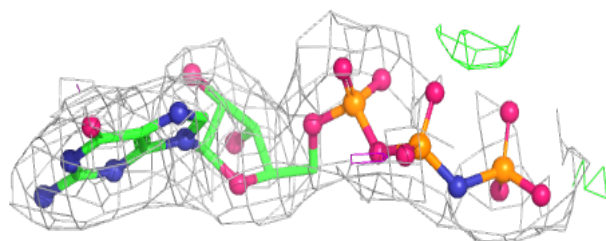
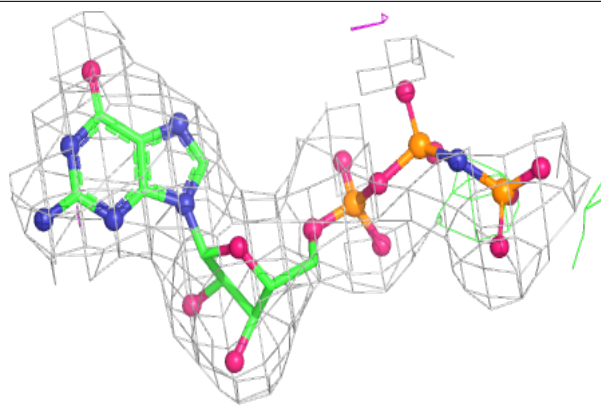
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GNP	C	201	32/32	0.97	0.22	38,45,56,59	0
3	GNP	A	201	32/32	0.97	0.20	41,46,51,52	0
4	MG	D	202	1/1	0.99	0.18	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

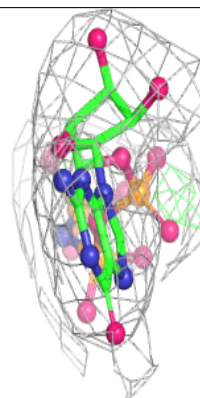
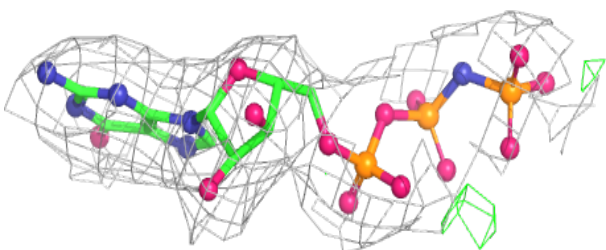
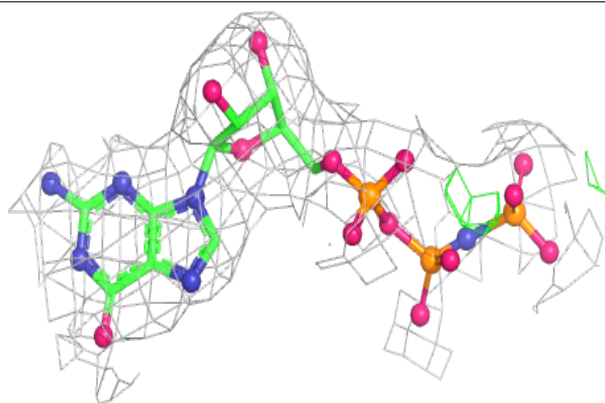


