



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 07:53 pm GMT

PDB ID : 9RKJ / pdb\_00009rkj  
Title : Crystal Structure of compound 3-mediated ternary complex of KRAS G12R  
GCP with pVHL:ElonginC:ElonginB  
Authors : Wijaya, A.J.; Karolak, N.K.; Ciulli, A.  
Deposited on : 2025-06-13  
Resolution : 2.89 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 : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

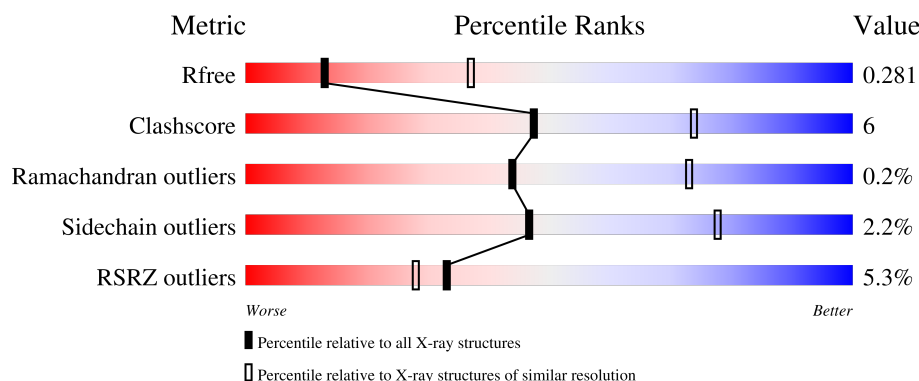
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	104	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	E	104	<div> <div>5%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	B	97	<div> <div>4%</div> <div>71%</div> <div>18%</div> <div>11%</div> </div>
2	F	97	<div> <div>5%</div> <div>77%</div> <div>11%</div> <div>11%</div> </div>
3	C	162	<div> <div>2%</div> <div>78%</div> <div>14%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	162	
4	D	170	
4	H	170	

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
5	FLC	B	201	-	X	-	-
5	FLC	C	302	-	X	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7708 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			764	487	127	146	4			
1	E	103	Total	C	N	O	S	0	0	0
			771	491	126	149	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			675	438	106	125	6			
2	F	86	Total	C	N	O	S	0	0	0
			662	430	104	122	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
F	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	148	Total	C	N	O	S	0	0	0
			1174	750	215	207	2			
3	G	147	Total	C	N	O	S	0	0	0
			1113	713	198	200	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
G	52	GLY	-	expression tag	UNP P40337
G	53	SER	-	expression tag	UNP P40337

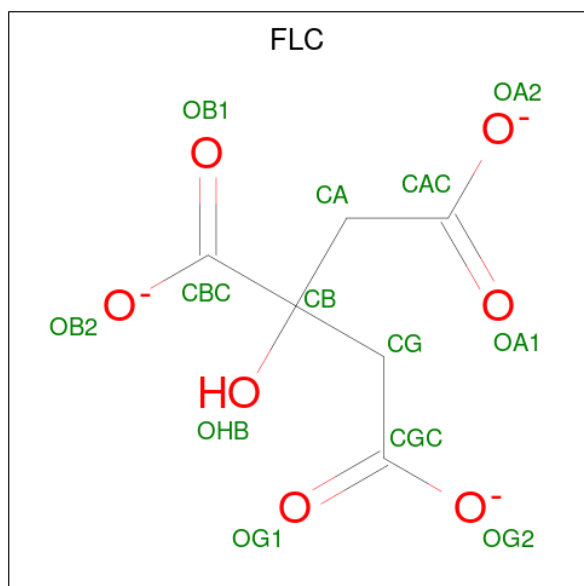
- Molecule 4 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	158	Total	C	N	O	S	0	1	0
			1213	766	211	229	7			
4	H	153	Total	C	N	O	S	0	0	0
			1081	675	193	208	5			

There are 4 discrepancies between the modelled and reference sequences:

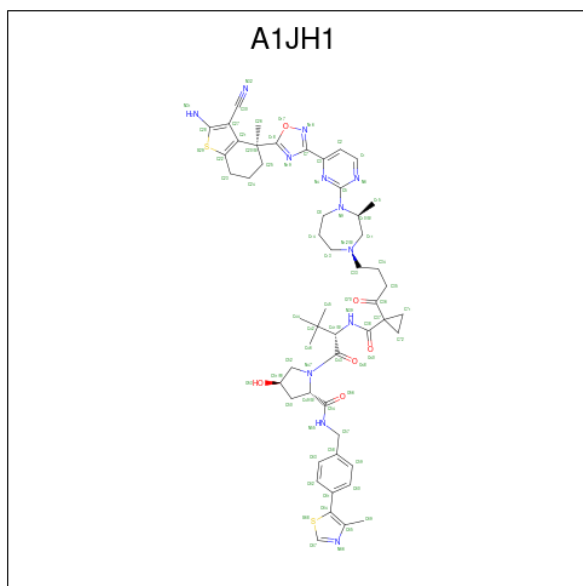
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP P01116
D	12	ARG	GLY	engineered mutation	UNP P01116
H	0	GLY	-	expression tag	UNP P01116
H	12	ARG	GLY	engineered mutation	UNP P01116

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula:  $C_6H_5O_7^-$ ).



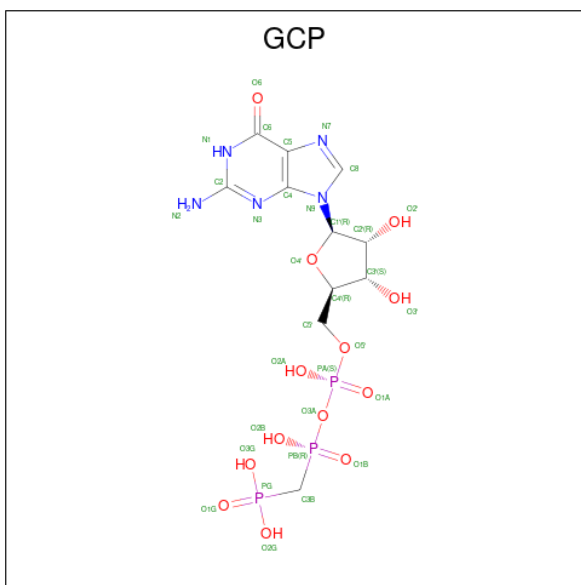
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		
5	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is (2 {S},4 {R})-1-[(2 {S})-2-[[1-[4-[(3 {S})-4-[4-[5-[(4 {S})-2-azanyl-3-cyano-4-methyl-6,7-dihydro-5 {H}-1-benzothiophen-4-yl]-1,2,4-oxadiazol-3-yl]pyrimidin-2-yl]-3-methyl-1,4-diazepan-1-yl]butanoyl]cyclopropyl]carbonylamino]-3,3-dimethyl-butanoyl]-{N}-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: A1JH1) (formula: C<sub>52</sub>H<sub>64</sub>N<sub>12</sub>O<sub>6</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			72	52	12	6	2		
6	G	1	Total	C	N	O	S	0	0
			72	52	12	6	2		

