



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2025 – 12:12 pm GMT

PDB ID : 8P11  
Title : X-ray structure of acetylcholine-binding protein (AChBP) in complex with FL003044.  
Authors : Cederfelt, D.; Boronat, P.; Dobritsch, D.; Hennig, S.; Fitzgerald, E.A.; de Esch, I.J.P.; Danielson, U.H.  
Deposited on : 2023-05-11  
Resolution : 1.90 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:

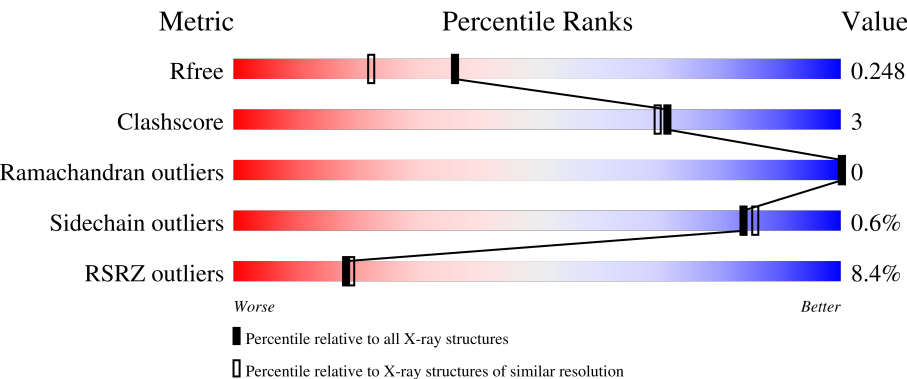
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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 <sub>free</sub>	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	237	<div><div>12%</div><div><div></div><div>81%</div><div>.</div><div>15%</div></div></div>
1	B	237	<div><div>14%</div><div><div></div><div>80%</div><div>5%</div><div>15%</div></div></div>
1	C	237	<div><div>10%</div><div><div></div><div>79%</div><div>5%</div><div>15%</div></div></div>
1	D	237	<div><div>5%</div><div><div></div><div>78%</div><div>8%</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	E	237	<div><div></div><div>4%</div><div>80%</div><div>16%</div></div>
1	F	237	<div><div></div><div>7%</div><div>81%</div><div>15%</div></div>
1	G	237	<div><div></div><div>3%</div><div>78%</div><div>13%</div></div>
1	H	237	<div><div></div><div>4%</div><div>81%</div><div>14%</div></div>
1	I	237	<div><div></div><div>6%</div><div>80%</div><div>15%</div></div>
1	J	237	<div><div></div><div>6%</div><div>80%</div><div>16%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16962 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1612	1010	276	321	5			
1	B	201	Total	C	N	O	S	0	0	0
			1609	1009	275	320	5			
1	C	201	Total	C	N	O	S	0	1	0
			1610	1010	275	320	5			
1	D	202	Total	C	N	O	S	0	0	0
			1612	1010	276	321	5			
1	E	199	Total	C	N	O	S	0	2	0
			1604	1009	273	317	5			
1	F	202	Total	C	N	O	S	0	0	0
			1612	1010	276	321	5			
1	G	206	Total	C	N	O	S	0	4	0
			1669	1046	287	331	5			
1	H	205	Total	C	N	O	S	0	3	0
			1655	1035	284	331	5			
1	I	202	Total	C	N	O	S	0	5	0
			1638	1031	279	323	5			
1	J	200	Total	C	N	O	S	0	3	0
			1619	1018	277	319	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLY	-	expression tag	UNP P58154
A	231	SER	-	expression tag	UNP P58154
A	232	HIS	-	expression tag	UNP P58154
A	233	HIS	-	expression tag	UNP P58154
A	234	HIS	-	expression tag	UNP P58154
A	235	HIS	-	expression tag	UNP P58154
A	236	HIS	-	expression tag	UNP P58154
A	237	HIS	-	expression tag	UNP P58154
B	230	GLY	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	SER	-	expression tag	UNP P58154
B	232	HIS	-	expression tag	UNP P58154
B	233	HIS	-	expression tag	UNP P58154
B	234	HIS	-	expression tag	UNP P58154
B	235	HIS	-	expression tag	UNP P58154
B	236	HIS	-	expression tag	UNP P58154
B	237	HIS	-	expression tag	UNP P58154
C	230	GLY	-	expression tag	UNP P58154
C	231	SER	-	expression tag	UNP P58154
C	232	HIS	-	expression tag	UNP P58154
C	233	HIS	-	expression tag	UNP P58154
C	234	HIS	-	expression tag	UNP P58154
C	235	HIS	-	expression tag	UNP P58154
C	236	HIS	-	expression tag	UNP P58154
C	237	HIS	-	expression tag	UNP P58154
D	230	GLY	-	expression tag	UNP P58154
D	231	SER	-	expression tag	UNP P58154
D	232	HIS	-	expression tag	UNP P58154
D	233	HIS	-	expression tag	UNP P58154
D	234	HIS	-	expression tag	UNP P58154
D	235	HIS	-	expression tag	UNP P58154
D	236	HIS	-	expression tag	UNP P58154
D	237	HIS	-	expression tag	UNP P58154
E	230	GLY	-	expression tag	UNP P58154
E	231	SER	-	expression tag	UNP P58154
E	232	HIS	-	expression tag	UNP P58154
E	233	HIS	-	expression tag	UNP P58154
E	234	HIS	-	expression tag	UNP P58154
E	235	HIS	-	expression tag	UNP P58154
E	236	HIS	-	expression tag	UNP P58154
E	237	HIS	-	expression tag	UNP P58154
F	230	GLY	-	expression tag	UNP P58154
F	231	SER	-	expression tag	UNP P58154
F	232	HIS	-	expression tag	UNP P58154
F	233	HIS	-	expression tag	UNP P58154
F	234	HIS	-	expression tag	UNP P58154
F	235	HIS	-	expression tag	UNP P58154
F	236	HIS	-	expression tag	UNP P58154
F	237	HIS	-	expression tag	UNP P58154
G	230	GLY	-	expression tag	UNP P58154
G	231	SER	-	expression tag	UNP P58154
G	232	HIS	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
G	233	HIS	-	expression tag	UNP P58154
G	234	HIS	-	expression tag	UNP P58154
G	235	HIS	-	expression tag	UNP P58154
G	236	HIS	-	expression tag	UNP P58154
G	237	HIS	-	expression tag	UNP P58154
H	230	GLY	-	expression tag	UNP P58154
H	231	SER	-	expression tag	UNP P58154
H	232	HIS	-	expression tag	UNP P58154
H	233	HIS	-	expression tag	UNP P58154
H	234	HIS	-	expression tag	UNP P58154
H	235	HIS	-	expression tag	UNP P58154
H	236	HIS	-	expression tag	UNP P58154
H	237	HIS	-	expression tag	UNP P58154
I	230	GLY	-	expression tag	UNP P58154
I	231	SER	-	expression tag	UNP P58154
I	232	HIS	-	expression tag	UNP P58154
I	233	HIS	-	expression tag	UNP P58154
I	234	HIS	-	expression tag	UNP P58154
I	235	HIS	-	expression tag	UNP P58154
I	236	HIS	-	expression tag	UNP P58154
I	237	HIS	-	expression tag	UNP P58154
J	230	GLY	-	expression tag	UNP P58154
J	231	SER	-	expression tag	UNP P58154
J	232	HIS	-	expression tag	UNP P58154
J	233	HIS	-	expression tag	UNP P58154
J	234	HIS	-	expression tag	UNP P58154
J	235	HIS	-	expression tag	UNP P58154
J	236	HIS	-	expression tag	UNP P58154
J	237	HIS	-	expression tag	UNP P58154