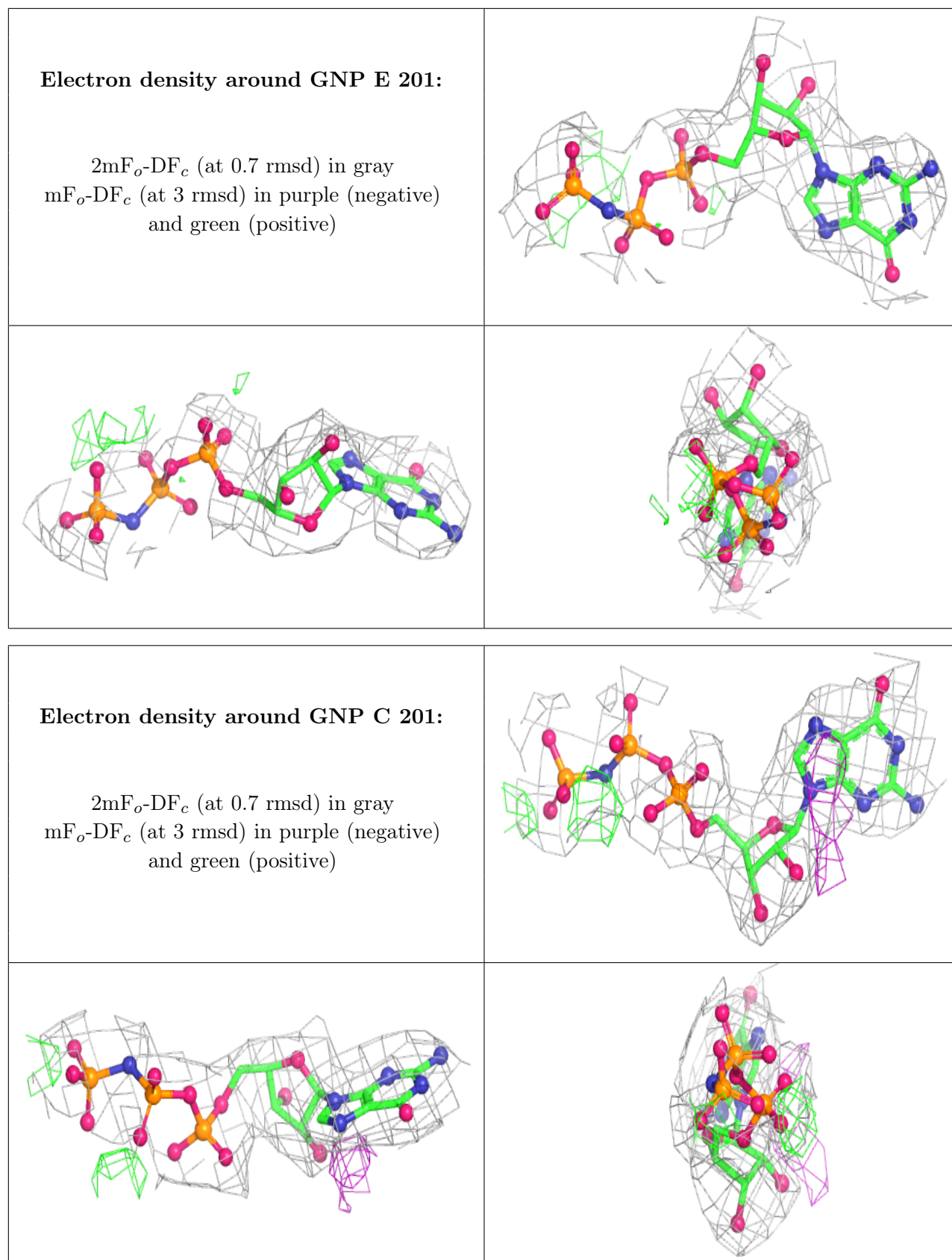
**Electron density around GNP B 201:**

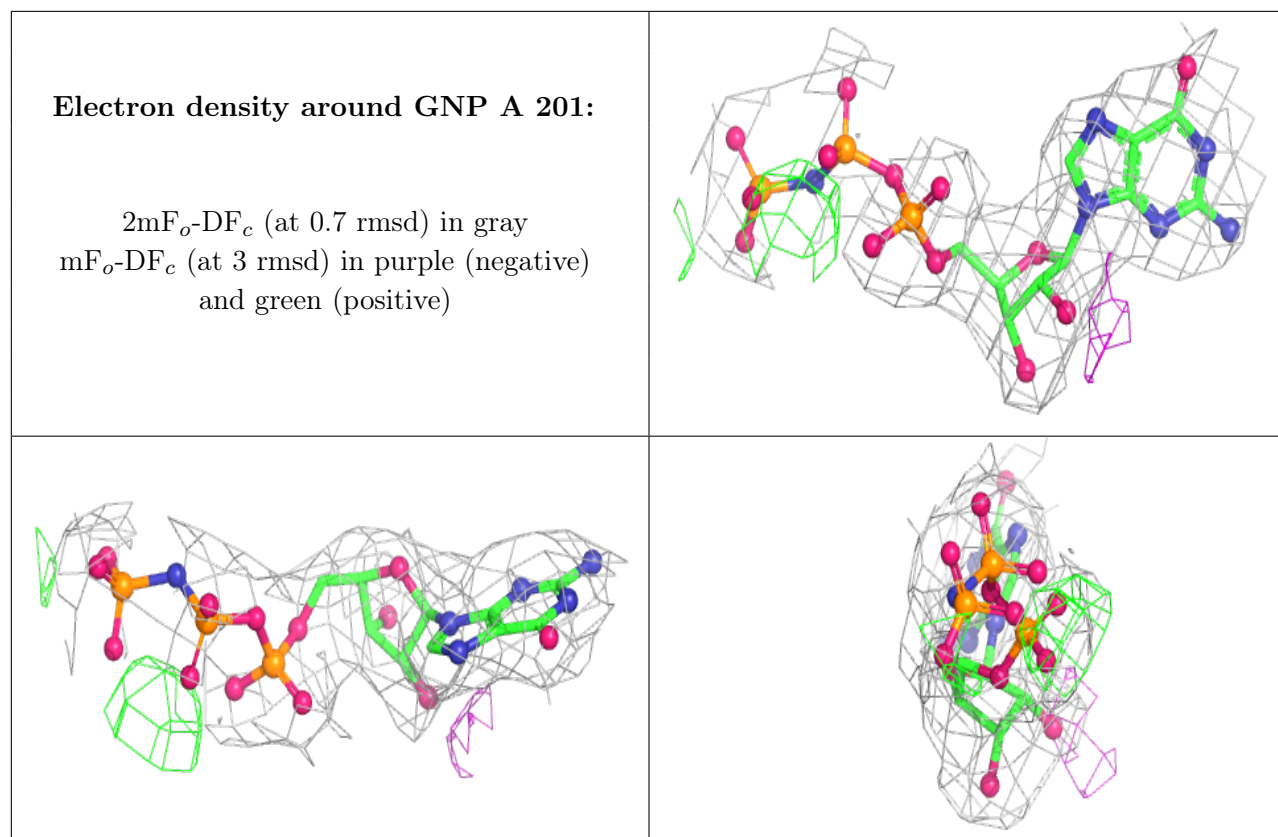
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GNP D 201:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.