- Molecule 7 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total 32	C 11	N 5	O 13	P 3	0	0
7	H	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

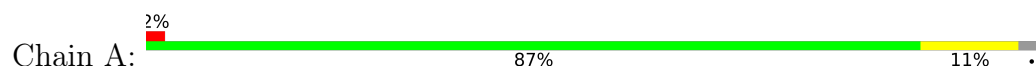
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	O	0	0
			2	2		
10	B	1	Total	O	0	0
			1	1		
10	C	5	Total	O	0	0
			5	5		
10	D	1	Total	O	0	0
			1	1		
10	F	1	Total	O	0	0
			1	1		
10	G	3	Total	O	0	0
			3	3		



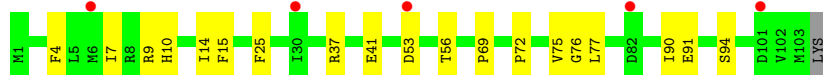
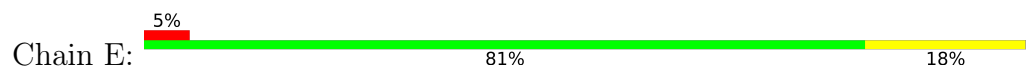
### 3 Residue-property plots [i](#)

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.

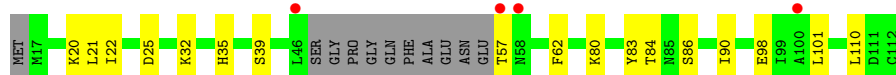
- Molecule 1: Elongin-B



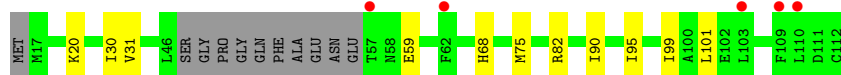
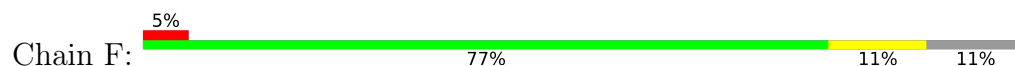
- Molecule 1: Elongin-B



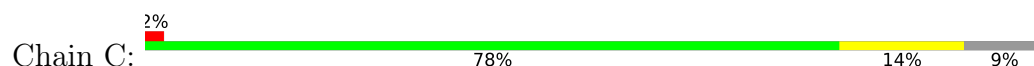
- Molecule 2: Elongin-C



- Molecule 2: Elongin-C

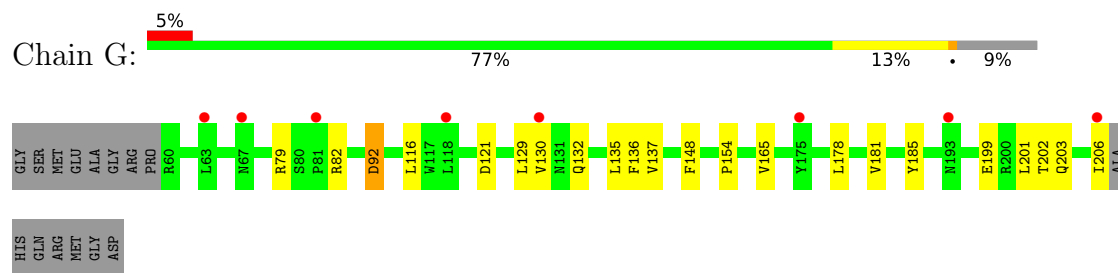


- Molecule 3: von Hippel-Lindau disease tumor suppressor

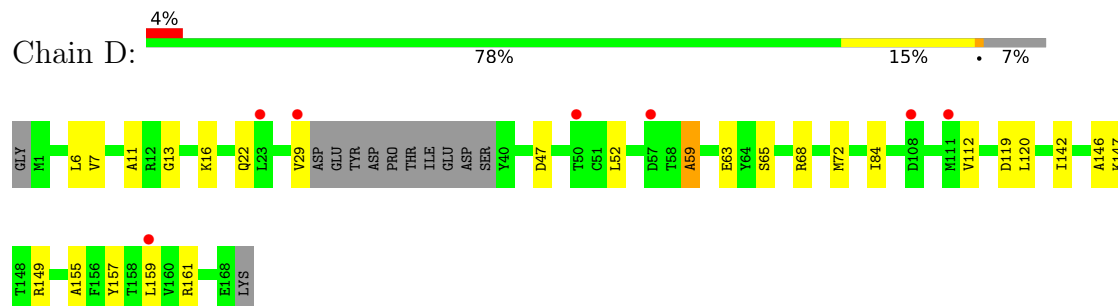


ASP

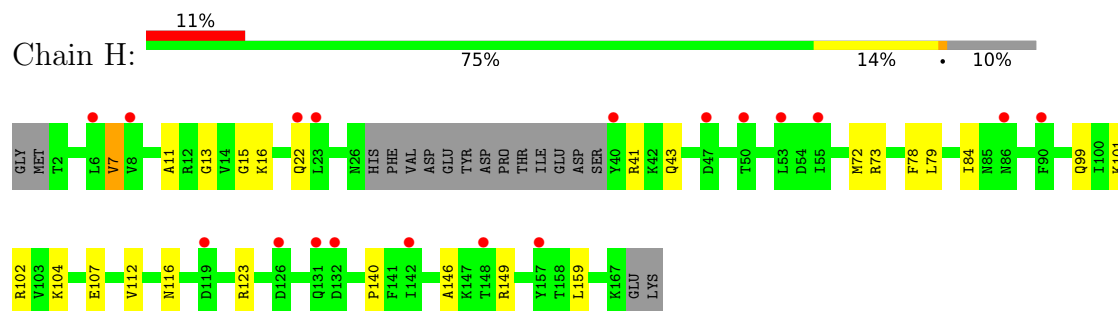
- Molecule 3: von Hippel-Lindau disease tumor suppressor



- Molecule 4: Isoform 2B of GTPase KRas



- Molecule 4: Isoform 2B of GTPase KRas



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.60Å 110.61Å 114.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.50 – 2.89 79.50 – 2.89	Depositor EDS
% Data completeness (in resolution range)	65.1 (79.50-2.89) 65.2 (79.50-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.237 , 0.288 0.233 , 0.281	Depositor DCC
$R_{free}$ test set	936 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: A1JH1, FLC, MG, GCP, 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	0.07	0/779	0.26	0/1055
1	E	0.08	0/787	0.26	0/1072
2	B	0.08	0/689	0.24	0/931
2	F	0.07	0/676	0.26	0/915
3	C	0.08	0/1205	0.25	0/1650
3	G	0.08	0/1143	0.27	0/1573
4	D	0.08	0/1231	0.24	0/1665
4	H	0.08	0/1095	0.27	0/1488
All	All	0.08	0/7605	0.26	0/10349

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	764	0	737	6	0
1	E	771	0	737	13	0
2	B	675	0	671	9	0
2	F	662	0	645	7	0
3	C	1174	0	1158	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1113	0	1044	14	0
4	D	1213	0	1170	15	0
4	H	1081	0	954	14	0
5	B	13	0	5	0	0
5	C	13	0	5	1	0
6	C	72	0	0	0	0
6	G	72	0	0	0	0
7	D	32	0	14	2	0
7	H	32	0	14	3	0
8	D	1	0	0	0	0
8	H	1	0	0	0	0
9	D	6	0	8	0	0
10	A	2	0	0	0	0
10	B	1	0	0	0	0
10	C	5	0	0	0	0
10	D	1	0	0	0	0
10	F	1	0	0	0	0
10	G	3	0	0	0	0
All	All	7708	0	7162	82	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 6.

