



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:06 PM JST

PDB ID : 7XRK  
Title : Diol dehydratase complexed with AdoMeCbl  
Authors : Shibata, N.; Toraya, T.  
Deposited on : 2022-05-10  
Resolution : 2.30 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 : 2.36  
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) : 2.36

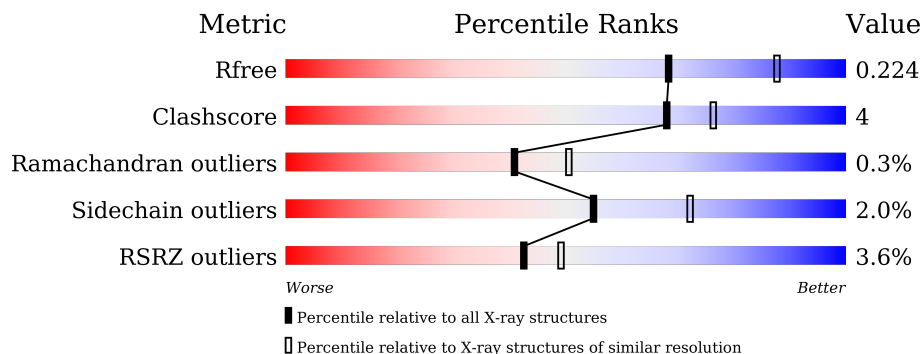
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	554	 90% 10%
1	D	554	 90% 10%
2	B	200	 80% 9% 11%
2	E	200	 80% 8% 11%
3	C	137	 94% 5%
3	F	137	 88% 9%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 13940 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 Diol dehydrase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	Total	C	N	O	S	0	0	0
			4210	2624	728	830	28			
1	D	553	Total	C	N	O	S	0	0	0
			4218	2629	729	831	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	ASP	ILE	conflict	UNP Q59470
D	553	ASP	ILE	conflict	UNP Q59470

- Molecule 2 is a protein called Diol dehydrase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	178	Total	C	N	O	S	0	0	0
			1358	859	244	253	2			
2	E	178	Total	C	N	O	S	0	0	0
			1357	859	244	252	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	MET	-	expression tag	UNP Q59471
B	26	SER	-	expression tag	UNP Q59471
B	27	SER	-	expression tag	UNP Q59471
B	28	HIS	-	expression tag	UNP Q59471
B	29	HIS	-	expression tag	UNP Q59471
B	30	HIS	-	expression tag	UNP Q59471
B	31	HIS	-	expression tag	UNP Q59471
B	32	HIS	-	expression tag	UNP Q59471
B	33	HIS	-	expression tag	UNP Q59471
B	34	SER	-	expression tag	UNP Q59471

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Chain	Residue	Modelled	Actual	Comment	Reference
B	35	ALA	-	expression tag	UNP Q59471
B	36	ALA	-	expression tag	UNP Q59471
B	37	LEU	-	expression tag	UNP Q59471
B	38	GLU	-	expression tag	UNP Q59471
B	39	VAL	-	expression tag	UNP Q59471
B	40	LEU	-	expression tag	UNP Q59471
B	41	PHE	-	expression tag	UNP Q59471
B	42	GLN	-	expression tag	UNP Q59471
B	43	GLY	-	expression tag	UNP Q59471
B	44	PRO	-	expression tag	UNP Q59471
B	45	GLY	-	expression tag	UNP Q59471
E	25	MET	-	expression tag	UNP Q59471
E	26	SER	-	expression tag	UNP Q59471
E	27	SER	-	expression tag	UNP Q59471
E	28	HIS	-	expression tag	UNP Q59471
E	29	HIS	-	expression tag	UNP Q59471
E	30	HIS	-	expression tag	UNP Q59471
E	31	HIS	-	expression tag	UNP Q59471
E	32	HIS	-	expression tag	UNP Q59471
E	33	HIS	-	expression tag	UNP Q59471
E	34	SER	-	expression tag	UNP Q59471
E	35	ALA	-	expression tag	UNP Q59471
E	36	ALA	-	expression tag	UNP Q59471
E	37	LEU	-	expression tag	UNP Q59471
E	38	GLU	-	expression tag	UNP Q59471
E	39	VAL	-	expression tag	UNP Q59471
E	40	LEU	-	expression tag	UNP Q59471
E	41	PHE	-	expression tag	UNP Q59471
E	42	GLN	-	expression tag	UNP Q59471
E	43	GLY	-	expression tag	UNP Q59471
E	44	PRO	-	expression tag	UNP Q59471
E	45	GLY	-	expression tag	UNP Q59471