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

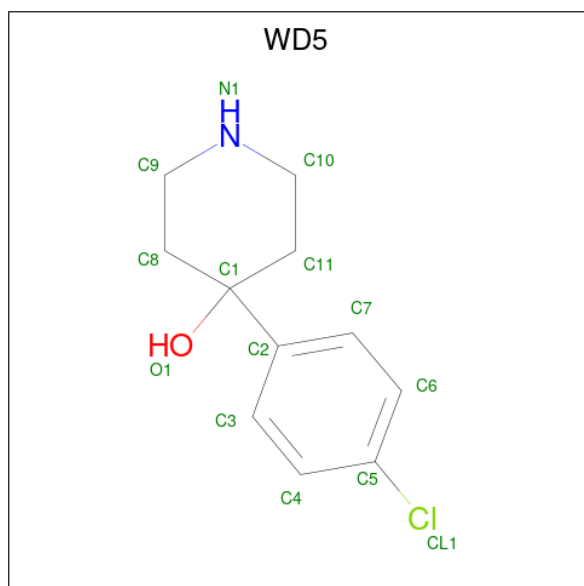
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	Cl	0	0
			1	1		
2	G	1	Total	Cl	0	0
			1	1		
2	H	1	Total	Cl	0	0
			1	1		
2	I	1	Total	Cl	0	0
			1	1		
2	J	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 4-(4-chlorophenyl)piperidin-4-ol (three-letter code: WD5) (formula:  $C_{11}H_{14}ClNO$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
3	F	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
3	G	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
3	H	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	21	Total	O	0	0
			21	21		
5	C	37	Total	O	0	0
			37	37		
5	D	76	Total	O	0	0
			76	76		
5	E	69	Total	O	0	1
			70	70		
5	F	56	Total	O	0	0
			56	56		
5	G	92	Total	O	0	0
			92	92		
5	H	92	Total	O	0	1
			93	93		
5	I	72	Total	O	0	1
			73	73		
5	J	78	Total	O	0	0
			78	78		

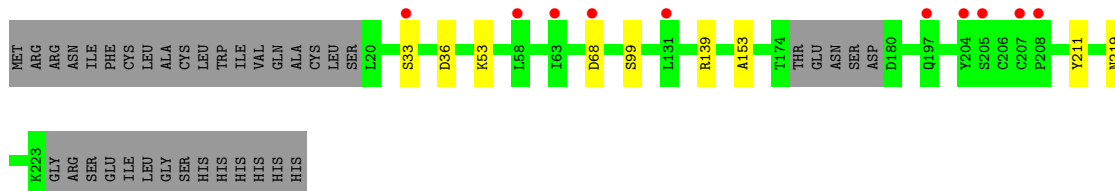
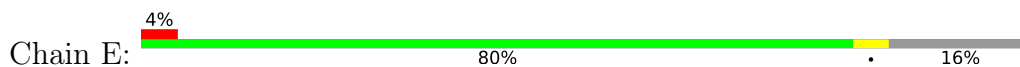




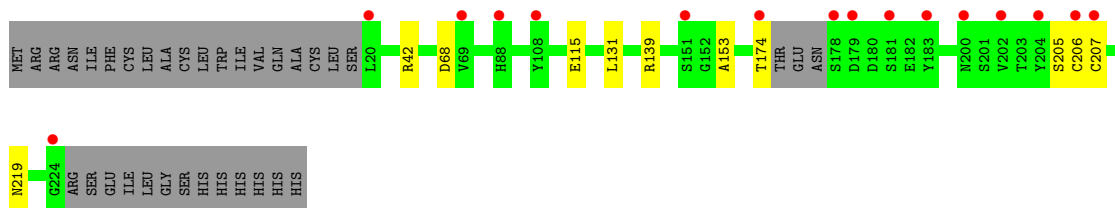
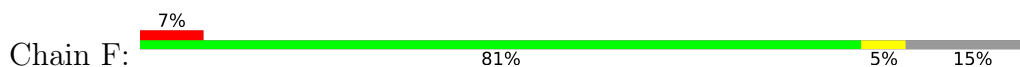
- Molecule 1: Acetylcholine-binding protein



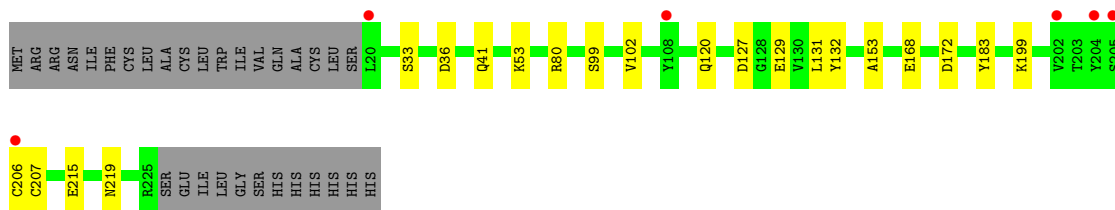
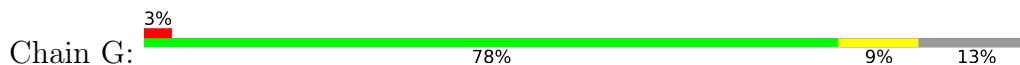
- Molecule 1: Acetylcholine-binding protein