All (82) 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:A:100:PRO:HD2	1:A:103:MET:HE2	1.67	0.75
3:G:116:LEU:HD22	3:G:135:LEU:HD12	1.70	0.72
4:H:11:ALA:O	4:H:16:LYS:NZ	2.29	0.66
1:E:7:ILE:HB	1:E:14:ILE:HB	1.77	0.66
2:F:20:LYS:HB3	2:F:59:GLU:HG2	1.76	0.66
4:H:7:VAL:HG21	4:H:72:MET:HE1	1.76	0.66
3:C:134:GLU:OE1	3:C:200:ARG:NH1	2.30	0.64
1:E:9:ARG:HB2	1:E:77:LEU:HB3	1.80	0.64
1:E:37:ARG:NH1	1:E:41:GLU:OE1	2.29	0.62
2:B:83:TYR:HB3	2:B:90:ILE:HD12	1.83	0.61
4:D:119:ASP:OD2	4:D:147:LYS:HE3	2.02	0.60
4:H:84:ILE:HB	4:H:123:ARG:HG3	1.84	0.60
3:G:82:ARG:NE	3:G:121:ASP:OD2	2.35	0.59
4:D:13:GLY:H	7:D:301:GCP:H3B1	1.67	0.59
1:A:99:LEU:HD12	2:B:98:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:112:VAL:HG22	4:H:140:PRO:HG2	1.84	0.58
4:H:22:GLN:O	4:H:149:ARG:NH1	2.36	0.58
3:C:127:GLY:O	3:C:156:TYR:OH	2.22	0.56
1:A:2:ASP:OD1	1:A:19:LYS:NZ	2.32	0.56
4:H:13:GLY:H	7:H:301:GCP:H3B1	1.70	0.56
3:C:84:VAL:HG11	3:C:151:ILE:HD13	1.88	0.55
4:D:22:GLN:HG3	4:D:146:ALA:O	2.06	0.55
4:H:73:ARG:O	4:H:104:LYS:NZ	2.37	0.54
4:D:47:ASP:OD1	4:D:161:ARG:NH1	2.41	0.54
3:G:129:LEU:HD13	3:G:154:PRO:HB3	1.89	0.54
3:G:92:ASP:N	3:G:92:ASP:OD1	2.40	0.53
1:E:14:ILE:HG12	2:F:30:ILE:HD12	1.89	0.53
1:E:94:SER:OG	2:F:68:HIS:ND1	2.35	0.53
3:C:148:PHE:HB3	3:G:148:PHE:HB3	1.91	0.53
4:D:6:LEU:HD22	4:D:159:LEU:HD23	1.92	0.52
4:D:11:ALA:O	4:D:16:LYS:NZ	2.43	0.51
1:E:25:PHE:HB2	1:E:53:ASP:HB2	1.91	0.51
2:B:20:LYS:HE3	2:B:22:ILE:HD11	1.94	0.50
3:G:116:LEU:HD23	3:G:137:VAL:HG22	1.93	0.50
3:C:79:ARG:HG3	3:G:79:ARG:NH2	2.26	0.50
3:G:178:LEU:O	3:G:185:TYR:OH	2.27	0.49
3:C:116:LEU:HD23	3:C:137:VAL:HG22	1.94	0.49
2:B:80:LYS:O	2:B:84:THR:OG1	2.24	0.48
5:C:302:FLC:HA1	2:F:82:ARG:HH12	1.78	0.48
1:E:4:PHE:CE1	1:E:69:PRO:HG3	2.49	0.48
3:C:120:ARG:NH2	3:C:197:ASP:OD2	2.42	0.47
2:B:86:SER:HB2	2:B:90:ILE:HD11	1.95	0.47
1:A:42:GLN:HG2	1:A:79:PHE:HE1	1.78	0.47
3:C:90:ASN:OD1	3:C:94:GLU:N	2.45	0.47
4:D:157:TYR:O	4:D:161:ARG:HG3	2.14	0.47
3:C:84:VAL:HG22	3:C:128:LEU:HD13	1.97	0.47
4:D:22:GLN:O	4:D:149:ARG:NH1	2.47	0.47
1:E:15:PHE:HB2	2:F:31:VAL:HG12	1.97	0.47
4:D:63:GLU:OE2	4:D:65:SER:OG	2.31	0.47
3:G:199:GLU:O	3:G:202:THR:OG1	2.33	0.47
1:A:80:ARG:HA	1:A:85:PHE:HA	1.96	0.47
4:D:59:ALA:HB3	4:D:68:ARG:HH22	1.80	0.46
1:E:53:ASP:OD1	1:E:53:ASP:N	2.47	0.46
4:H:7:VAL:HG22	4:H:78:PHE:HD1	1.81	0.46
4:H:101:LYS:HE3	4:H:107:GLU:HG3	1.98	0.46
2:B:32:LYS:HD3	2:B:35:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ILE:HA	1:E:75:VAL:HG23	1.98	0.45
4:D:7:VAL:HG11	4:D:72:MET:HE1	1.97	0.45
4:D:142:ILE:HD12	4:D:155:ALA:HA	1.98	0.44
4:H:146:ALA:N	7:H:301:GCP:O6	2.51	0.44
1:E:76:GLY:HA2	1:E:90:ILE:HD11	1.99	0.44
3:G:135:LEU:HD23	3:G:201:LEU:HD22	1.99	0.44
2:B:25:ASP:OD1	2:B:25:ASP:N	2.46	0.44
4:H:99:GLN:OE1	4:H:102:ARG:NH1	2.51	0.43
4:H:84:ILE:H	4:H:84:ILE:HG13	1.68	0.42
3:C:81:PRO:HD2	3:C:153:LEU:HG	2.01	0.42
4:H:13:GLY:N	7:H:301:GCP:H3B1	2.34	0.42
4:D:112:VAL:HG12	4:D:159:LEU:HD13	2.01	0.42
4:H:15:GLY:HA3	4:H:116:ASN:ND2	2.35	0.42
3:C:135:LEU:HD23	3:C:135:LEU:HA	1.85	0.42
4:D:13:GLY:N	7:D:301:GCP:H3B1	2.34	0.42
1:E:10:HIS:O	1:E:91:GLU:HB2	2.20	0.42
3:G:203:GLN:HA	3:G:206:ILE:HD13	2.03	0.41
1:E:72:PRO:HD2	2:F:75:MET:HE2	2.02	0.41
2:F:95:ILE:HB	3:G:165:VAL:HG21	2.02	0.41
3:G:130:VAL:HG11	3:G:136:PHE:HB2	2.02	0.41
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.92	0.41
3:G:129:LEU:HD23	3:G:132:GLN:HA	2.02	0.41
3:C:176:ARG:NH2	3:C:189:GLU:OE2	2.54	0.40
1:A:26:GLU:O	1:A:30:ILE:HG12	2.22	0.40
2:B:21:LEU:HD22	2:B:62:PHE:HE2	1.86	0.40
2:B:39:SER:HB2	2:B:110:LEU:O	2.22	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	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
1	E	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
2	B	82/97 (84%)	80 (98%)	2 (2%)	0	100	100
2	F	82/97 (84%)	79 (96%)	3 (4%)	0	100	100
3	C	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
3	G	145/162 (90%)	139 (96%)	6 (4%)	0	100	100
4	D	155/170 (91%)	151 (97%)	3 (2%)	1 (1%)	22	52
4	H	149/170 (88%)	144 (97%)	4 (3%)	1 (1%)	19	49
All	All	957/1066 (90%)	920 (96%)	35 (4%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	59	ALA
4	H	43	GLN