- Molecule 3 is a protein called Diol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	136	1087	678	194	212	3	0	0	0
3	F	135	1078	674	193	208	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	MET	-	expression tag	UNP Q59472
F	37	MET	-	expression tag	UNP Q59472

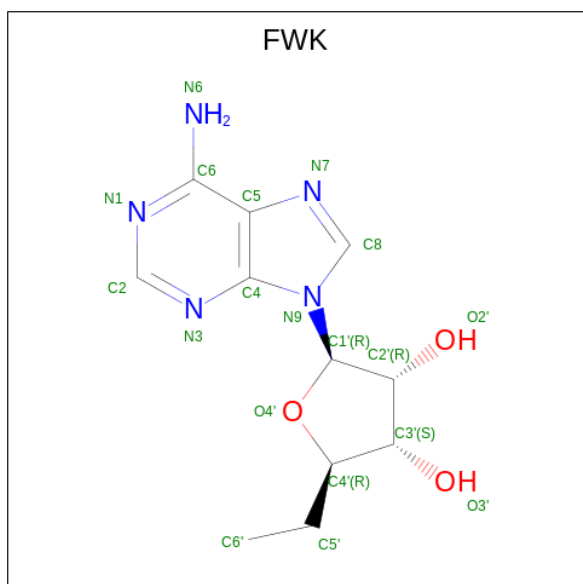
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0

- Molecule 6 is (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-ethyl-oxolane-3,4-diol (three-letter code: FWK) (formula: C<sub>11</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



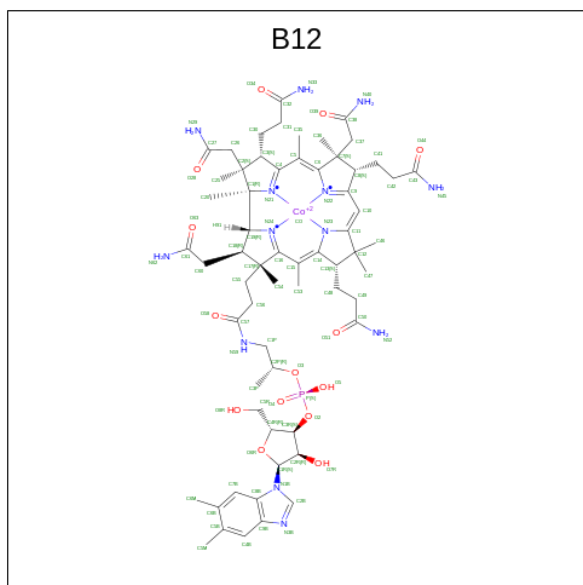
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 19 11 5 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	D	1	19	11	5	3	0	0

- Molecule 7 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
7	B	1	91	62	1	13	14	1	0	0
7	E	1	91	62	1	13	14	1	0	0

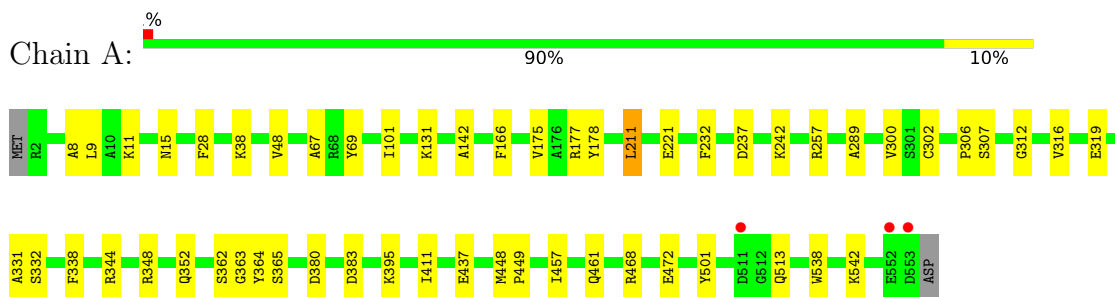
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	150	Total	O	0	0
			150	150		
8	B	36	Total	O	0	0
			36	36		
8	C	29	Total	O	0	0
			29	29		
8	D	140	Total	O	0	0
			140	140		
8	E	28	Total	O	0	0
			28	28		
8	F	25	Total	O	0	0
			25	25		

