



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 02:38 PM EDT

PDB ID : 7T7M  
Title : Structure of human GLP SET-domain (EHMT1) in complex with covalent inhibitor (Compound 1)  
Authors : Park, K.-S.; Kumar, P.  
Deposited on : 2021-12-15  
Resolution : 2.85 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

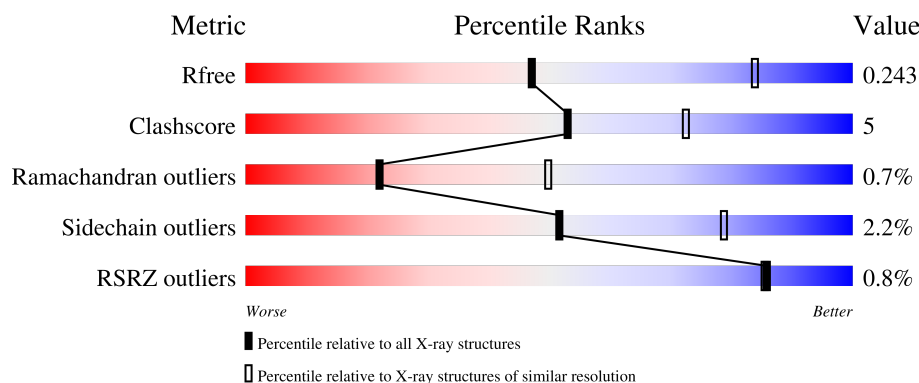
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	287	
1	B	287	
1	C	287	
1	D	287	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8611 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 Histone-lysine N-methyltransferase EHMT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2100	1310	379	386	25			
1	B	259	Total	C	N	O	S	0	0	0
			2094	1305	378	386	25			
1	C	260	Total	C	N	O	S	0	0	0
			2102	1310	379	388	25			
1	D	262	Total	C	N	O	S	0	0	0
			2109	1316	378	390	25			

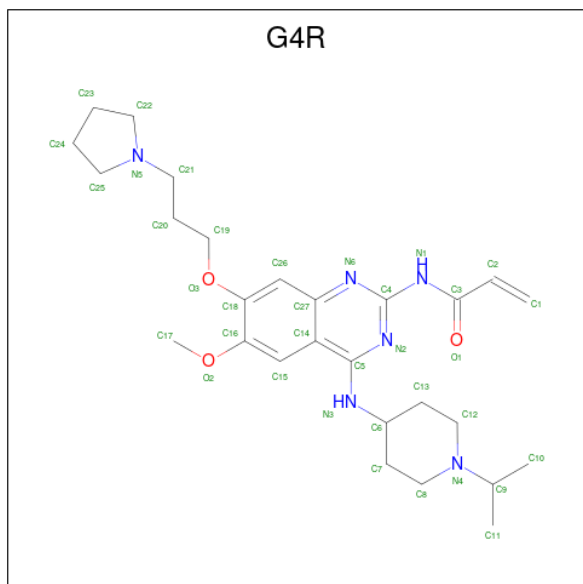
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	980	GLY	-	expression tag	UNP Q9H9B1
A	981	SER	-	expression tag	UNP Q9H9B1
B	980	GLY	-	expression tag	UNP Q9H9B1
B	981	SER	-	expression tag	UNP Q9H9B1
C	980	GLY	-	expression tag	UNP Q9H9B1
C	981	SER	-	expression tag	UNP Q9H9B1
D	980	GLY	-	expression tag	UNP Q9H9B1
D	981	SER	-	expression tag	UNP Q9H9B1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

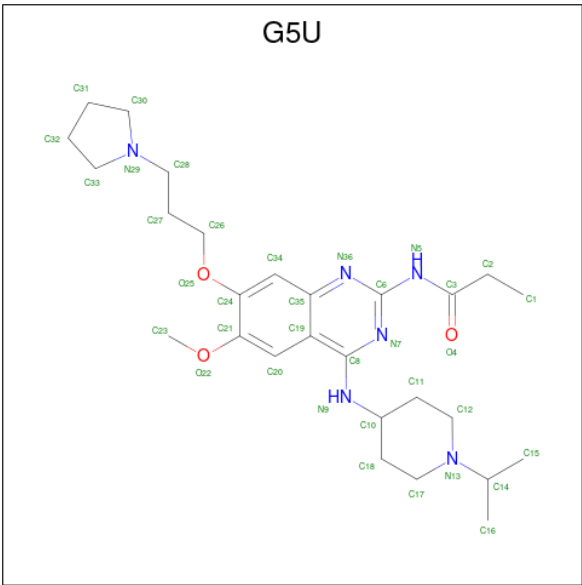
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	B	4	Total	Zn	0	0
			4	4		
2	C	4	Total	Zn	0	0
			4	4		
2	D	4	Total	Zn	0	0
			4	4		

- Molecule 3 is N-(6-methoxy-4-{[1-(propan-2-yl)piperidin-4-yl]amino}-7-[3-(pyrrolidin-1-yl)propoxy]quinazolin-2-yl)prop-2-enamide (three-letter code: G4R) (formula: C<sub>27</sub>H<sub>40</sub>N<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			36	27	6	3		
3	B	1	Total	C	N	O	0	0
			36	27	6	3		
3	C	1	Total	C	N	O	0	0
			36	27	6	3		

- Molecule 4 is N-(6-methoxy-4-{[1-(propan-2-yl)piperidin-4-yl]amino}-7-[3-(pyrrolidin-1-yl)propoxy]quinazolin-2-yl)propanamide (three-letter code: G5U) (formula: C<sub>27</sub>H<sub>42</sub>N<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			36	27	6	3		


- Molecule 5 is water.

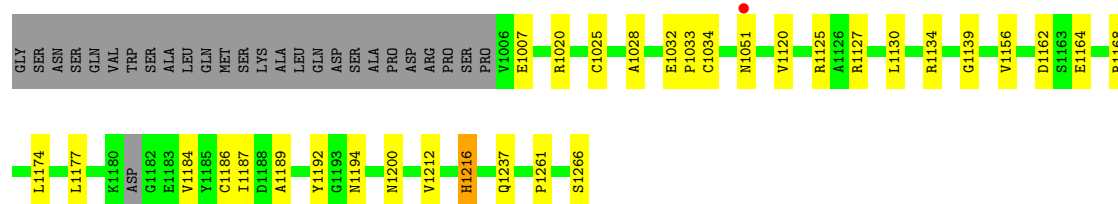
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	7	Total	O	0	0
			7	7		
5	C	14	Total	O	0	0
			14	14		
5	D	5	Total	O	0	0
			5	5		

### 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.

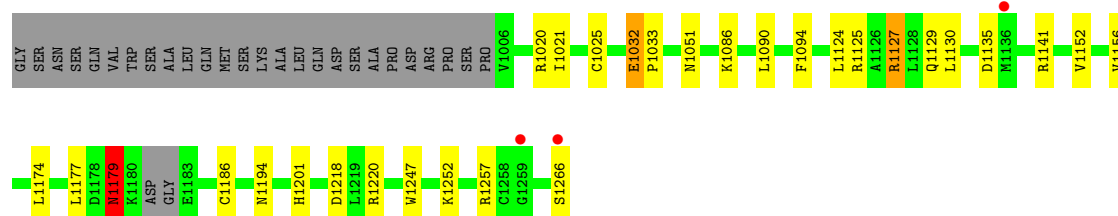
- Molecule 1: Histone-lysine N-methyltransferase EHMT1