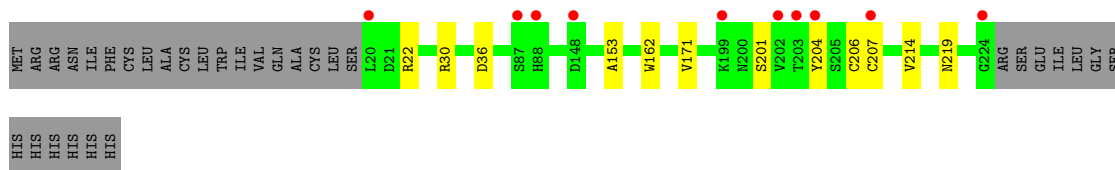
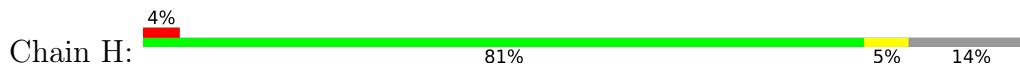
- Molecule 1: Acetylcholine-binding protein



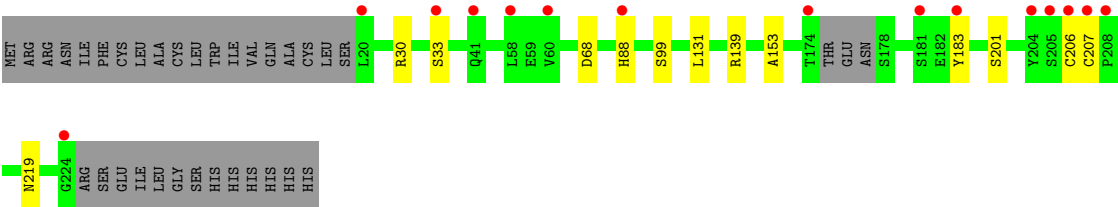
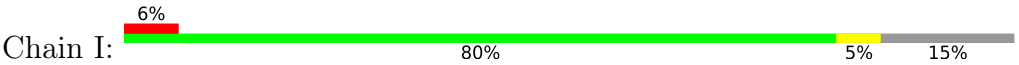
- Molecule 1: Acetylcholine-binding protein



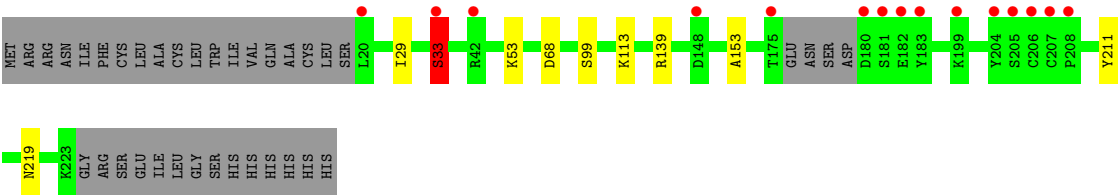
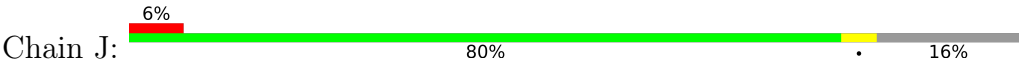
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



• Molecule 1: Acetylcholine-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.25Å 120.64Å 240.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 1.90 47.31 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.31-1.90) 100.0 (47.31-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.217 , 0.244 0.225 , 0.248	Depositor DCC
$R_{free}$ test set	8730 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.9	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	0.96	EDS
Total number of atoms	16962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1096e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, WD5

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	0.68	0/1647	0.84	0/2246
1	B	0.66	0/1644	0.80	0/2243
1	C	0.66	0/1648	0.81	0/2248
1	D	0.65	0/1647	0.83	0/2246
1	E	0.67	0/1645	0.85	2/2244 (0.1%)
1	F	0.69	0/1647	0.82	0/2246
1	G	0.69	0/1717	0.84	0/2342
1	H	0.74	0/1700	0.88	0/2319
1	I	0.67	0/1688	0.82	0/2303
1	J	0.68	1/1663 (0.1%)	0.84	1/2269 (0.0%)
All	All	0.68	1/16646 (0.0%)	0.83	3/22706 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	33	SER	CA-CB	-5.14	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	J	211	TYR	CB-CG-CD1	-5.70	117.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	TYR	CB-CG-CD2	5.64	124.38	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	88	HIS	Sidechain