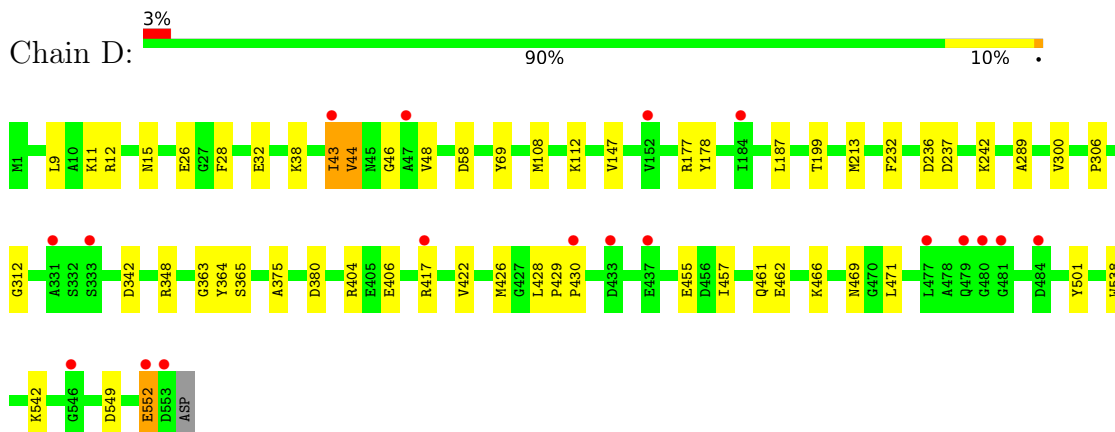
### 3 Residue-property plots [i](#)

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.

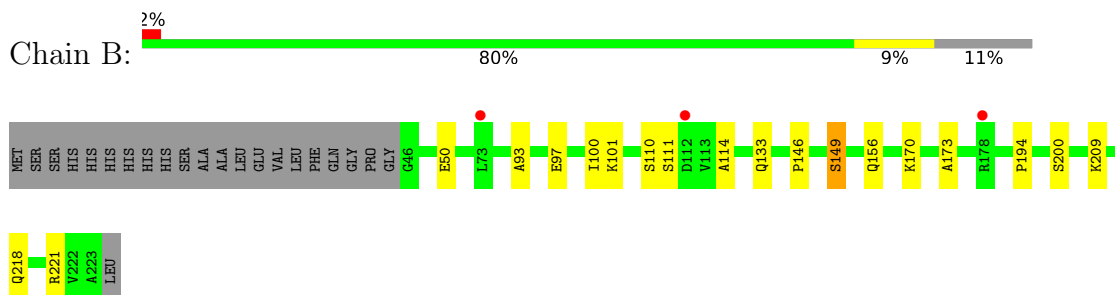
- Molecule 1: Diol dehydrase alpha subunit



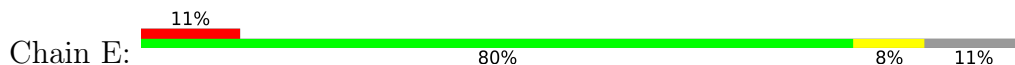
- Molecule 1: Diol dehydrase alpha subunit