Chain A: 




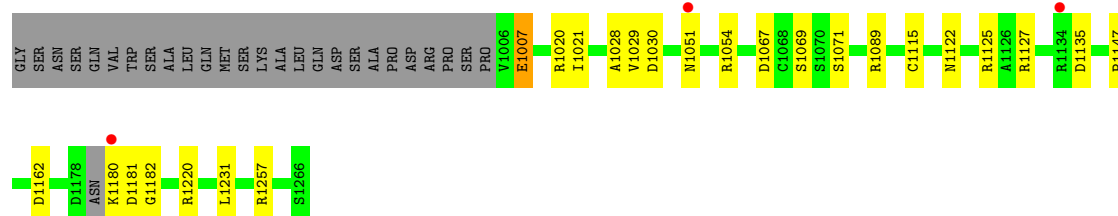
- Molecule 1: Histone-lysine N-methyltransferase EHMT1

Chain B: 



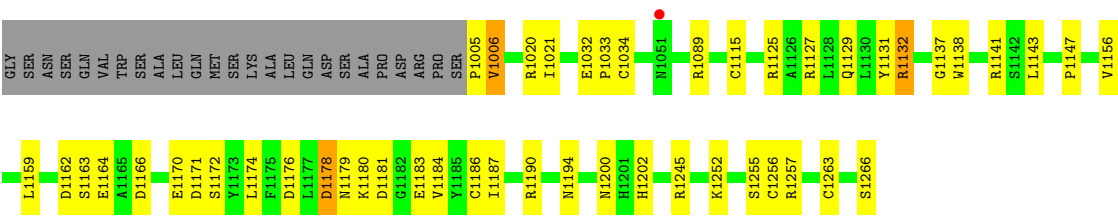
- Molecule 1: Histone-lysine N-methyltransferase EHMT1

Chain C: 



- Molecule 1: Histone-lysine N-methyltransferase EHMT1

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.49Å 128.73Å 132.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.69 – 2.85 77.47 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.69-2.85) 100.0 (77.47-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.199 , 0.244 0.200 , 0.243	Depositor DCC
$R_{free}$ test set	2008 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8611	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: G5U, G4R, ZN

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	0.52	0/2150	0.55	0/2905
1	B	0.34	0/2144	0.49	0/2899
1	C	0.33	0/2152	0.50	0/2908
1	D	0.38	0/2161	0.53	0/2923
All	All	0.40	0/8607	0.52	0/11635

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	2100	0	1992	27	0
1	B	2094	0	1980	19	0
1	C	2102	0	1992	18	0
1	D	2109	0	1994	31	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	0	3	0
3	C	36	0	0	0	0
4	D	36	0	0	4	0
5	A	20	0	0	0	0
5	B	7	0	0	0	0
5	C	14	0	0	0	0
5	D	5	0	0	0	0
All	All	8611	0	7958	89	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 5.

All (89) 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:1020:ARG:HH12	1:B:1266:SER:HB2	1.38	0.87
1:D:1245:ARG:O	1:D:1245:ARG:HG3	1.85	0.76
1:A:1020:ARG:CZ	1:A:1125:ARG:HH21	2.04	0.69
1:A:1127:ARG:HH22	1:B:1257:ARG:HB3	1.61	0.65
1:D:1263:CYS:SG	1:D:1266:SER:HB3	2.37	0.65
1:D:1020:ARG:HH12	1:D:1125:ARG:CZ	2.10	0.64
1:B:1179:ASN:C	1:B:1179:ASN:HD22	2.04	0.61
1:C:1051:ASN:HD21	1:C:1220:ARG:HH12	1.48	0.61
1:C:1029:VAL:HG23	1:C:1030:ASP:H	1.66	0.60
1:C:1020:ARG:NH2	1:C:1122:ASN:O	2.29	0.60
1:A:1020:ARG:NH1	1:B:1266:SER:HB2	2.12	0.59
1:B:1051:ASN:OD1	1:B:1220:ARG:NH2	2.36	0.59
1:D:1129:GLN:HB2	1:D:1143:LEU:HD21	1.85	0.58
1:A:1032:GLU:HG3	1:A:1033:PRO:HD2	1.85	0.56
1:D:1164:GLU:O	1:D:1164:GLU:HG3	2.05	0.56
1:D:1171:ASP:HB3	4:D:1305:G5U:C11	2.36	0.55
1:A:1261:PRO:O	1:C:1125:ARG:NH1	2.41	0.54
1:A:1134:ARG:HH11	1:A:1134:ARG:HG2	1.73	0.53
1:D:1021:ILE:HD13	1:D:1127:ARG:HA	1.89	0.53
1:D:1129:GLN:CB	1:D:1143:LEU:HD21	2.39	0.52
1:B:1174:LEU:HD13	3:B:1305:G4R:C1	2.41	0.51
1:A:1164:GLU:O	1:A:1168:ARG:HG3	2.10	0.51
1:C:1021:ILE:HD13	1:C:1127:ARG:HA	1.93	0.51
1:D:1256:CYS:SG	1:D:1257:ARG:N	2.84	0.50
1:D:1032:GLU:HG3	1:D:1033:PRO:HD2	1.93	0.50
1:C:1007:GLU:HA	1:C:1028:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1135:ASP:HB3	1:C:1257:ARG:HE	1.75	0.50
1:B:1124:LEU:HD12	1:B:1152:VAL:O	2.11	0.50
1:D:1020:ARG:NH1	1:D:1125:ARG:CZ	2.74	0.50
1:D:1131:TYR:CD1	1:D:1141:ARG:HD2	2.47	0.49
1:A:1162:ASP:HB3	1:A:1184:VAL:HG23	1.95	0.49
1:A:1200:ASN:HD22	1:A:1237:GLN:NE2	2.11	0.49
1:D:1159:LEU:HD22	1:D:1187:ILE:HG12	1.95	0.49
1:B:1201:HIS:CE1	1:B:1247:TRP:HE1	2.32	0.48
1:C:1051:ASN:ND2	1:C:1220:ARG:HH22	2.12	0.48
1:D:1162:ASP:HB3	1:D:1184:VAL:HG13	1.95	0.47
1:A:1051:ASN:N	1:A:1051:ASN:OD1	2.45	0.47
1:B:1129:GLN:OE1	1:B:1141:ARG:NH1	2.48	0.47
1:D:1131:TYR:CG	1:D:1141:ARG:HD2	2.50	0.46
1:D:1162:ASP:OD1	1:D:1184:VAL:CG1	2.63	0.46
1:D:1005:PRO:O	1:D:1006:VAL:HG12	2.15	0.46
1:A:1177:LEU:HD11	1:A:1187:ILE:HG13	1.96	0.46
1:B:1218:ASP:OD2	1:B:1220:ARG:NH1	2.49	0.46
1:B:1020:ARG:HH12	1:B:1125:ARG:HG2	1.80	0.46
1:A:1266:SER:OG	1:C:1020:ARG:HD3	2.16	0.45
1:D:1156:VAL:HG22	1:D:1194:ASN:CG	2.37	0.45
1:B:1252:LYS:HG2	1:D:1125:ARG:CZ	2.47	0.45
1:B:1021:ILE:HD13	1:B:1127:ARG:HA	1.98	0.45
1:D:1138:TRP:O	1:D:1200:ASN:ND2	2.49	0.45
1:A:1020:ARG:NH1	1:A:1125:ARG:HH21	2.15	0.45
1:B:1025:CYS:HA	1:B:1130:LEU:O	2.17	0.44
1:B:1032:GLU:HG3	1:B:1033:PRO:HD2	1.99	0.44
1:D:1089:ARG:HD3	1:D:1147:PRO:HB2	1.98	0.44
1:C:1051:ASN:ND2	1:C:1220:ARG:HH12	2.15	0.44
1:D:1166:ASP:O	4:D:1305:G5U:C16	2.65	0.44
1:A:1156:VAL:HG22	1:A:1194:ASN:CG	2.38	0.44
1:D:1176:ASP:OD2	4:D:1305:G5U:O4	2.36	0.44
1:A:1186:CYS:SG	3:A:1305:G4R:C2	3.06	0.43
1:C:1051:ASN:HD21	1:C:1220:ARG:NH1	2.12	0.43
1:C:1089:ARG:NH2	1:C:1147:PRO:HG2	2.34	0.43
1:D:1178:ASP:O	1:D:1184:VAL:HG23	2.18	0.43
1:A:1130:LEU:HD12	1:A:1139:GLY:O	2.19	0.43
1:C:1029:VAL:HG23	1:C:1030:ASP:N	2.31	0.43
1:D:1132:ARG:HH21	1:D:1137:GLY:HA2	1.82	0.43
1:A:1020:ARG:NH2	1:A:1125:ARG:HH21	2.17	0.43
1:C:1067:ASP:OD1	1:C:1069:SER:OG	2.33	0.42
1:D:1162:ASP:CG	1:D:1184:VAL:HG13	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:GLU:HA	1:A:1028:ALA:HB2	2.00	0.42
1:A:1216:HIS:ND1	1:A:1216:HIS:C	2.73	0.42
1:C:1180:LYS:O	1:C:1182:GLY:N	2.53	0.42
1:A:1200:ASN:HD22	1:A:1237:GLN:HE22	1.66	0.42
1:A:1025:CYS:HA	1:A:1130:LEU:O	2.20	0.41
1:A:1134:ARG:HG2	1:A:1134:ARG:NH1	2.35	0.41
1:B:1186:CYS:SG	3:B:1305:G4R:C2	3.08	0.41
1:A:1189:ALA:HA	1:A:1192:TYR:O	2.20	0.41
1:C:1021:ILE:H	1:C:1021:ILE:HG13	1.81	0.41
1:A:1186:CYS:SG	3:A:1305:G4R:C1	3.09	0.41
1:B:1090:LEU:HD13	1:B:1094:PHE:CD2	2.56	0.41
1:D:1174:LEU:HD12	4:D:1305:G5U:C6	2.51	0.41
1:C:1162:ASP:OD1	1:C:1162:ASP:N	2.53	0.41
1:B:1156:VAL:HG22	1:B:1194:ASN:CG	2.40	0.41
1:D:1170:GLU:HG3	1:D:1172:SER:H	1.86	0.41
1:D:1252:LYS:HE2	1:D:1252:LYS:N	2.35	0.41
1:A:1120:VAL:HG21	1:A:1212:VAL:HG21	2.02	0.40
1:A:1174:LEU:HB3	3:A:1305:G4R:C1	2.51	0.40
1:D:1020:ARG:HH11	1:D:1125:ARG:HG2	1.86	0.40
1:D:1266:SER:O	1:D:1266:SER:OG	2.29	0.40
1:B:1186:CYS:SG	3:B:1305:G4R:C1	3.10	0.40
1:C:1147:PRO:HA	1:C:1231:LEU:HD12	2.04	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	256/287 (89%)	237 (93%)	19 (7%)	0	100	100
1	B	255/287 (89%)	234 (92%)	19 (8%)	2 (1%)	19	46
1	C	256/287 (89%)	234 (91%)	20 (8%)	2 (1%)	19	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	260/287 (91%)	232 (89%)	25 (10%)	3 (1%)	13	35
All	All	1027/1148 (90%)	937 (91%)	83 (8%)	7 (1%)	22	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1179	ASN
1	C	1007	GLU
1	D	1006	VAL
1	C	1181	ASP
1	B	1135	ASP
1	D	1181	ASP
1	D	1178	ASP