### 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	80/92 (87%)	80 (100%)	0	100	100
1	E	80/92 (87%)	79 (99%)	1 (1%)	65	88
2	B	75/86 (87%)	73 (97%)	2 (3%)	40	73
2	F	71/86 (83%)	68 (96%)	3 (4%)	25	59
3	C	129/148 (87%)	127 (98%)	2 (2%)	58	84
3	G	115/148 (78%)	113 (98%)	2 (2%)	56	83
4	D	125/150 (83%)	122 (98%)	3 (2%)	44	76
4	H	94/150 (63%)	90 (96%)	4 (4%)	25	57
All	All	769/952 (81%)	752 (98%)	17 (2%)	47	78

All (17) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	B	57	THR
2	B	101	LEU
3	C	118	LEU
3	C	142	VAL
4	D	29	VAL
4	D	52	LEU
4	D	84	ILE
1	E	56	THR
2	F	90	ILE
2	F	99	ILE
2	F	101	LEU
3	G	92	ASP
3	G	181	VAL
4	H	7	VAL
4	H	41	ARG
4	H	79	LEU
4	H	159	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	27	HIS
3	G	96	GLN
3	G	191	HIS
4	H	43	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
7	GCP	D	301	8	27,34,34	1.28	3 (11%)	34,54,54	2.04	7 (20%)
5	FLC	C	302	-	12,12,12	1.86	6 (50%)	17,17,17	2.50	6 (35%)
7	GCP	H	301	8	27,34,34	1.41	3 (11%)	34,54,54	2.03	6 (17%)
9	GOL	D	303	-	5,5,5	0.93	0	5,5,5	1.00	0
6	A1JH1	G	301	-	66,80,80	0.95	2 (3%)	73,120,120	0.84	4 (5%)
5	FLC	B	201	-	12,12,12	1.87	6 (50%)	17,17,17	2.50	6 (35%)
6	A1JH1	C	301	-	66,80,80	1.00	2 (3%)	73,120,120	0.75	5 (6%)

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
7	GCP	D	301	8	-	0/15/38/38	0/3/3/3
5	FLC	C	302	-	-	7/16/16/16	-
7	GCP	H	301	8	-	2/15/38/38	0/3/3/3
9	GOL	D	303	-	-	2/4/4/4	-
6	A1JH1	G	301	-	-	11/52/108/108	0/9/9/9
5	FLC	B	201	-	-	9/16/16/16	-
6	A1JH1	C	301	-	-	3/52/108/108	0/9/9/9

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	301	A1JH1	C5-N9	6.09	1.47	1.36
6	C	301	A1JH1	C5-N9	5.80	1.46	1.36
7	H	301	GCP	PB-O3A	4.98	1.63	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	A1JH1	C11-N12	4.89	1.51	1.46
6	G	301	A1JH1	C11-N12	3.84	1.50	1.46
7	D	301	GCP	PB-O3A	3.84	1.62	1.58
7	D	301	GCP	C6-N1	3.17	1.38	1.33
7	H	301	GCP	C6-N1	3.16	1.38	1.33
5	B	201	FLC	OB1-CBC	2.80	1.31	1.22
5	C	302	FLC	OB1-CBC	2.79	1.31	1.22
5	B	201	FLC	OG1-CGC	2.77	1.31	1.22
5	C	302	FLC	OA1-CAC	2.76	1.31	1.22
5	B	201	FLC	OA1-CAC	2.75	1.31	1.22
5	C	302	FLC	OG1-CGC	2.74	1.31	1.22
5	B	201	FLC	OG2-CGC	-2.66	1.21	1.30
5	C	302	FLC	OG2-CGC	-2.64	1.21	1.30
5	B	201	FLC	OA2-CAC	-2.63	1.21	1.30
5	C	302	FLC	OA2-CAC	-2.63	1.21	1.30
7	D	301	GCP	PB-O2B	-2.55	1.50	1.56
7	H	301	GCP	PB-O2B	-2.52	1.50	1.56
5	B	201	FLC	OB2-CBC	-2.20	1.22	1.30
5	C	302	FLC	OB2-CBC	-2.19	1.22	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	301	GCP	C5-C6-N1	-8.31	112.07	123.43
7	H	301	GCP	C5-C6-N1	-8.19	112.23	123.43
5	B	201	FLC	OB1-CBC-CB	-6.47	113.09	122.25
5	C	302	FLC	OB1-CBC-CB	-6.44	113.14	122.25
7	D	301	GCP	C2-N1-C6	5.84	125.22	115.93
7	H	301	GCP	C2-N1-C6	5.79	125.13	115.93
5	C	302	FLC	OB2-CBC-CB	5.55	122.69	113.05
5	B	201	FLC	OB2-CBC-CB	5.54	122.67	113.05
5	C	302	FLC	OA1-CAC-CA	-3.18	113.66	122.94
6	C	301	A1JH1	C14-C13-N12	3.17	121.34	115.35
5	B	201	FLC	OG1-CGC-CG	-3.17	113.69	122.94
5	C	302	FLC	OG1-CGC-CG	-3.16	113.70	122.94
6	G	301	A1JH1	C14-C13-N12	3.14	121.27	115.35
5	B	201	FLC	OA1-CAC-CA	-3.13	113.79	122.94
7	H	301	GCP	N3-C2-N1	-2.86	123.41	127.22
7	D	301	GCP	N3-C2-N1	-2.81	123.47	127.22
5	C	302	FLC	OG2-CGC-CG	2.67	122.94	114.35
5	C	302	FLC	OA2-CAC-CA	2.66	122.91	114.35
5	B	201	FLC	OA2-CAC-CA	2.64	122.83	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	201	FLC	OG2-CGC-CG	2.64	122.83	114.35
7	D	301	GCP	C4-C5-C6	-2.51	118.40	120.80
7	H	301	GCP	C2-N3-C4	-2.47	112.54	115.36
7	H	301	GCP	C4-C5-C6	-2.41	118.49	120.80
7	D	301	GCP	C2-N3-C4	-2.39	112.63	115.36
6	G	301	A1JH1	C25-C20-C18	-2.32	104.95	110.39
6	G	301	A1JH1	C24-C23-C22	-2.32	109.72	113.53
6	C	301	A1JH1	C24-C23-C22	-2.31	109.74	113.53
6	C	301	A1JH1	C25-C20-C18	-2.31	104.98	110.39
6	C	301	A1JH1	C7-N19-C18	2.28	104.61	101.38
7	D	301	GCP	O2B-PB-O1B	2.26	117.63	110.07
7	D	301	GCP	O1G-PG-C3B	-2.26	106.38	111.24
7	H	301	GCP	O1G-PG-C3B	-2.22	106.45	111.24
6	G	301	A1JH1	C7-N19-C18	2.20	104.50	101.38
6	C	301	A1JH1	C26-C20-C21	2.18	112.91	107.66