## 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	1612	0	1560	5	0
1	B	1609	0	1559	6	0
1	C	1610	0	1562	13	0
1	D	1612	0	1560	20	0
1	E	1604	0	1563	6	0
1	F	1612	0	1560	10	0
1	G	1669	0	1630	19	0
1	H	1655	0	1605	12	0
1	I	1638	0	1606	11	0
1	J	1619	0	1583	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	D	14	0	0	2	0
3	F	14	0	0	0	0
3	G	14	0	0	0	0
3	H	14	0	0	1	0
4	G	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	54	0	0	1	0
5	B	21	0	0	1	0
5	C	37	0	0	0	0
5	D	76	0	0	5	0
5	E	70	0	0	1	0
5	F	56	0	0	1	0
5	G	92	0	0	1	0
5	H	93	0	0	0	0
5	I	73	0	0	0	0
5	J	78	0	0	0	0
All	All	16962	0	15796	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HG12	1:C:214:VAL:HG23	1.57	0.84
1:D:171:VAL:HG12	1:D:214:VAL:HG23	1.61	0.83
1:H:171:VAL:HG12	1:H:214:VAL:HG23	1.62	0.82
1:H:204:TYR:HD1	1:I:183:TYR:HE1	1.34	0.76
1:H:206:CYS:HG	1:H:207:CYS:HG	0.78	0.76
1:G:206:CYS:HG	1:G:207:CYS:HG	0.74	0.73
1:H:204:TYR:CD1	1:I:183:TYR:CE1	2.76	0.73
1:I:206:CYS:HG	1:I:207:CYS:HG	0.73	0.72
1:A:206:CYS:HG	1:A:207:CYS:HG	0.72	0.71
1:E:36[A]:ASP:OD1	5:E:401:HOH:O	2.12	0.68
1:B:206:CYS:HG	1:B:207:CYS:HG	0.67	0.66
1:H:36[B]:ASP:OD2	1:I:30:ARG:NH1	2.28	0.65
1:D:206:CYS:HG	1:D:207:CYS:HG	0.71	0.64
1:C:206:CYS:HG	1:C:207:CYS:HG	0.66	0.64
1:H:204:TYR:HD1	1:I:183:TYR:CE1	2.13	0.63
1:D:33:SER:HA	5:D:419:HOH:O	1.99	0.62
1:G:41:GLN:NE2	1:G:80:ARG:HG3	2.14	0.62
1:F:206:CYS:HG	1:F:207:CYS:HG	0.67	0.62
1:G:41:GLN:HE21	1:G:80:ARG:CG	2.12	0.61
1:C:171:VAL:CG1	1:C:214:VAL:HG23	2.30	0.61
1:C:204:TYR:HD1	1:D:183:TYR:CE1	2.20	0.60
1:G:41:GLN:NE2	1:G:80:ARG:CG	2.66	0.58
1:D:171:VAL:CG1	1:D:214:VAL:HG23	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:HIS:CE1	1:F:42:ARG:HH21	2.24	0.56
1:G:41:GLN:HE21	1:G:80:ARG:HG3	1.71	0.55
1:D:131:LEU:HD12	1:D:131:LEU:N	2.23	0.54
1:C:131:LEU:N	1:C:131:LEU:HD12	2.22	0.54
1:F:205:SER:H	1:G:183:TYR:HH	1.53	0.53
1:H:171:VAL:CG1	1:H:214:VAL:HG23	2.37	0.52
1:F:131:LEU:HD12	1:F:131:LEU:N	2.25	0.52
1:C:184:PHE:CD2	1:C:192:ILE:HD11	2.44	0.52
1:J:68:ASP:HB2	1:J:139:ARG:NH1	2.25	0.52
1:J:68:ASP:HB2	1:J:139:ARG:HH11	1.74	0.51
1:J:33:SER:OG	1:J:99:SER:O	2.14	0.51
1:G:33:SER:HB2	1:G:99:SER:O	2.10	0.50
1:F:174:THR:CG2	5:F:431:HOH:O	2.60	0.50
1:G:41:GLN:NE2	1:G:80:ARG:HB2	2.26	0.50
1:D:88:HIS:CE1	1:F:42:ARG:NH2	2.79	0.49
1:C:171:VAL:HG12	1:C:214:VAL:CG2	2.37	0.49
1:I:68:ASP:HB2	1:I:139:ARG:NH2	2.28	0.49
1:C:204:TYR:HD1	1:D:183:TYR:HE1	1.62	0.48
1:D:206:CYS:SG	3:D:301:WD5:C4	3.01	0.48
1:E:68:ASP:HB2	1:E:139:ARG:NH1	2.28	0.48
1:A:162:TRP:CZ2	1:B:118:THR:HG21	2.49	0.48
1:E:68:ASP:HB2	1:E:139:ARG:HH11	1.79	0.47
1:H:204:TYR:HB3	1:I:183:TYR:OH	2.14	0.47
1:B:33:SER:HB2	1:B:99:SER:O	2.15	0.47
3:D:301:WD5:CL1	1:E:53:LYS:HE2	2.51	0.47
1:F:68:ASP:HB2	1:F:139:ARG:NH2	2.29	0.47
1:G:120:GLN:OE1	1:G:132:TYR:OH	2.10	0.47
1:D:113:LYS:NZ	5:D:402:HOH:O	2.38	0.47
1:B:74:GLN:HG3	1:B:133:MET:HE2	1.97	0.46
1:D:33:SER:HB2	1:D:99:SER:O	2.16	0.46
1:I:68:ASP:HB2	1:I:139:ARG:HH21	1.80	0.46
1:D:33:SER:HB2	5:D:419:HOH:O	2.16	0.46
1:J:53:LYS:HB3	1:J:53:LYS:HE3	1.85	0.45
1:C:193:LEU:HD12	1:C:219:ASN:OD1	2.17	0.45
1:G:215:GLU:CD	5:G:451:HOH:O	2.54	0.45
1:G:41:GLN:HE22	1:G:80:ARG:HB2	1.82	0.44
1:I:33:SER:HB2	1:I:99:SER:O	2.17	0.44
1:D:33:SER:CB	5:D:419:HOH:O	2.64	0.44
1:F:153:ALA:O	1:F:219:ASN:HA	2.18	0.44
1:E:33:SER:HB2	1:E:99:SER:O	2.18	0.44
1:D:153:ALA:O	1:D:219:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:ALA:O	1:H:219:ASN:HA	2.18	0.43
1:A:153:ALA:O	1:A:219:ASN:HA	2.18	0.43
1:B:153:ALA:O	1:B:219:ASN:HA	2.18	0.43
1:C:153:ALA:O	1:C:219:ASN:HA	2.19	0.43
1:J:153:ALA:O	1:J:219:ASN:HA	2.19	0.43
1:A:33:SER:HB3	5:A:426:HOH:O	2.18	0.43
1:D:130:VAL:C	1:D:131:LEU:HD12	2.38	0.43
1:F:68:ASP:HB2	1:F:139:ARG:HH21	1.83	0.43
1:A:31:GLN:HA	1:A:31:GLN:OE1	2.18	0.43
1:D:41:GLN:CD	1:D:80:ARG:HD3	2.39	0.43
1:C:130:VAL:C	1:C:131:LEU:HD12	2.39	0.43
1:D:171:VAL:HG12	1:D:214:VAL:CG2	2.41	0.43
1:B:115:GLU:OE2	5:B:501:HOH:O	2.22	0.43
1:E:153:ALA:O	1:E:219:ASN:HA	2.18	0.42
1:G:53:LYS:HG2	1:G:183:TYR:HD2	1.84	0.42
1:G:102:VAL:O	4:G:303:GOL:H32	2.19	0.42
1:G:36[A]:ASP:OD2	1:H:30:ARG:NH1	2.52	0.42
1:C:184:PHE:CD2	1:C:192:ILE:CD1	3.01	0.42
1:G:153:ALA:O	1:G:219:ASN:HA	2.19	0.42
1:I:153:ALA:O	1:I:219:ASN:HA	2.18	0.42
1:G:172:ASP:OD1	1:G:199:LYS:HD2	2.20	0.41
1:F:115:GLU:HG3	1:J:113:LYS:HE3	2.02	0.41
1:J:29:ILE:O	1:J:33:SER:HB2	2.21	0.41
1:G:127:ASP:OD2	1:G:129:GLU:OE1	2.39	0.41
1:D:189:ARG:NH2	5:D:406:HOH:O	2.54	0.40
1:H:162:TRP:O	3:H:301:WD5:C11	2.69	0.40
1:C:204:TYR:CD1	1:D:183:TYR:CE1	3.06	0.40
1:G:168:GLU:OE2	1:H:22:ARG:NH2	2.55	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	198/237 (84%)	197 (100%)	1 (0%)	0	100	100
1	B	197/237 (83%)	196 (100%)	1 (0%)	0	100	100
1	C	198/237 (84%)	197 (100%)	1 (0%)	0	100	100
1	D	198/237 (84%)	197 (100%)	1 (0%)	0	100	100
1	E	197/237 (83%)	196 (100%)	1 (0%)	0	100	100
1	F	198/237 (84%)	197 (100%)	1 (0%)	0	100	100
1	G	208/237 (88%)	206 (99%)	2 (1%)	0	100	100
1	H	206/237 (87%)	204 (99%)	2 (1%)	0	100	100
1	I	203/237 (86%)	201 (99%)	2 (1%)	0	100	100
1	J	199/237 (84%)	197 (99%)	2 (1%)	0	100	100
All	All	2002/2370 (84%)	1988 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/220 (86%)	185 (98%)	3 (2%)	58	56
1	B	188/220 (86%)	186 (99%)	2 (1%)	70	71
1	C	188/220 (86%)	187 (100%)	1 (0%)	86	88
1	D	188/220 (86%)	186 (99%)	2 (1%)	70	71
1	E	188/220 (86%)	188 (100%)	0	100	100
1	F	188/220 (86%)	188 (100%)	0	100	100
1	G	196/220 (89%)	196 (100%)	0	100	100
1	H	194/220 (88%)	193 (100%)	1 (0%)	86	88
1	I	193/220 (88%)	192 (100%)	1 (0%)	86	88
1	J	190/220 (86%)	189 (100%)	1 (0%)	86	88
All	All	1901/2200 (86%)	1890 (99%)	11 (1%)	84	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	156	ARG
1	A	201	SER
1	B	80	ARG
1	B	179	ASP
1	C	201	SER
1	D	43	ASP
1	D	201	SER
1	H	201	SER
1	I	201	SER
1	J	33	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	B	74	GLN
1	D	120	GLN
1	G	41	GLN
1	H	74	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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	WD5	D	301	-	15,15,15	0.36	0	21,21,21	0.63	0
3	WD5	H	301	-	15,15,15	0.47	0	21,21,21	0.92	1 (4%)
4	GOL	G	303	-	5,5,5	0.20	0	5,5,5	0.59	0
3	WD5	F	301	-	15,15,15	0.59	0	21,21,21	0.64	0
3	WD5	G	301	-	15,15,15	0.58	0	21,21,21	0.58	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
3	WD5	D	301	-	-	0/6/16/16	0/2/2/2
3	WD5	H	301	-	-	0/6/16/16	0/2/2/2
4	GOL	G	303	-	-	2/4/4/4	-
3	WD5	F	301	-	-	4/6/16/16	1/2/2/2
3	WD5	G	301	-	-	2/6/16/16	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	WD5	C11-C1-C8	-2.46	105.46	108.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	303	GOL	C1-C2-C3-O3
4	G	303	GOL	O2-C2-C3-O3
3	G	301	WD5	O1-C1-C2-C3
3	F	301	WD5	O1-C1-C2-C3
3	G	301	WD5	O1-C1-C2-C7
3	F	301	WD5	O1-C1-C2-C7