### 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	234/258 (91%)	232 (99%)	2 (1%)	78	92
1	B	234/258 (91%)	229 (98%)	5 (2%)	53	79
1	C	235/258 (91%)	232 (99%)	3 (1%)	69	88
1	D	235/258 (91%)	224 (95%)	11 (5%)	26	56
All	All	938/1032 (91%)	917 (98%)	21 (2%)	52	79

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

Mol	Chain	Res	Type
1	A	1034	CYS
1	A	1216	HIS
1	B	1032	GLU
1	B	1086	LYS
1	B	1127	ARG
1	B	1177	LEU
1	B	1179	ASN

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Mol	Chain	Res	Type
1	C	1054	ARG
1	C	1071	SER
1	C	1115	CYS
1	D	1034	CYS
1	D	1115	CYS
1	D	1132	ARG
1	D	1163	SER
1	D	1179	ASN
1	D	1180	LYS
1	D	1183	GLU
1	D	1186	CYS
1	D	1190	ARG
1	D	1202	HIS
1	D	1255	SER

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

Mol	Chain	Res	Type
1	A	1129	GLN
1	A	1200	ASN
1	B	1179	ASN
1	C	1051	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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$
3	G4R	B	1305	-	38,39,39	4.48	15 (39%)	52,53,53	2.71	21 (40%)
4	G5U	D	1305	1	38,39,39	4.40	14 (36%)	53,53,53	1.86	12 (22%)
3	G4R	A	1305	-	38,39,39	4.38	14 (36%)	52,53,53	2.13	17 (32%)
3	G4R	C	1305	-	38,39,39	4.42	14 (36%)	52,53,53	2.51	21 (40%)

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
3	G4R	B	1305	-	-	12/23/40/40	0/4/4/4
4	G5U	D	1305	1	-	15/23/40/40	0/4/4/4
3	G4R	A	1305	-	-	9/23/40/40	0/4/4/4
3	G4R	C	1305	-	-	9/23/40/40	0/4/4/4