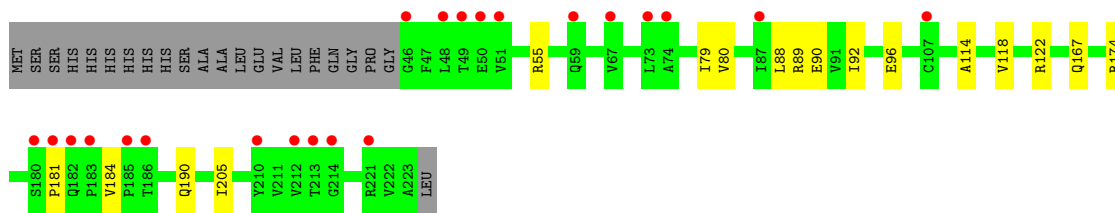


- Molecule 2: Diol dehydrase beta subunit



- Molecule 2: Diol dehydrase beta subunit





- Molecule 3: Diol dehydrase gamma subunit

Chain C: 94% 5%



- Molecule 3: Diol dehydrase gamma subunit

Chain F: 12% 88% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.31Å 111.56Å 197.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.07 – 2.30 45.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.07-2.30) 99.5 (45.07-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.165 , 0.225 0.166 , 0.224	Depositor DCC
$R_{free}$ test set	1992 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtrriage
Anisotropy	1.212	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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 30.90 % 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 1.2106e-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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FWK, B12, K

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	0.29	0/4282	0.53	0/5800
1	D	0.29	0/4290	0.53	0/5810
2	B	0.28	0/1380	0.53	0/1868
2	E	0.29	0/1379	0.52	0/1867
3	C	0.30	0/1102	0.54	0/1489
3	F	0.26	0/1093	0.53	0/1478
All	All	0.29	0/13526	0.53	0/18312

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	43	ILE	Peptide

### 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	4210	0	4136	27	0
1	D	4218	0	4149	36	0
2	B	1358	0	1408	12	0
2	E	1357	0	1408	12	0
3	C	1087	0	1096	4	0
3	F	1078	0	1092	9	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	19	0	0	0	0
6	D	19	0	0	0	0
7	B	91	0	88	7	0
7	E	91	0	88	9	0
8	A	150	0	0	0	0
8	B	36	0	0	1	0
8	C	29	0	0	0	0
8	D	140	0	0	4	0
8	E	28	0	0	0	0
8	F	25	0	0	0	0
All	All	13940	0	13465	103	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 4.