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	201	FLC	CA-CB-CBC-OB1
5	B	201	FLC	CA-CB-CBC-OB2
5	B	201	FLC	OHB-CB-CBC-OB1
5	B	201	FLC	OHB-CB-CBC-OB2
5	B	201	FLC	OHB-CB-CG-CGC
5	C	302	FLC	CAC-CA-CB-CBC
5	C	302	FLC	CAC-CA-CB-CG
5	C	302	FLC	CAC-CA-CB-OHB
5	C	302	FLC	CG-CB-CBC-OB1
5	C	302	FLC	CG-CB-CBC-OB2
5	C	302	FLC	OHB-CB-CBC-OB1
5	C	302	FLC	OHB-CB-CBC-OB2
6	C	301	A1JH1	O70-C36-C37-C38
6	C	301	A1JH1	O70-C36-C37-C71
6	G	301	A1JH1	C72-C37-C38-N39
6	G	301	A1JH1	C42-C41-N39-C38
9	D	303	GOL	C1-C2-C3-O3
5	B	201	FLC	CA-CB-CG-CGC
5	B	201	FLC	CBC-CB-CG-CGC
9	D	303	GOL	O2-C2-C3-O3
6	G	301	A1JH1	C43-C41-N39-C38
6	G	301	A1JH1	C71-C37-C38-N39

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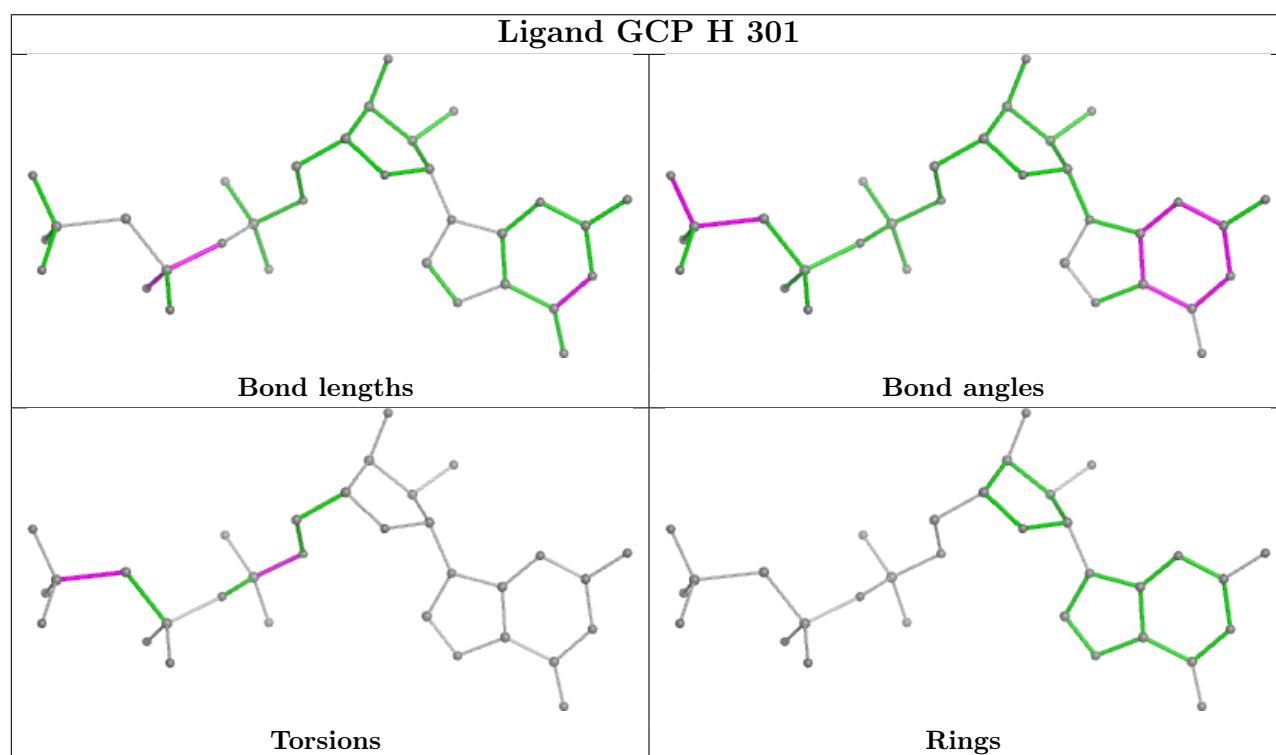
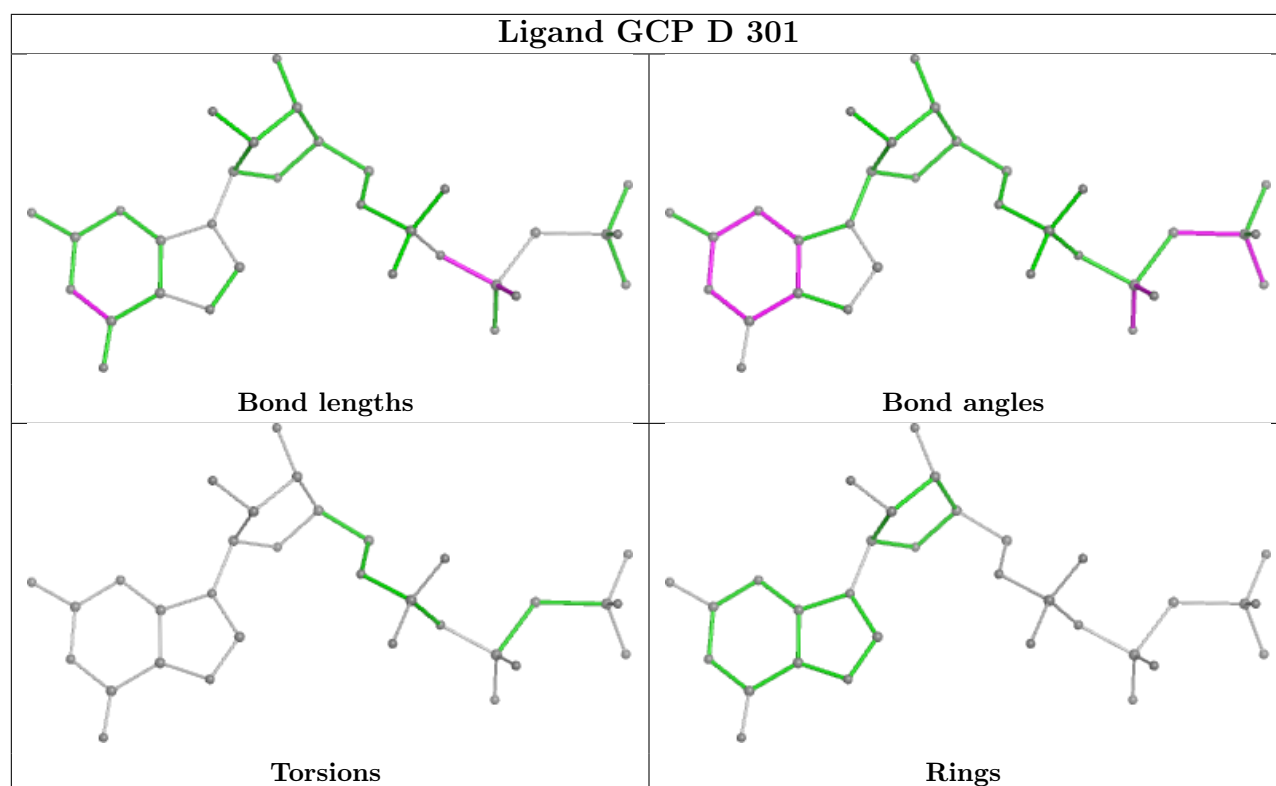
Mol	Chain	Res	Type	Atoms
6	G	301	A1JH1	C71-C37-C38-O40
6	C	301	A1JH1	C34-C33-N12-C11
5	B	201	FLC	CG-CB-CBC-OB1
5	B	201	FLC	CG-CB-CBC-OB2
6	G	301	A1JH1	N4-C5-N9-C8
6	G	301	A1JH1	N6-C5-N9-C8
6	G	301	A1JH1	C36-C37-C38-O40
6	G	301	A1JH1	C36-C37-C38-N39
7	H	301	GCP	PB-C3B-PG-O1G
6	G	301	A1JH1	C72-C37-C38-O40
7	H	301	GCP	C5'-O5'-PA-O1A
6	G	301	A1JH1	O70-C36-C37-C72