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1305	G4R	C21-N5	-17.63	1.06	1.47
3	A	1305	G4R	C21-N5	-17.31	1.07	1.47
3	C	1305	G4R	C21-N5	-16.98	1.08	1.47
4	D	1305	G5U	C14-N13	-13.52	1.21	1.48
3	A	1305	G4R	C9-N4	-13.19	1.21	1.48
3	C	1305	G4R	C9-N4	-12.98	1.22	1.48
3	B	1305	G4R	C9-N4	-12.90	1.22	1.48
4	D	1305	G5U	C28-N29	-12.82	1.17	1.47
4	D	1305	G5U	C33-N29	-11.49	1.26	1.47
3	C	1305	G4R	C4-N1	8.23	1.49	1.38
3	B	1305	G4R	C4-N1	8.00	1.49	1.38
4	D	1305	G5U	C6-N5	7.82	1.49	1.38
3	A	1305	G4R	C4-N1	6.82	1.47	1.38
4	D	1305	G5U	C30-N29	6.20	1.59	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1305	G4R	C23-C22	-6.02	1.30	1.51
3	C	1305	G4R	C23-C22	-5.97	1.30	1.51
3	A	1305	G4R	C23-C22	-5.89	1.31	1.51
3	B	1305	G4R	C24-C25	-5.83	1.31	1.51
3	C	1305	G4R	C24-C25	-5.77	1.31	1.51
3	A	1305	G4R	C24-C25	-5.68	1.32	1.51
4	D	1305	G5U	C3-N5	5.63	1.48	1.35
4	D	1305	G5U	C31-C30	-5.50	1.32	1.51
3	A	1305	G4R	O1-C3	-5.19	1.14	1.24
3	B	1305	G4R	O1-C3	-5.16	1.14	1.24
3	B	1305	G4R	C3-N1	5.10	1.44	1.35
3	C	1305	G4R	O1-C3	-4.99	1.14	1.24
3	C	1305	G4R	C15-C16	4.85	1.45	1.36
3	C	1305	G4R	C3-N1	4.75	1.43	1.35
3	A	1305	G4R	C15-C16	4.58	1.44	1.36
3	B	1305	G4R	C15-C16	4.48	1.44	1.36
4	D	1305	G5U	C10-N9	4.37	1.56	1.46
3	A	1305	G4R	C3-N1	4.28	1.42	1.35
3	B	1305	G4R	C26-C27	3.82	1.47	1.41
3	A	1305	G4R	C26-C27	3.70	1.47	1.41
3	C	1305	G4R	C5-N2	3.59	1.37	1.32
3	B	1305	G4R	C6-N3	3.59	1.54	1.46
3	A	1305	G4R	C6-N3	3.57	1.54	1.46
3	C	1305	G4R	C6-N3	3.48	1.54	1.46
3	C	1305	G4R	C26-C27	3.29	1.47	1.41
4	D	1305	G5U	C20-C21	3.23	1.42	1.36
4	D	1305	G5U	C11-C10	-3.14	1.44	1.52
4	D	1305	G5U	O25-C24	3.10	1.43	1.37
4	D	1305	G5U	C8-N7	3.06	1.37	1.32
4	D	1305	G5U	C19-C35	-2.60	1.38	1.42
3	B	1305	G4R	C7-C6	-2.60	1.45	1.52
3	B	1305	G4R	C5-N2	2.51	1.36	1.32
3	C	1305	G4R	O3-C18	2.48	1.42	1.37
3	B	1305	G4R	O3-C18	2.45	1.42	1.37
4	D	1305	G5U	O4-C3	-2.44	1.18	1.23
3	B	1305	G4R	C13-C6	-2.42	1.46	1.52
3	A	1305	G4R	O3-C18	2.41	1.42	1.37
3	A	1305	G4R	C5-N2	2.41	1.36	1.32
3	B	1305	G4R	C26-C18	2.25	1.40	1.36
3	C	1305	G4R	C22-N5	2.12	1.51	1.47
3	C	1305	G4R	C7-C6	-2.10	1.47	1.52
3	A	1305	G4R	C7-C6	-2.06	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1305	G4R	C26-C18	2.04	1.40	1.36

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1305	G4R	C2-C3-N1	9.15	119.87	113.84
3	B	1305	G4R	C2-C3-N1	8.72	119.58	113.84
3	B	1305	G4R	C8-N4-C12	6.04	120.11	109.08
3	B	1305	G4R	C5-C14-C27	5.99	119.65	115.88
3	A	1305	G4R	C2-C3-N1	5.80	117.66	113.84
4	D	1305	G5U	C6-N5-C3	-5.73	121.60	130.28
3	B	1305	G4R	C15-C14-C5	-5.65	119.78	124.88
3	A	1305	G4R	C5-C14-C27	5.60	119.41	115.88
3	C	1305	G4R	O2-C16-C15	-4.96	118.82	125.24
4	D	1305	G5U	O22-C21-C20	-4.77	119.07	125.24
3	C	1305	G4R	C5-C14-C27	4.74	118.86	115.88
3	B	1305	G4R	C14-C27-N6	-4.71	117.82	122.81
3	B	1305	G4R	O2-C16-C15	-4.55	119.36	125.24
3	A	1305	G4R	O2-C16-C15	-4.48	119.45	125.24
3	A	1305	G4R	C15-C14-C5	-4.42	120.89	124.88
3	A	1305	G4R	C14-C27-N6	-4.11	118.45	122.81
3	C	1305	G4R	C4-N6-C27	4.09	122.27	115.60
3	C	1305	G4R	C14-C27-N6	-3.98	118.58	122.81
3	B	1305	G4R	C13-C6-N3	3.85	116.59	110.60
3	C	1305	G4R	O3-C18-C26	-3.80	118.76	125.19
3	C	1305	G4R	C15-C14-C5	-3.77	121.48	124.88
3	C	1305	G4R	O2-C16-C18	3.70	120.56	115.41
3	B	1305	G4R	C13-C12-N4	3.66	117.05	111.43
3	B	1305	G4R	O2-C16-C18	3.66	120.51	115.41
4	D	1305	G5U	O25-C24-C34	-3.62	119.07	125.19
3	B	1305	G4R	C4-N6-C27	3.59	121.45	115.60
3	C	1305	G4R	N6-C4-N2	-3.55	120.62	126.23
3	A	1305	G4R	O2-C16-C18	3.55	120.35	115.41
3	C	1305	G4R	C14-C5-N3	-3.35	117.47	120.63
3	C	1305	G4R	O1-C3-N1	-3.32	119.25	123.05
4	D	1305	G5U	C11-C10-N9	3.30	115.75	110.60
4	D	1305	G5U	N5-C6-N7	3.18	125.76	116.46
3	A	1305	G4R	C4-N6-C27	3.15	120.74	115.60
3	B	1305	G4R	N6-C4-N2	-3.12	121.29	126.23
4	D	1305	G5U	O25-C24-C21	3.10	122.13	115.73
3	B	1305	G4R	C14-C5-N3	-3.01	117.79	120.63
4	D	1305	G5U	O22-C21-C24	2.96	119.53	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1305	G5U	C8-C19-C35	2.90	117.71	115.88
3	B	1305	G4R	C7-C8-N4	2.90	115.87	111.43
3	C	1305	G4R	O3-C18-C16	2.86	121.65	115.73
3	A	1305	G4R	O1-C3-N1	-2.85	119.78	123.05
3	A	1305	G4R	C7-C6-N3	-2.78	106.26	110.60
3	A	1305	G4R	C14-C5-N2	-2.74	117.49	121.98
3	C	1305	G4R	C7-C6-N3	-2.74	106.33	110.60
4	D	1305	G5U	C18-C10-C11	2.72	115.53	110.82
3	C	1305	G4R	N1-C4-N2	2.65	124.21	116.46
3	C	1305	G4R	C17-O2-C16	-2.63	113.56	117.53
3	B	1305	G4R	O1-C3-N1	-2.61	120.06	123.05
4	D	1305	G5U	C23-O22-C21	-2.58	113.64	117.53
3	B	1305	G4R	C17-O2-C16	-2.52	113.72	117.53
3	C	1305	G4R	N3-C5-N2	2.51	124.23	118.90
3	A	1305	G4R	C24-C25-N5	2.49	106.83	103.92
4	D	1305	G5U	C6-N36-C35	2.47	119.63	115.60
3	B	1305	G4R	N3-C5-N2	2.46	124.12	118.90
3	A	1305	G4R	N6-C4-N2	-2.45	122.36	126.23
3	B	1305	G4R	C14-C5-N2	-2.37	118.09	121.98
3	B	1305	G4R	C4-N2-C5	2.32	121.70	116.39
3	A	1305	G4R	C4-N2-C5	2.26	121.56	116.39
3	C	1305	G4R	C14-C5-N2	-2.24	118.30	121.98
4	D	1305	G5U	C34-C35-C19	2.22	122.20	119.65
3	B	1305	G4R	C24-C25-N5	2.18	106.47	103.92
3	C	1305	G4R	C4-N2-C5	2.17	121.36	116.39
3	A	1305	G4R	C13-C6-N3	-2.17	107.22	110.60
3	A	1305	G4R	O3-C18-C26	-2.16	121.54	125.19
3	C	1305	G4R	C24-C25-N5	2.14	106.42	103.92
3	B	1305	G4R	C5-N3-C6	2.12	128.20	124.16
3	C	1305	G4R	C1-C2-C3	-2.06	119.92	122.27
3	C	1305	G4R	C13-C6-N3	-2.05	107.40	110.60
3	B	1305	G4R	C26-C27-N6	2.03	121.81	118.72
3	A	1305	G4R	C17-O2-C16	-2.02	114.48	117.53
3	A	1305	G4R	C8-C7-C6	2.00	114.02	110.50