All (103) 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:D:462:GLU:HG3	1:D:466:LYS:HD2	1.58	0.85
7:E:301:B12:C2B	7:E:301:B12:H492	2.23	0.69
1:D:455:GLU:OE1	8:D:701:HOH:O	2.12	0.67
7:B:301:B12:C2B	7:B:301:B12:H492	2.25	0.66
1:D:417:ARG:NH1	8:D:703:HOH:O	2.24	0.65
2:E:89:ARG:HH11	2:E:89:ARG:HG2	1.61	0.64
7:B:301:B12:H552	7:B:301:B12:H531	1.79	0.63
7:E:301:B12:H552	7:E:301:B12:H531	1.81	0.62
1:A:8:ALA:HA	1:A:11:LYS:HE3	1.80	0.62
2:B:101:LYS:NZ	8:B:401:HOH:O	2.31	0.62
1:D:177:ARG:HG3	1:D:177:ARG:HH11	1.64	0.62
7:B:301:B12:H362	7:B:301:B12:H351	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ILE:O	1:D:44:VAL:HG23	2.02	0.59
1:A:177:ARG:HG2	1:A:461:GLN:HG2	1.84	0.58
2:E:79:ILE:HG23	2:E:80:VAL:HG13	1.84	0.58
1:D:236:ASP:OD2	3:F:130:ARG:NH2	2.31	0.58
1:D:426:MET:HE2	1:D:428:LEU:HD11	1.84	0.58
2:E:167:GLN:HG3	2:E:184:VAL:HG22	1.85	0.58
1:D:177:ARG:HD2	1:D:461:GLN:CG	2.34	0.57
2:B:111:SER:O	2:B:133:GLN:NE2	2.30	0.57
7:E:301:B12:H601	7:E:301:B12:H262	1.86	0.56
1:A:331:ALA:HB1	1:A:362:SER:HB3	1.87	0.56
1:D:11:LYS:NZ	8:D:705:HOH:O	2.40	0.55
3:F:132:THR:OG1	3:F:135:GLU:HG3	2.07	0.55
7:E:301:B12:H492	7:E:301:B12:H2B	1.89	0.55
1:D:538:TRP:NE1	1:D:542:LYS:HE3	2.22	0.55
1:D:43:ILE:HG22	1:D:44:VAL:N	2.23	0.54
1:D:26:GLU:HG3	2:E:205:ILE:HG21	1.89	0.53
1:A:175:VAL:HB	1:A:178:TYR:HD2	1.74	0.53
1:A:365:SER:HB3	1:A:380:ASP:HA	1.90	0.53
7:E:301:B12:H362	7:E:301:B12:H351	1.89	0.53
1:A:468:ARG:NH2	1:A:472:GLU:OE2	2.28	0.53
2:E:174:ARG:HD3	2:E:181:PRO:HB3	1.89	0.52
2:B:146:PRO:HG2	2:B:149:SER:HB2	1.90	0.52
1:D:469:ASN:OD1	1:D:471:LEU:HB2	2.10	0.51
1:D:375:ALA:O	2:E:190:GLN:HG2	2.10	0.51
7:E:301:B12:C6	7:E:301:B12:H4B	2.41	0.51
3:F:62:ASP:OD1	3:F:62:ASP:N	2.43	0.51
1:A:338:PHE:HA	2:B:194:PRO:HB3	1.93	0.50
1:A:513:GLN:NE2	3:C:47:ASN:OD1	2.44	0.50
1:D:69:TYR:HB2	1:D:289:ALA:HB1	1.93	0.50
1:D:306:PRO:O	1:D:312:GLY:HA3	2.12	0.50
2:B:50:GLU:HG2	2:B:218:GLN:HB3	1.93	0.49
1:D:43:ILE:HD11	1:D:48:VAL:HG22	1.94	0.49
1:D:422:VAL:O	1:D:426:MET:HG3	2.13	0.48
2:B:114:ALA:HB2	7:B:301:B12:HM62	1.95	0.48
2:E:89:ARG:NH1	2:E:90:GLU:OE2	2.47	0.48
3:F:164:VAL:HG22	3:F:169:LEU:HD11	1.96	0.48
1:A:457:ILE:HD13	1:A:457:ILE:HA	1.72	0.47
1:A:69:TYR:HB2	1:A:289:ALA:HB1	1.94	0.47
1:D:365:SER:HB3	1:D:380:ASP:HA	1.94	0.47
1:D:177:ARG:HD2	1:D:461:GLN:HG2	1.95	0.47
1:A:9:LEU:O	1:A:15:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASP:CG	1:A:242:LYS:HE2	2.35	0.47
1:D:471:LEU:HD12	3:F:75:THR:HA	1.96	0.47
3:F:55:THR:HG23	3:F:59:LYS:O	2.15	0.47
3:C:164:VAL:HG22	3:C:169:LEU:HD11	1.97	0.47
1:D:342:ASP:OD2	8:D:702:HOH:O	2.21	0.46
7:E:301:B12:H262	7:E:301:B12:H91	1.71	0.46
7:B:301:B12:H4B	7:B:301:B12:C6	2.45	0.46
3:C:67:GLU:H	3:C:67:GLU:CD	2.19	0.46
1:A:302:CYS:O	1:A:306:PRO:HD2	2.17	0.45
2:E:89:ARG:HG2	2:E:89:ARG:NH1	2.26	0.45
2:B:170:LYS:HE3	2:B:170:LYS:HB3	1.78	0.45
1:D:237:ASP:CG	1:D:242:LYS:HE2	2.36	0.45
3:F:65:THR:O	3:F:69:VAL:HG23	2.17	0.45
1:A:538:TRP:NE1	1:A:542:LYS:HE3	2.32	0.45
1:D:187:LEU:HA	1:D:199:THR:HG21	1.99	0.45
2:E:92:ILE:O	2:E:96:GLU:HG3	2.18	0.44
1:A:383:ASP:OD1	1:D:12:ARG:NH2	2.45	0.44
1:A:48:VAL:HB	1:A:67:ALA:HB1	1.99	0.44
1:A:307:SER:O	1:A:344:ARG:NH2	2.50	0.44
1:A:306:PRO:O	1:A:312:GLY:HA3	2.17	0.44
2:B:100:ILE:HG13	2:B:173:ALA:HB1	1.99	0.44
1:A:395:LYS:NZ	1:D:32:GLU:OE2	2.51	0.43
1:D:549:ASP:O	1:D:552:GLU:HG3	2.18	0.43
1:A:316:VAL:O	1:A:319:GLU:HG2	2.18	0.43
1:A:221:GLU:OE2	1:A:257:ARG:NH1	2.50	0.43
1:D:471:LEU:HD13	3:F:69:VAL:HG13	2.00	0.43
1:D:9:LEU:O	1:D:15:ASN:ND2	2.52	0.43
1:D:108:MET:HB3	1:D:112:LYS:HB3	2.00	0.42
1:D:471:LEU:HD23	1:D:471:LEU:HA	1.83	0.42
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.95	0.42
1:D:43:ILE:CD1	1:D:48:VAL:HG22	2.50	0.42
2:E:114:ALA:HB2	7:E:301:B12:HM62	2.02	0.42
2:B:50:GLU:HG2	2:B:218:GLN:CB	2.50	0.42
2:B:93:ALA:O	2:B:97:GLU:HB2	2.20	0.42
1:D:69:TYR:OH	3:F:158:GLU:OE1	2.15	0.42
1:A:395:LYS:HE3	1:A:538:TRP:CE2	2.55	0.42
2:B:200:SER:OG	7:B:301:B12:O5	2.36	0.41
2:E:118:VAL:O	2:E:122:ARG:HD3	2.21	0.41
1:D:404:ARG:NH1	1:D:406:GLU:OE2	2.54	0.41
1:A:448:MET:HE3	1:A:449:PRO:HD2	2.02	0.41
7:E:301:B12:H531	7:E:301:B12:C55	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HD12	1:A:131:LYS:HE3	2.02	0.41
1:A:332:SER:HB2	1:A:352:GLN:HG2	2.03	0.41
1:D:429:PRO:HA	1:D:430:PRO:HD3	1.93	0.41
1:A:142:ALA:HB2	1:A:166:PHE:CG	2.56	0.41
2:B:209:LYS:HD3	2:B:209:LYS:HA	1.84	0.41
7:B:301:B12:H4B	7:B:301:B12:C5	2.50	0.41
2:E:88:LEU:HD12	2:E:88:LEU:HA	1.89	0.40
3:C:55:THR:HG21	3:C:64:PHE:CE2	2.57	0.40
1:D:457:ILE:HD13	1:D:457:ILE:HA	1.89	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	550/554 (99%)	533 (97%)	15 (3%)	2 (0%)	34	42
1	D	551/554 (100%)	531 (96%)	16 (3%)	4 (1%)	22	26
2	B	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
2	E	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
3	C	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
3	F	133/137 (97%)	131 (98%)	2 (2%)	0	100	100
All	All	1720/1782 (96%)	1671 (97%)	43 (2%)	6 (0%)	41	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	VAL
1	D	363	GLY
1	A	300	VAL