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Mol	Chain	Res	Type	Atoms
3	F	301	WD5	C8-C1-C2-C3
3	F	301	WD5	C8-C1-C2-C7

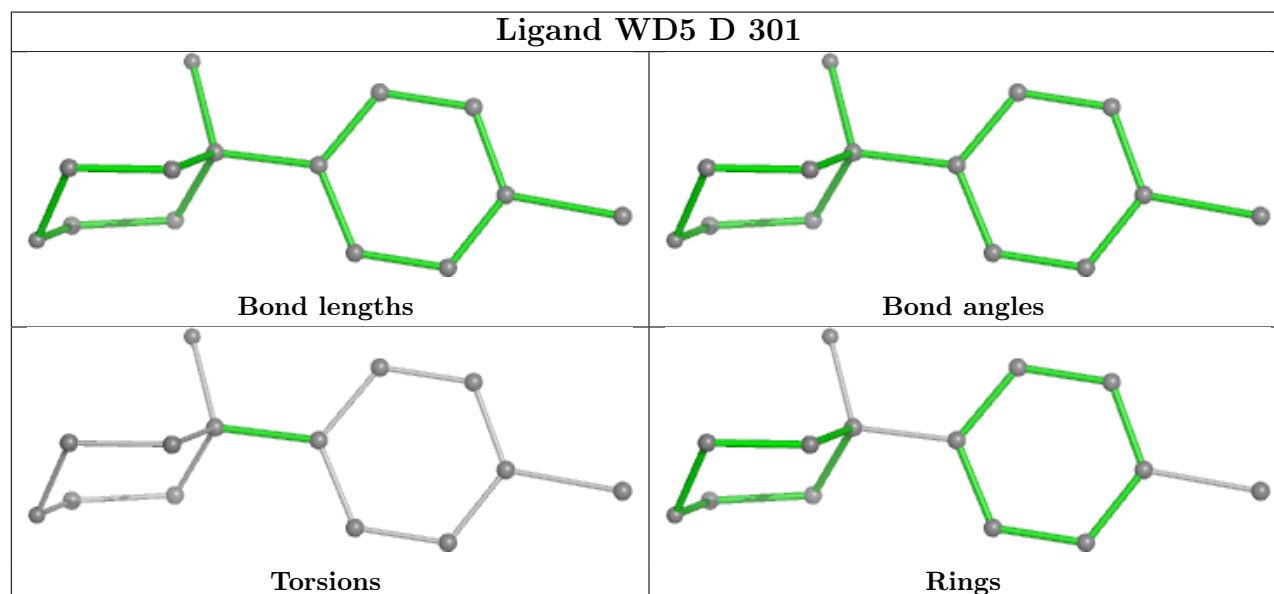
All (1) ring outliers are listed below:

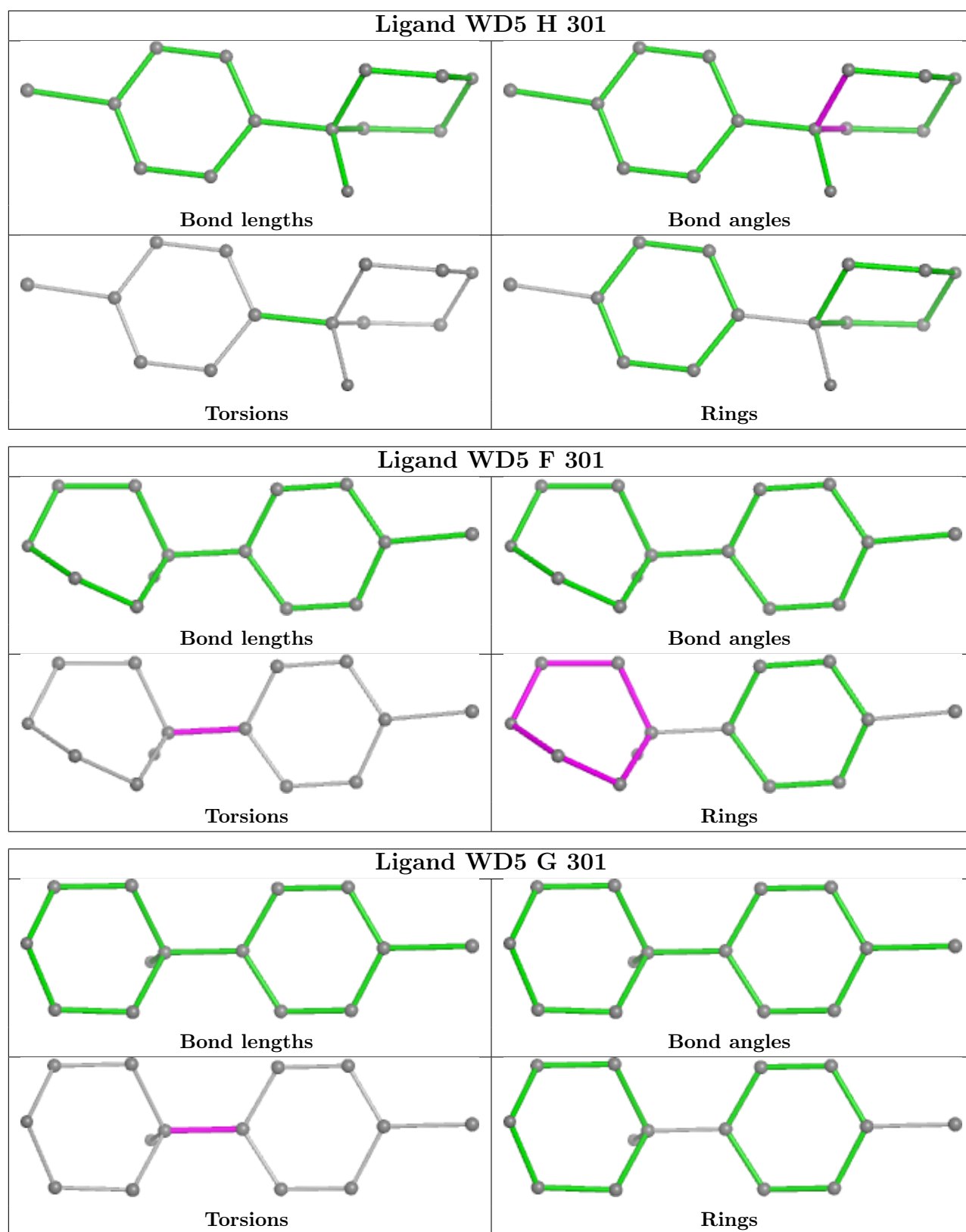
Mol	Chain	Res	Type	Atoms
3	F	301	WD5	C1-C10-C11-C8-C9-N1