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1305	G4R	C1-C2-C3-N1
3	A	1305	G4R	C1-C2-C3-O1
3	A	1305	G4R	C2-C3-N1-C4

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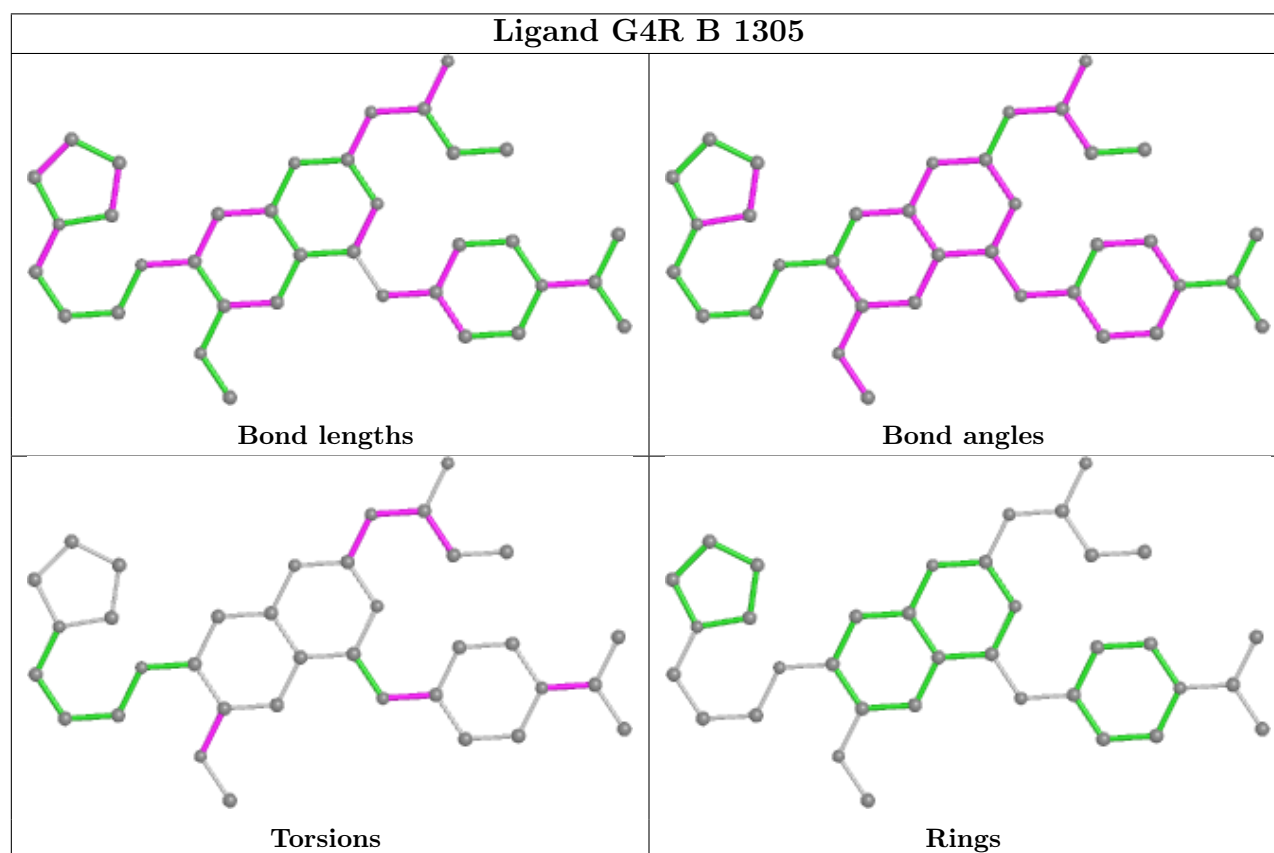
Mol	Chain	Res	Type	Atoms
3	A	1305	G4R	O1-C3-N1-C4
3	A	1305	G4R	N2-C4-N1-C3
3	A	1305	G4R	N6-C4-N1-C3
3	B	1305	G4R	C1-C2-C3-N1
3	B	1305	G4R	C1-C2-C3-O1
3	B	1305	G4R	C2-C3-N1-C4
3	B	1305	G4R	O1-C3-N1-C4
3	B	1305	G4R	N2-C4-N1-C3
3	B	1305	G4R	N6-C4-N1-C3
3	B	1305	G4R	C13-C6-N3-C5
3	B	1305	G4R	C10-C9-N4-C12
3	B	1305	G4R	C11-C9-N4-C12
3	C	1305	G4R	C1-C2-C3-N1
3	C	1305	G4R	C1-C2-C3-O1
3	C	1305	G4R	C2-C3-N1-C4
3	C	1305	G4R	O1-C3-N1-C4
4	D	1305	G5U	C11-C10-N9-C8
4	D	1305	G5U	C27-C28-N29-C30
4	D	1305	G5U	C27-C28-N29-C33
4	D	1305	G5U	N36-C6-N5-C3
4	D	1305	G5U	N7-C6-N5-C3
4	D	1305	G5U	C19-C8-N9-C10
4	D	1305	G5U	N7-C8-N9-C10
3	A	1305	G4R	O3-C19-C20-C21
3	C	1305	G4R	C19-C20-C21-N5
3	C	1305	G4R	C18-C16-O2-C17
3	A	1305	G4R	C18-C16-O2-C17
3	C	1305	G4R	C15-C16-O2-C17
4	D	1305	G5U	O25-C26-C27-C28
4	D	1305	G5U	C24-C21-O22-C23
3	A	1305	G4R	C15-C16-O2-C17
3	C	1305	G4R	O3-C19-C20-C21
4	D	1305	G5U	C1-C2-C3-O4
4	D	1305	G5U	C1-C2-C3-N5
4	D	1305	G5U	C20-C21-O22-C23
3	C	1305	G4R	C20-C19-O3-C18
3	B	1305	G4R	C18-C16-O2-C17
3	B	1305	G4R	C10-C9-N4-C8
4	D	1305	G5U	C15-C14-N13-C17
4	D	1305	G5U	C16-C14-N13-C12
3	B	1305	G4R	C15-C16-O2-C17
4	D	1305	G5U	C21-C24-O25-C26