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Mol	Chain	Res	Type
1	A	363	GLY
1	D	300	VAL
1	D	46	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/453 (100%)	442 (98%)	9 (2%)	55	72
1	D	452/453 (100%)	441 (98%)	11 (2%)	49	66
2	B	146/164 (89%)	142 (97%)	4 (3%)	44	61
2	E	146/164 (89%)	145 (99%)	1 (1%)	84	92
3	C	115/116 (99%)	114 (99%)	1 (1%)	78	89
3	F	114/116 (98%)	111 (97%)	3 (3%)	46	63
All	All	1424/1466 (97%)	1395 (98%)	29 (2%)	55	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	38	LYS
1	A	211	LEU
1	A	232	PHE
1	A	348	ARG
1	A	364	TYR
1	A	411	ILE
1	A	437	GLU
1	A	501	TYR
2	B	110	SER
2	B	149	SER
2	B	156	GLN
2	B	221	ARG
3	C	146	ARG
1	D	28	PHE

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Mol	Chain	Res	Type
1	D	38	LYS
1	D	58	ASP
1	D	147	VAL
1	D	178	TYR
1	D	213	MET
1	D	232	PHE
1	D	348	ARG
1	D	364	TYR
1	D	501	TYR
1	D	552	GLU
2	E	55	ARG
3	F	62	ASP
3	F	79	MET
3	F	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	479	GLN
1	A	513	GLN
1	A	543	ASN
3	C	68	ASN
1	D	467	ASN
1	D	479	GLN
2	E	56	GLN
2	E	190	GLN
3	F	124	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 8 ligands modelled in this entry, 4 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
7	B12	B	301	-	90,101,101	1.28	8 (8%)	137,166,166	1.19	13 (9%)
7	B12	E	301	-	90,101,101	1.29	8 (8%)	137,166,166	1.16	11 (8%)
6	FWK	D	603	-	18,21,21	1.03	1 (5%)	17,31,31	1.47	4 (23%)
6	FWK	A	603	-	18,21,21	1.05	1 (5%)	17,31,31	1.40	3 (17%)