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	WD5	2	0
3	H	301	WD5	1	0
4	G	303	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	202/237 (85%)	0.93	28 (13%) 7 7	33, 48, 91, 139	0
1	B	201/237 (84%)	1.16	33 (16%) 5 5	37, 56, 84, 115	0
1	C	201/237 (84%)	1.05	24 (11%) 10 10	24, 51, 89, 109	1 (0%)
1	D	202/237 (85%)	0.43	13 (6%) 27 28	29, 41, 77, 109	0
1	E	199/237 (83%)	0.40	10 (5%) 35 36	22, 40, 70, 103	2 (1%)
1	F	202/237 (85%)	0.62	16 (7%) 20 21	30, 43, 79, 104	0
1	G	206/237 (86%)	0.20	6 (2%) 54 56	20, 36, 62, 92	4 (1%)
1	H	205/237 (86%)	0.23	10 (4%) 36 37	18, 36, 70, 93	3 (1%)
1	I	202/237 (85%)	0.39	15 (7%) 22 23	22, 40, 76, 111	5 (2%)
1	J	200/237 (84%)	0.47	15 (7%) 22 23	21, 40, 74, 99	3 (1%)
All	All	2020/2370 (85%)	0.59	170 (8%) 18 19	18, 43, 81, 139	18 (0%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	TYR	9.3
1	F	204	TYR	6.9
1	J	175	THR	5.2
1	F	202	VAL	5.0
1	J	181	SER	4.7
1	C	203	THR	4.4
1	I	206	CYS	4.4
1	F	181	SER	4.4
1	F	207	CYS	4.2
1	A	202	VAL	4.2
1	C	175	THR	4.2
1	C	181	SER	4.1
1	B	63	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	204	TYR	4.1
1	A	172	ASP	4.0
1	G	204	TYR	3.9
1	J	207	CYS	3.9
1	B	131	LEU	3.9
1	B	203	THR	3.9
1	H	88	HIS	3.8
1	I	207	CYS	3.8
1	D	205	SER	3.6
1	A	208	PRO	3.6
1	C	183	TYR	3.6
1	I	205	SER	3.6
1	J	208	PRO	3.5
1	F	206	CYS	3.5
1	E	204	TYR	3.5
1	J	206	CYS	3.5
1	A	206	CYS	3.5
1	H	203	THR	3.4
1	C	202	VAL	3.4
1	B	202	VAL	3.3
1	J	33	SER	3.3
1	A	224	GLY	3.3
1	C	204	TYR	3.3
1	A	203	THR	3.3
1	A	153	ALA	3.3
1	C	20	LEU	3.1
1	A	174	THR	3.1
1	C	201	SER	3.1
1	H	199	LYS	3.1
1	E	208	PRO	3.1
1	J	183	TYR	3.1
1	A	201	SER	3.1
1	B	181	SER	3.1
1	I	174	THR	3.1
1	B	204	TYR	3.0
1	J	182	GLU	3.0
1	E	207	CYS	3.0
1	C	193	LEU	3.0
1	J	180	ASP	3.0
1	J	20	LEU	3.0
1	B	198	LYS	3.0
1	E	58	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	202	VAL	2.9
1	D	174	THR	2.9
1	H	202	VAL	2.9
1	A	178	SER	2.9
1	B	218	LEU	2.8
1	J	204	TYR	2.8
1	A	20	LEU	2.8
1	C	224	GLY	2.8
1	I	33	SER	2.8
1	J	205	SER	2.8
1	D	183	TYR	2.8
1	C	91	ASP	2.8
1	B	197	GLN	2.8
1	C	206	CYS	2.7
1	B	199	LYS	2.7
1	H	87	SER	2.7
1	B	60	VAL	2.7
1	C	205	SER	2.7
1	D	224	GLY	2.7
1	C	182	GLU	2.7
1	E	205	SER	2.6
1	B	67	VAL	2.6
1	D	207	CYS	2.6
1	J	148	ASP	2.6
1	F	151	SER	2.6
1	A	211	TYR	2.6
1	B	58	LEU	2.6
1	G	205	SER	2.6
1	C	149	THR	2.6
1	B	144	VAL	2.5
1	B	195	VAL	2.5
1	A	207	CYS	2.5
1	A	63	ILE	2.5
1	I	181	SER	2.5
1	B	175	THR	2.5
1	F	108	TYR	2.5
1	A	131	LEU	2.5
1	B	20	LEU	2.5
1	I	224	GLY	2.5
1	B	193	LEU	2.5
1	F	174	THR	2.5
1	F	178	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	108	TYR	2.4
1	B	223	LYS	2.4
1	H	207	CYS	2.4
1	C	180	ASP	2.4
1	B	149	THR	2.4
1	C	174	THR	2.4
1	G	20	LEU	2.4
1	B	158	LYS	2.3
1	H	148	ASP	2.3
1	C	208	PRO	2.3
1	A	69	VAL	2.3
1	A	200	ASN	2.3
1	E	131[A]	LEU	2.3
1	F	20	LEU	2.3
1	D	88	HIS	2.3
1	A	151	SER	2.3
1	D	151	SER	2.3
1	I	60	VAL	2.3
1	F	88	HIS	2.3
1	B	148	ASP	2.3
1	I	41	GLN	2.3
1	A	181	SER	2.3
1	B	192	ILE	2.3
1	C	219	ASN	2.3
1	D	193	LEU	2.3
1	B	160	GLY	2.2
1	I	183	TYR	2.2
1	J	199	LYS	2.2
1	B	154	THR	2.2
1	F	179	ASP	2.2
1	A	205	SER	2.2
1	B	201	SER	2.2
1	D	178	SER	2.2
1	B	183	TYR	2.2
1	C	80	ARG	2.2
1	A	60	VAL	2.2
1	F	69	VAL	2.2
1	G	206	CYS	2.2
1	F	224	GLY	2.2
1	H	224	GLY	2.2
1	A	173	PRO	2.2
1	E	63	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	42	ARG	2.2
1	A	44	ARG	2.2
1	E	197	GLN	2.1
1	B	150	GLU	2.1
1	C	153	ALA	2.1
1	I	20	LEU	2.1
1	I	88	HIS	2.1
1	C	57	ILE	2.1
1	D	91	ASP	2.1
1	F	183	TYR	2.1
1	E	33	SER	2.1
1	B	106	ALA	2.1
1	I	204	TYR	2.1
1	F	200	ASN	2.1
1	B	147	VAL	2.1
1	I	208	PRO	2.1
1	A	183	TYR	2.1
1	B	108	TYR	2.1
1	D	20	LEU	2.0
1	I	58	LEU	2.0
1	B	220	PHE	2.0
1	D	33	SER	2.0
1	C	187	TYR	2.0
1	B	88	HIS	2.0
1	C	152	GLY	2.0
1	A	180	ASP	2.0
1	E	68	ASP	2.0
1	A	171	VAL	2.0
1	D	60	VAL	2.0
1	H	20	LEU	2.0
1	J	42	ARG	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands