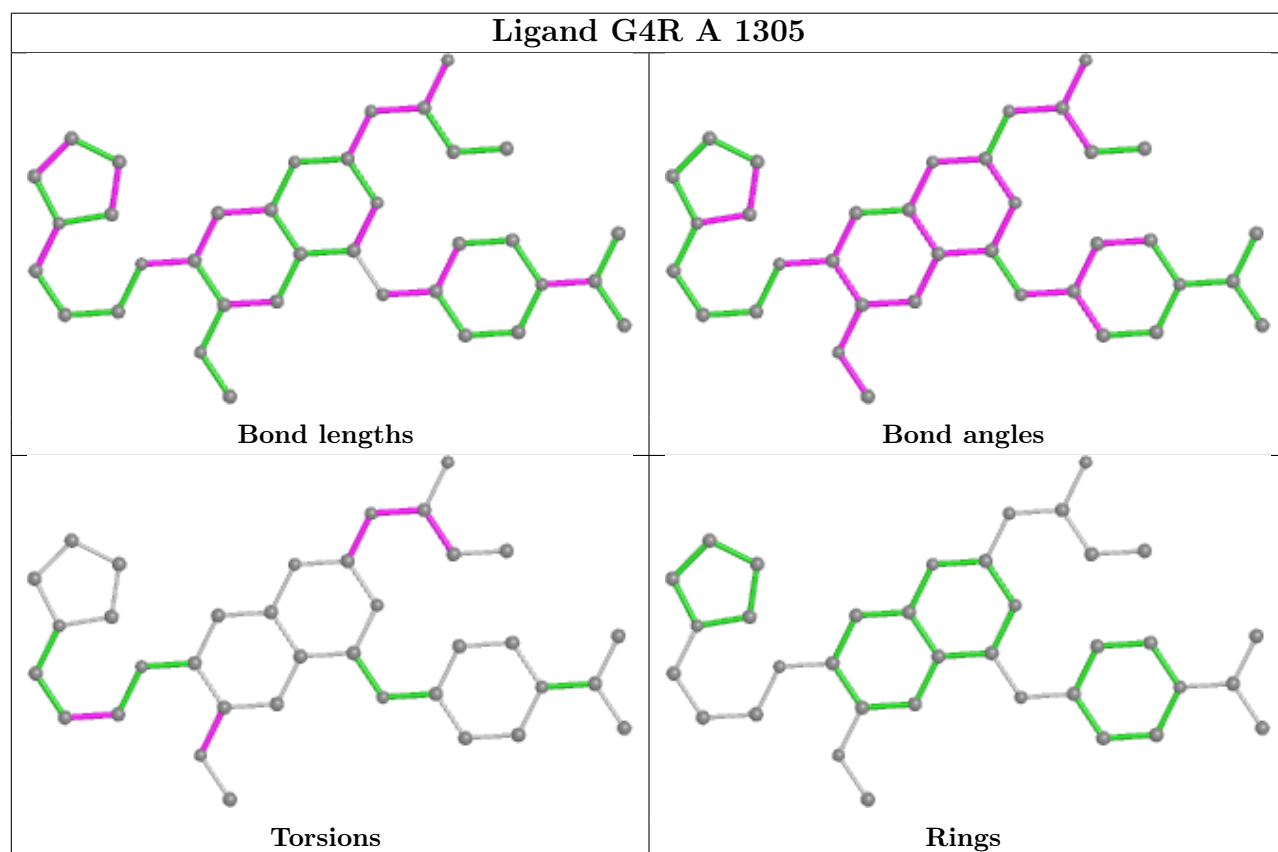
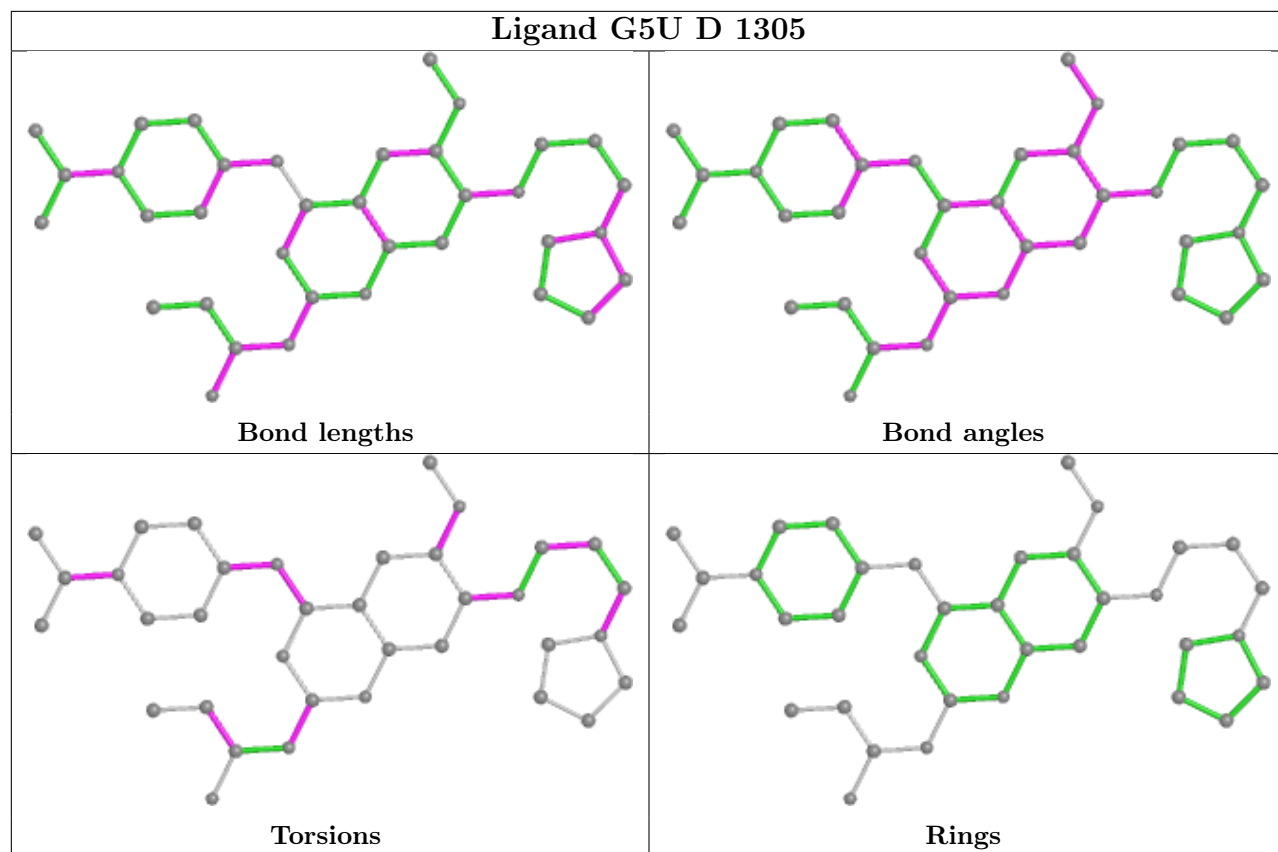
There are no ring outliers.