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	B12	B	301	-	-	3/52/223/223	0/3/11/11
7	B12	E	301	-	-	6/52/223/223	0/3/11/11
6	FWK	D	603	-	-	0/2/22/22	0/3/3/3
6	FWK	A	603	-	-	0/2/22/22	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	B12	C14-N23	-5.04	1.28	1.35
7	E	301	B12	C14-N23	-4.95	1.28	1.35
7	B	301	B12	C8B-C9B	4.40	1.49	1.40
7	E	301	B12	C8B-C9B	4.37	1.49	1.40
7	B	301	B12	C11-N23	4.36	1.45	1.37
7	E	301	B12	C11-N23	4.27	1.45	1.37
7	E	301	B12	C16-C15	-3.91	1.33	1.44
7	B	301	B12	C16-C15	-3.74	1.34	1.44
7	B	301	B12	C6B-C5B	3.22	1.48	1.40
7	E	301	B12	C6B-C5B	3.17	1.48	1.40
7	E	301	B12	C10-C9	2.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	B12	C14-C15	2.68	1.49	1.38
7	B	301	B12	C10-C9	2.66	1.46	1.39
6	A	603	FWK	C5-C4	2.65	1.47	1.40
7	E	301	B12	C14-C15	2.63	1.49	1.38
6	D	603	FWK	C5-C4	2.58	1.47	1.40
7	E	301	B12	C19-N24	-2.21	1.44	1.48
7	B	301	B12	C19-N24	-2.05	1.45	1.48

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	301	B12	C2P-C1P-N59	-4.41	106.43	112.93
7	B	301	B12	C9-C10-C11	-3.78	120.50	125.97
7	E	301	B12	C13-C14-N23	3.74	114.19	109.10
7	B	301	B12	C17-C16-C15	3.62	131.96	126.26
7	B	301	B12	C2P-C1P-N59	-3.53	107.73	112.93
7	E	301	B12	C17-C16-C15	3.50	131.77	126.26
7	B	301	B12	C13-C14-N23	3.49	113.85	109.10
7	E	301	B12	C13-C14-C15	-3.39	119.13	124.32
7	E	301	B12	C9-C10-C11	-3.22	121.31	125.97
6	D	603	FWK	N3-C2-N1	-3.17	123.73	128.68
7	B	301	B12	C13-C14-C15	-3.15	119.51	124.32
6	A	603	FWK	N3-C2-N1	-3.06	123.89	128.68
7	B	301	B12	C17-C16-N24	-2.77	106.87	111.15
7	E	301	B12	C17-C16-N24	-2.77	106.88	111.15
7	E	301	B12	C55-C56-C57	-2.73	105.28	111.23
6	D	603	FWK	C6'-C5'-C4'	-2.72	105.78	113.27
7	B	301	B12	C20-C1-N21	2.68	114.67	110.27
7	E	301	B12	C30-C3-C2	-2.62	113.55	119.09
7	B	301	B12	C48-C13-C14	2.58	114.91	108.49
7	B	301	B12	C53-C15-C16	2.53	124.73	120.38
7	E	301	B12	C48-C13-C14	2.53	114.78	108.49
7	E	301	B12	C20-C1-N21	2.50	114.37	110.27
7	B	301	B12	C55-C56-C57	-2.49	105.78	111.23
6	A	603	FWK	C4-C5-N7	-2.43	106.86	109.40
7	E	301	B12	C53-C15-C16	2.34	124.41	120.38
6	A	603	FWK	C6'-C5'-C4'	-2.26	107.04	113.27
7	B	301	B12	C4B-C9B-N3B	2.25	136.92	130.88
7	B	301	B12	C13-C12-C11	-2.17	98.51	100.97
6	D	603	FWK	C4-C5-N7	-2.09	107.22	109.40
7	B	301	B12	C8B-C9B-N3B	-2.03	103.55	107.83
6	D	603	FWK	C3'-C2'-C1'	2.01	104.01	100.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