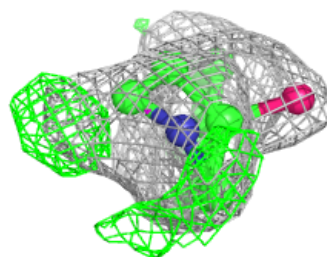
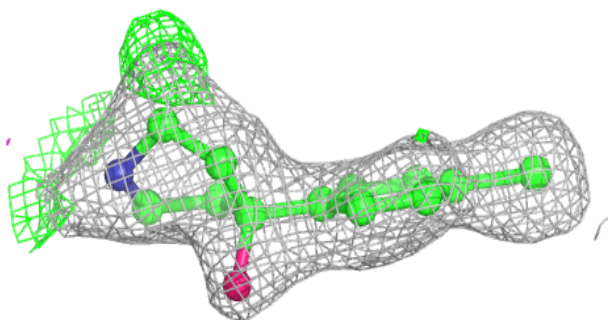
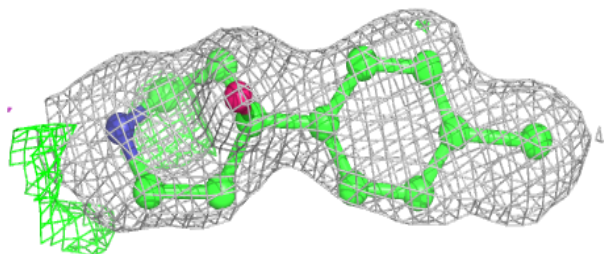
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	WD5	F	301	14/14	0.81	0.19	57,67,73,75	0
3	WD5	H	301	14/14	0.82	0.20	76,82,87,89	0
3	WD5	G	301	14/14	0.85	0.15	43,52,54,55	0
3	WD5	D	301	14/14	0.86	0.13	46,58,66,73	0
4	GOL	G	303	6/6	0.90	0.12	36,49,50,59	0
2	CL	G	302	1/1	0.96	0.07	36,36,36,36	0
2	CL	C	301	1/1	0.96	0.09	47,47,47,47	0
2	CL	B	301	1/1	0.97	0.07	46,46,46,46	0
2	CL	E	301	1/1	0.99	0.04	35,35,35,35	0
2	CL	A	301	1/1	0.99	0.09	40,40,40,40	0
2	CL	H	302	1/1	0.99	0.04	37,37,37,37	0
2	CL	D	302	1/1	0.99	0.04	42,42,42,42	0
2	CL	J	301	1/1	1.00	0.07	33,33,33,33	0
2	CL	F	302	1/1	1.00	0.03	36,36,36,36	0
2	CL	I	301	1/1	1.00	0.03	36,36,36,36	0

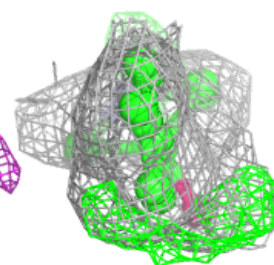
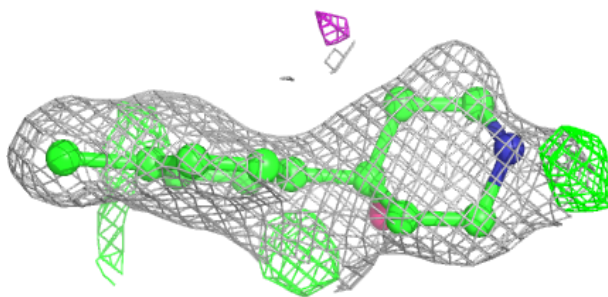
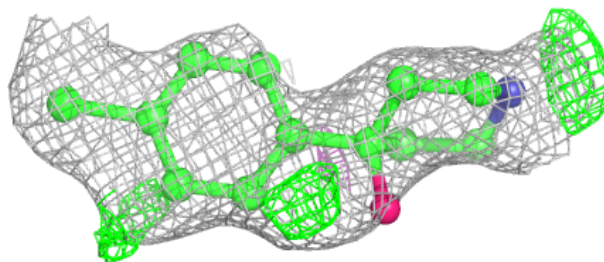
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around WD5 F 301:**

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

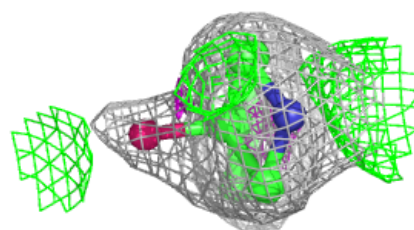
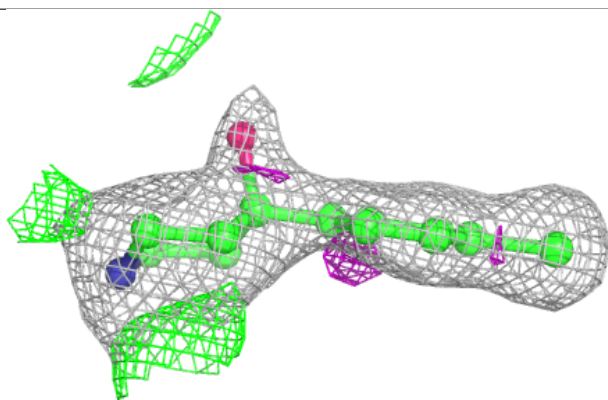
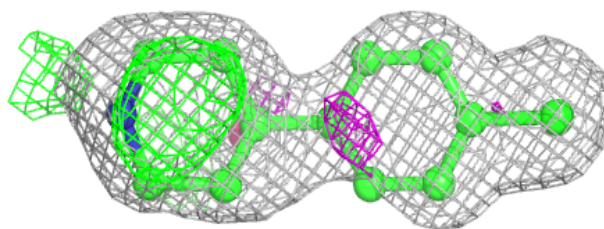
**Electron density around WD5 H 301:**

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

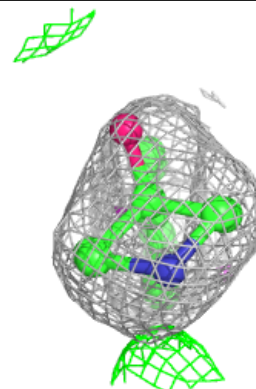
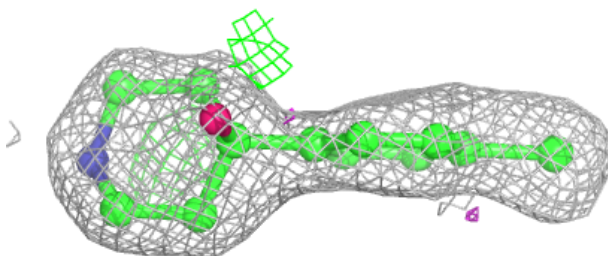
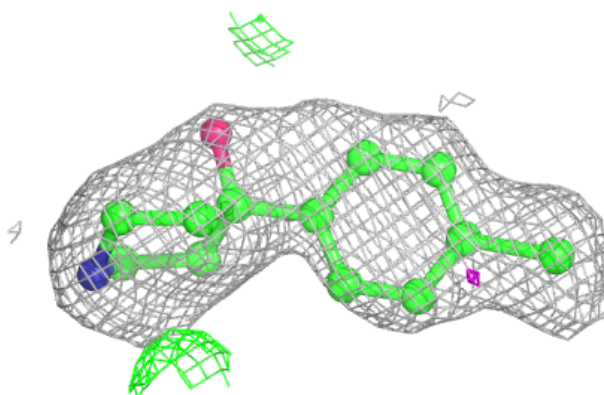


**Electron density around WD5 G 301:**

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

**Electron density around WD5 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.