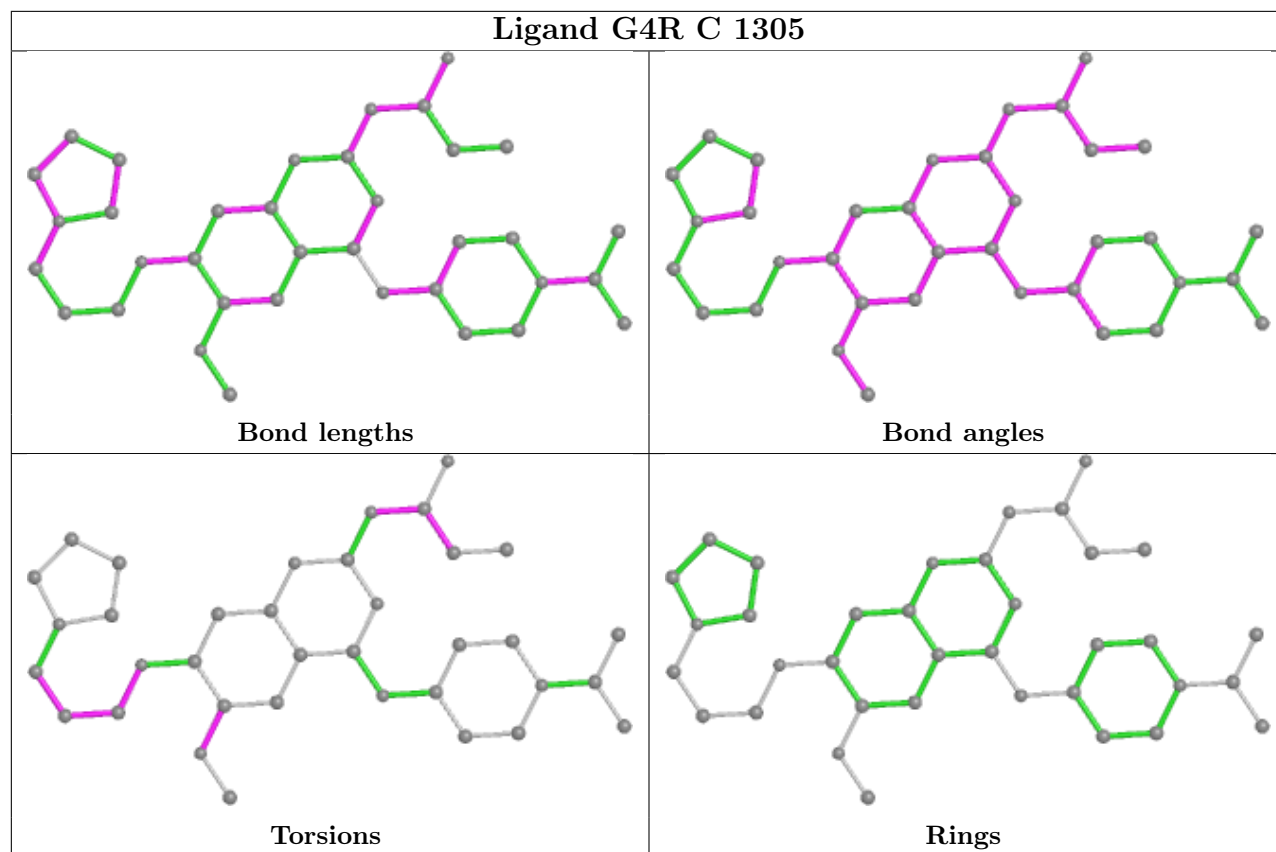
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1305	G4R	3	0
4	D	1305	G5U	4	0
3	A	1305	G4R	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.







## 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	260/287 (90%)	-0.13	1 (0%) 92 92	26, 40, 70, 99	0
1	B	259/287 (90%)	0.11	3 (1%) 79 78	24, 49, 84, 108	0
1	C	260/287 (90%)	0.03	3 (1%) 79 78	25, 43, 87, 111	0
1	D	262/287 (91%)	-0.11	1 (0%) 92 92	26, 51, 95, 105	0
All	All	1041/1148 (90%)	-0.02	8 (0%) 86 85	24, 45, 88, 111	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1266	SER	5.1
1	B	1136	MET	3.4
1	A	1051	ASN	3.0
1	B	1259	GLY	2.9
1	C	1134	ARG	2.6
1	C	1180	LYS	2.4
1	C	1051	ASN	2.2
1	D	1051	ASN	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

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.

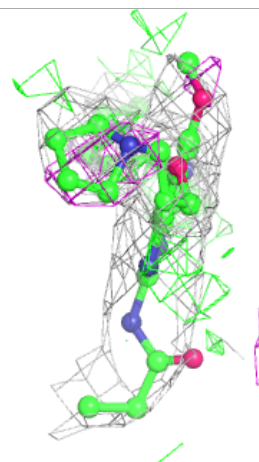
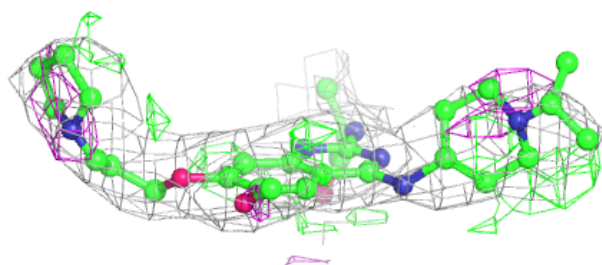
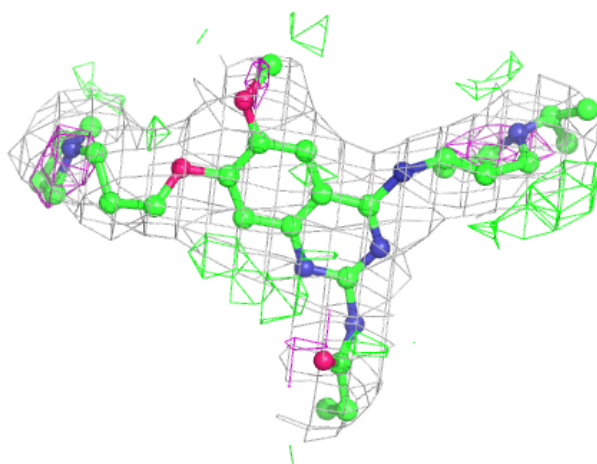
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	G5U	D	1305	36/36	0.82	0.26	33,54,66,68	3
3	G4R	B	1305	36/36	0.90	0.25	42,72,89,94	0
3	G4R	C	1305	36/36	0.91	0.22	48,64,84,88	0
2	ZN	C	1304	1/1	0.91	0.16	74,74,74,74	0
3	G4R	A	1305	36/36	0.92	0.20	35,56,78,80	0
2	ZN	D	1304	1/1	0.95	0.17	77,77,77,77	0
2	ZN	B	1304	1/1	0.96	0.16	66,66,66,66	0
2	ZN	A	1304	1/1	0.99	0.16	42,42,42,42	0
2	ZN	D	1301	1/1	0.99	0.17	33,33,33,33	0
2	ZN	D	1303	1/1	0.99	0.15	41,41,41,41	0
2	ZN	B	1302	1/1	0.99	0.19	30,30,30,30	0
2	ZN	A	1302	1/1	0.99	0.17	33,33,33,33	0
2	ZN	C	1301	1/1	0.99	0.15	38,38,38,38	0
2	ZN	C	1302	1/1	0.99	0.15	33,33,33,33	0
2	ZN	C	1303	1/1	0.99	0.15	37,37,37,37	0
2	ZN	B	1303	1/1	1.00	0.16	34,34,34,34	0
2	ZN	A	1301	1/1	1.00	0.16	37,37,37,37	0
2	ZN	B	1301	1/1	1.00	0.17	28,28,28,28	0
2	ZN	D	1302	1/1	1.00	0.16	35,35,35,35	0
2	ZN	A	1303	1/1	1.00	0.16	38,38,38,38	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.