There are no ring outliers.

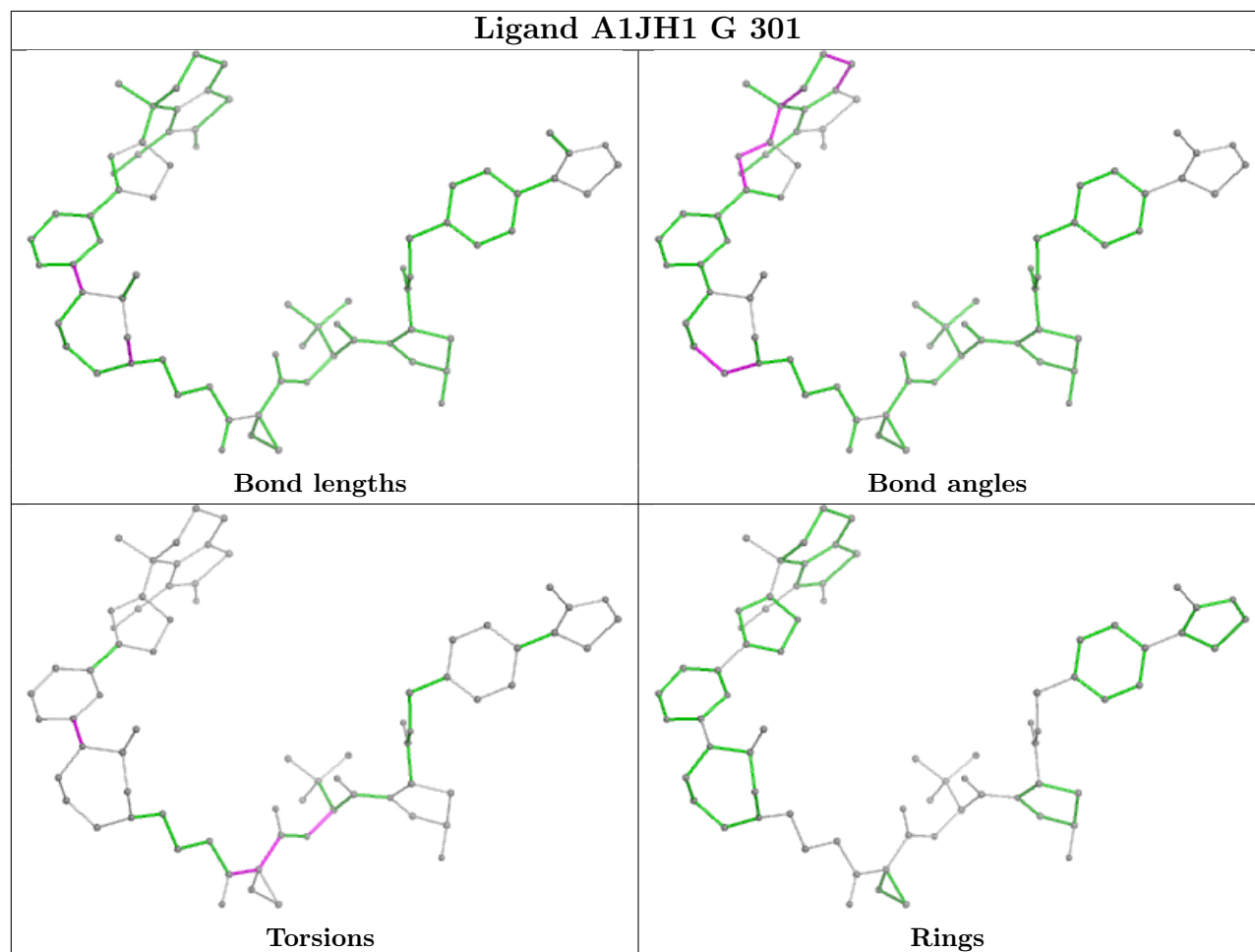
3 monomers are involved in 6 short contacts:

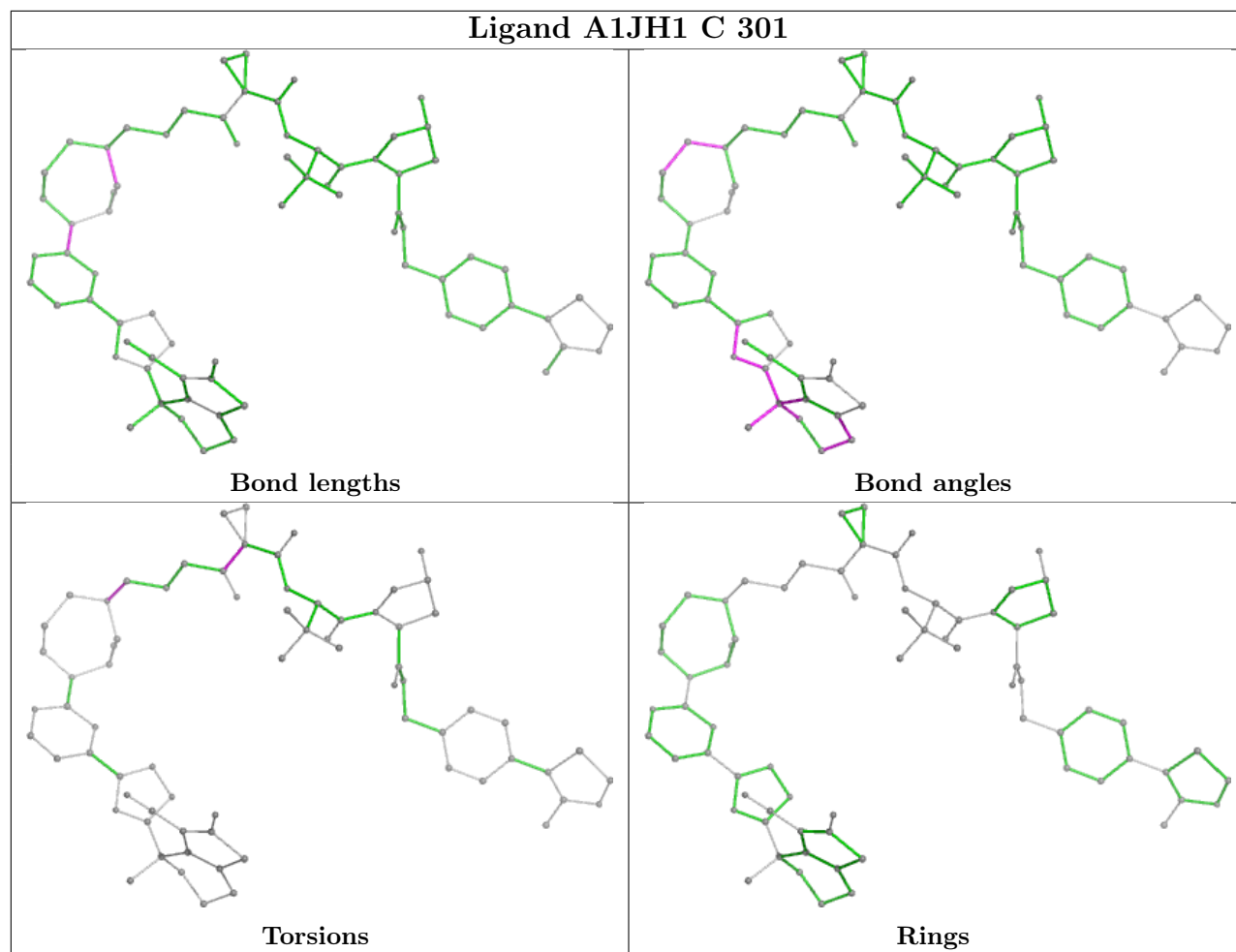
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	301	GCP	2	0
5	C	302	FLC	1	0
7	H	301	GCP	3	0

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.



## Ligand A1JH1 G 301





## 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	101/104 (97%)	0.36	2 (1%) 64 58	19, 45, 64, 72	0
1	E	103/104 (99%)	0.32	5 (4%) 36 30	34, 49, 80, 91	0
2	B	86/97 (88%)	0.17	4 (4%) 37 31	18, 33, 52, 71	0
2	F	86/97 (88%)	0.53	5 (5%) 30 26	27, 48, 61, 74	0
3	C	148/162 (91%)	0.14	3 (2%) 64 58	16, 32, 64, 81	0
3	G	147/162 (90%)	0.54	8 (5%) 32 28	27, 49, 79, 105	0
4	D	158/170 (92%)	0.37	7 (4%) 39 33	24, 40, 58, 73	1 (0%)
4	H	153/170 (90%)	0.99	18 (11%) 10 9	43, 71, 92, 113	0
All	All	982/1066 (92%)	0.45	52 (5%) 33 28	16, 46, 81, 113	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	53	LEU	3.5
4	H	40	TYR	3.4
4	H	47	ASP	3.3
4	H	90	PHE	3.2
4	H	119	ASP	3.2
4	H	126	ASP	3.1
2	F	109	PHE	3.0
2	F	57	THR	3.0
4	D	29	VAL	3.0
1	A	53	ASP	3.0
3	G	81	PRO	2.9
4	D	57	ASP	2.9
3	G	193	ASN	2.9
4	H	22	GLN	2.7
2	B	46	LEU	2.7
3	G	206	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	159	LEU	2.6
2	B	58	ASN	2.5
4	H	8	VAL	2.5
3	C	140	LEU	2.5
2	F	103	LEU	2.5
3	C	137	VAL	2.5
4	H	55	ILE	2.5
4	H	23	LEU	2.4
3	G	130	VAL	2.4
3	C	207	ALA	2.4
4	D	108	ASP	2.4
4	D	23	LEU	2.4
1	E	82	ASP	2.4
2	B	100	ALA	2.4
4	H	131	GLN	2.4
2	F	62	PHE	2.4
3	G	63	LEU	2.3
1	E	53	ASP	2.3
4	D	111	MET	2.3
1	E	101	ASP	2.3
4	H	132	ASP	2.3
4	H	50	THR	2.3
4	H	148	THR	2.2
3	G	67	ASN	2.2
2	F	110	LEU	2.2
3	G	118	LEU	2.2
3	G	175	TYR	2.2
4	D	50	THR	2.2
2	B	57	THR	2.1
1	E	6	MET	2.1
1	E	30	ILE	2.1
1	A	62	PHE	2.1
4	H	6	LEU	2.1
4	H	86	ASN	2.0
4	H	142	ILE	2.0
4	H	157	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