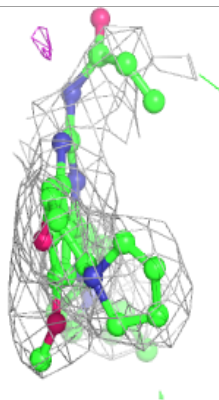
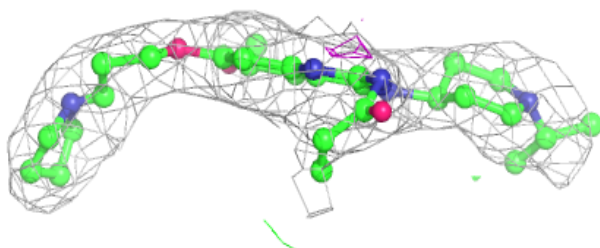
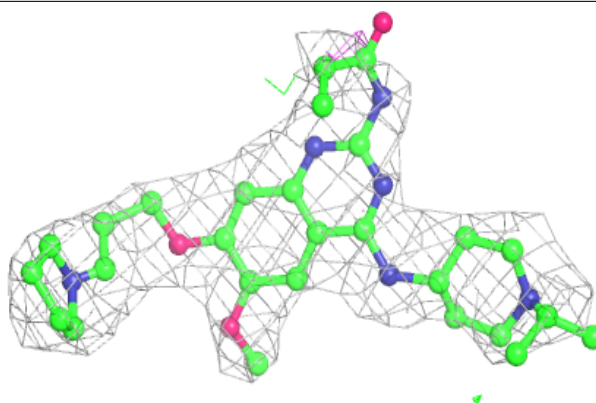
**Electron density around G5U D 1305:**

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

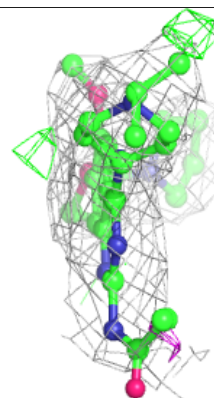
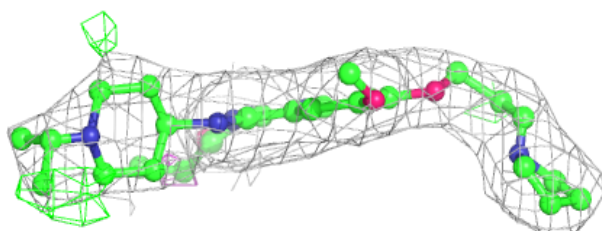
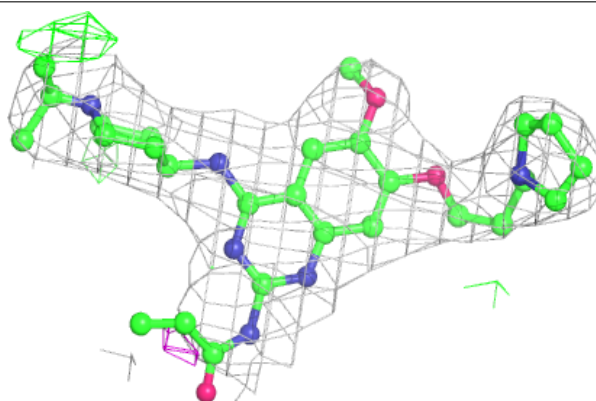


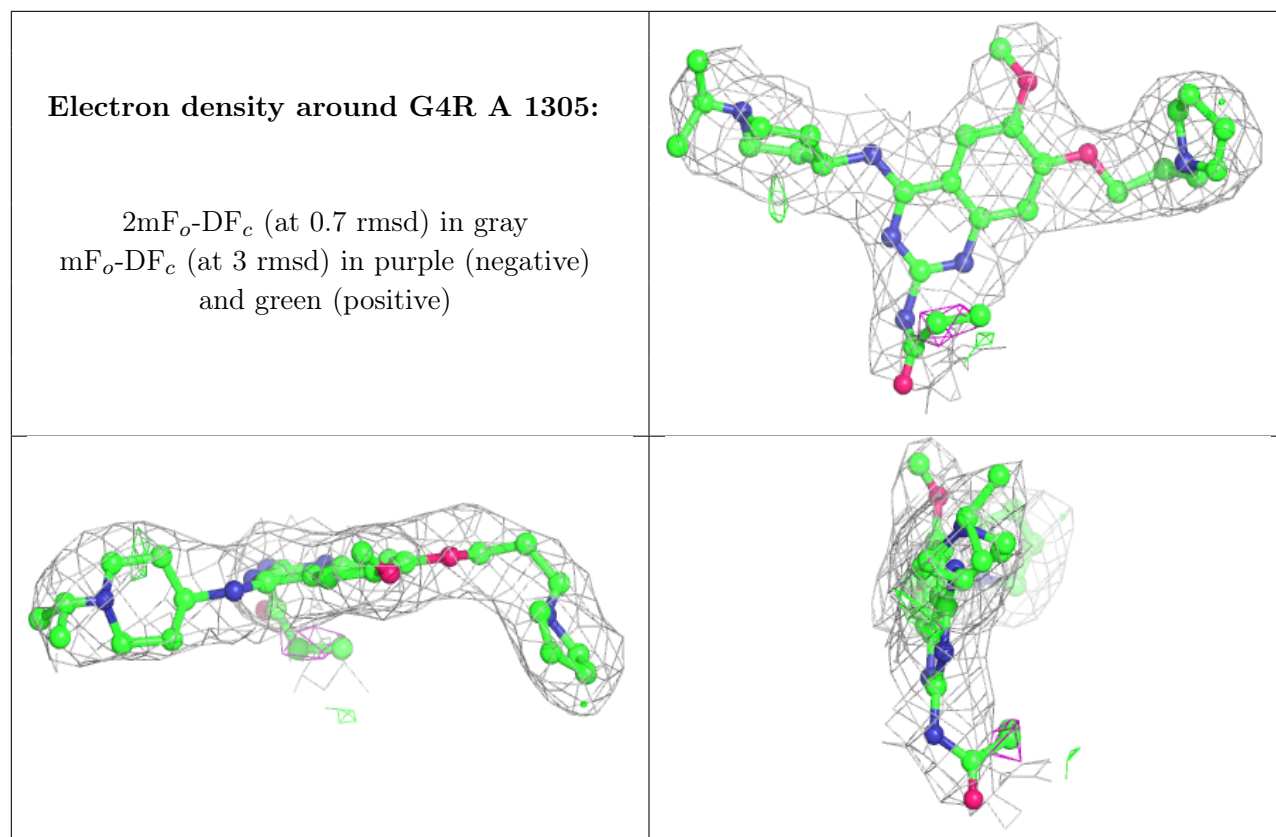
**Electron density around G4R B 1305:**

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

**Electron density around G4R C 1305:**

$2mF_o-DF_c$  (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.