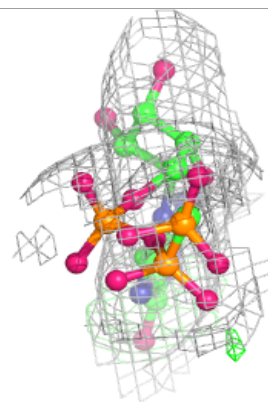
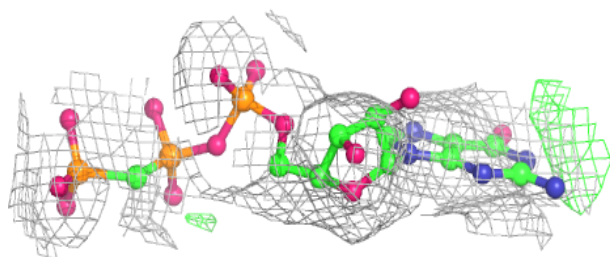
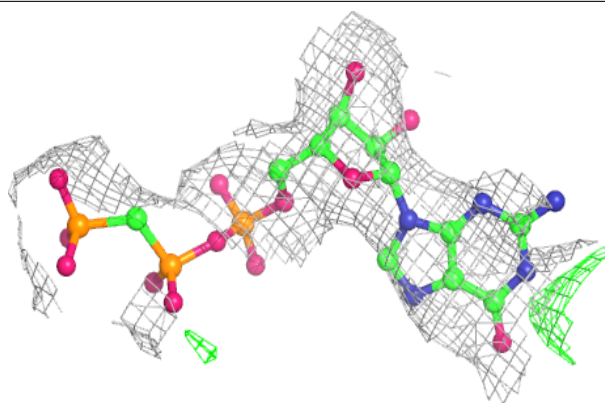
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	FLC	C	302	13/13	0.77	0.16	37,42,65,76	0
5	FLC	B	201	13/13	0.80	0.13	59,67,79,91	0
9	GOL	D	303	6/6	0.83	0.18	26,45,48,53	0
8	MG	H	302	1/1	0.87	0.10	67,67,67,67	0
7	GCP	H	301	32/32	0.89	0.10	50,70,94,106	0
8	MG	D	302	1/1	0.90	0.12	51,51,51,51	0
6	A1JH1	G	301	72/72	0.93	0.11	27,49,69,77	0
7	GCP	D	301	32/32	0.93	0.09	28,40,52,62	0
6	A1JH1	C	301	72/72	0.93	0.10	17,29,42,46	0

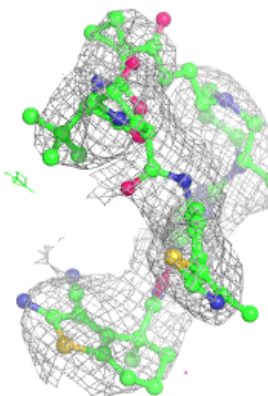
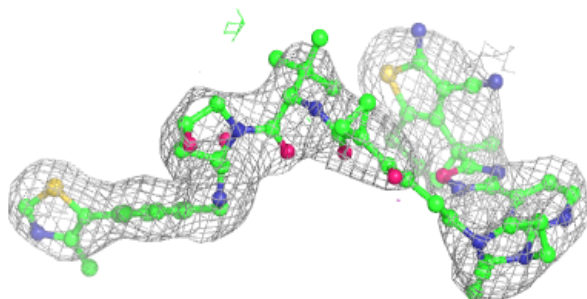
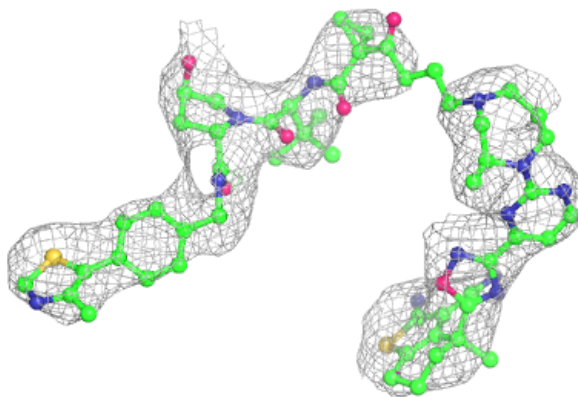
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GCP H 301:**

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

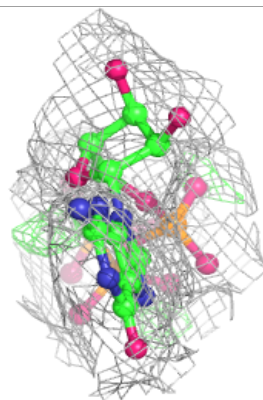
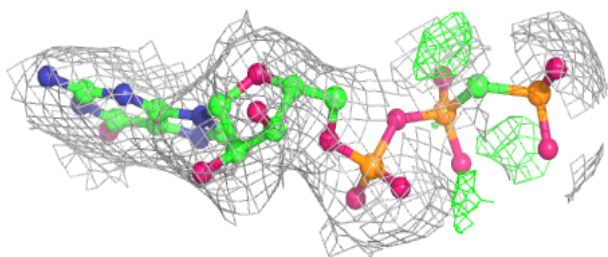
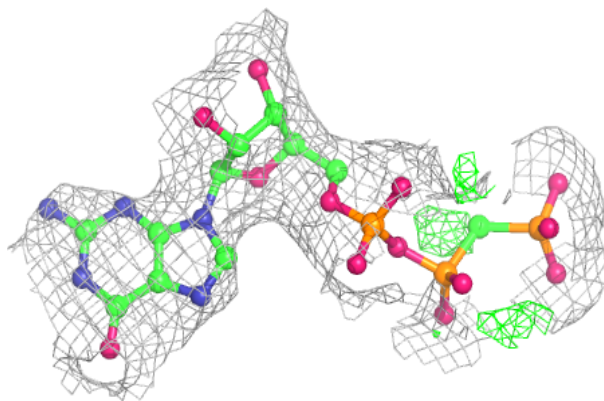
**Electron density around A1JH1 G 301:**

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

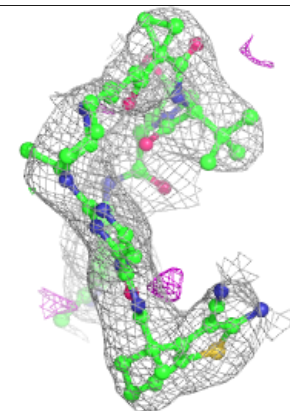
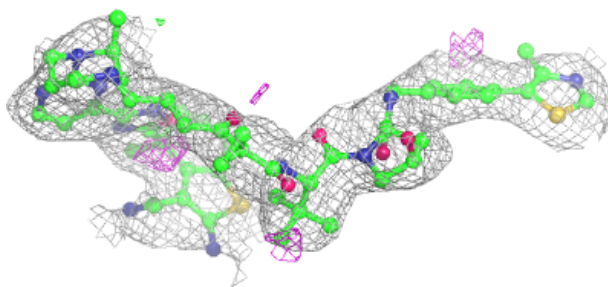
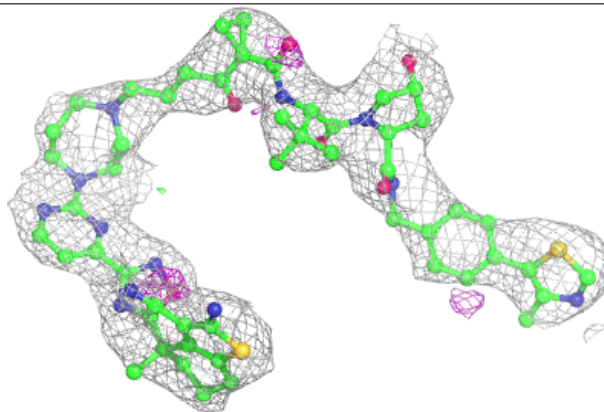


**Electron density around GCP D 301:**

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

**Electron density around A1JH1 C 301:**

$2mF_o-DF_c$  (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.