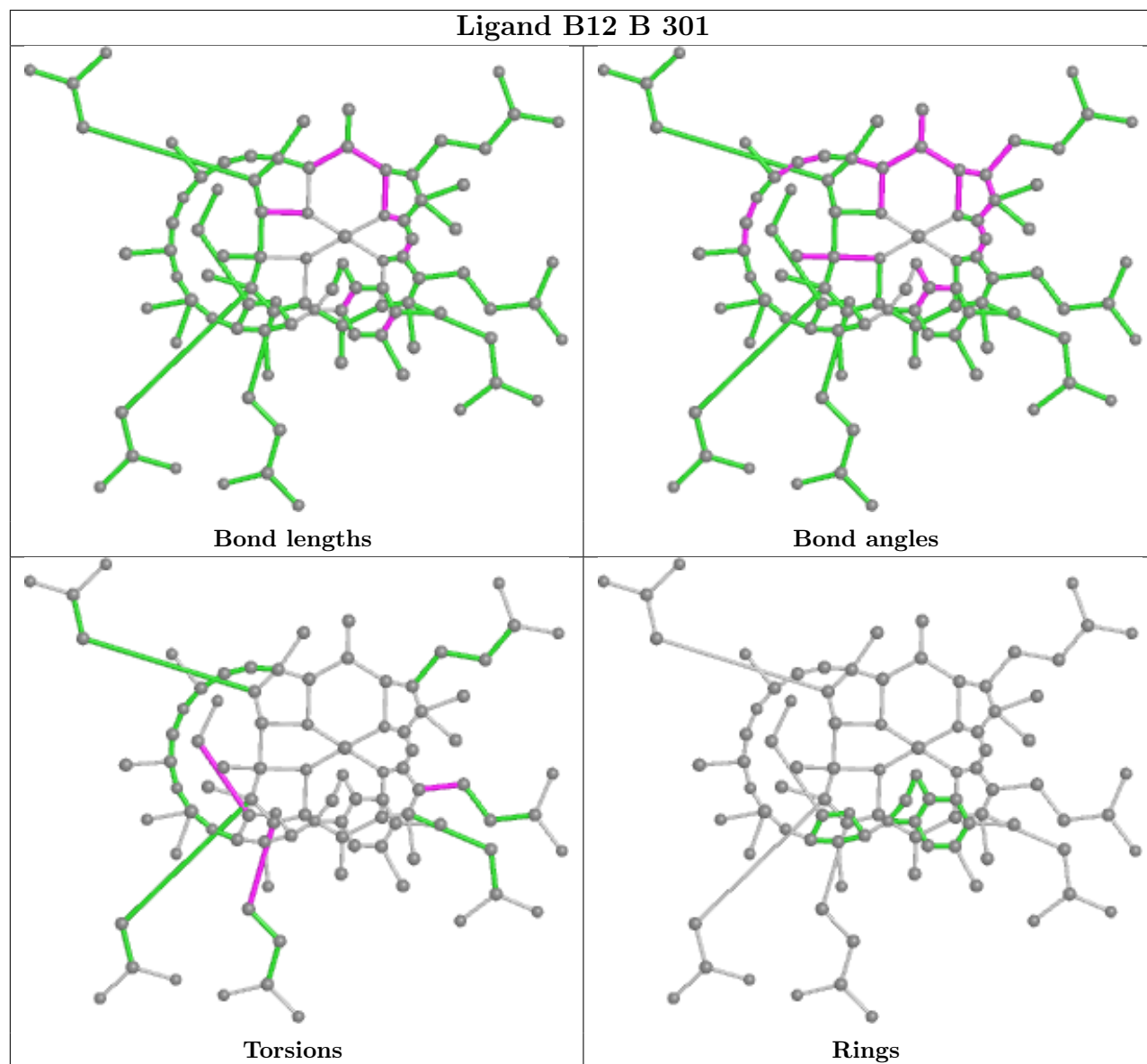
Mol	Chain	Res	Type	Atoms
7	E	301	B12	C3R-C4R-C5R-O8R
7	E	301	B12	O6R-C4R-C5R-O8R
7	E	301	B12	C2-C3-C30-C31
7	B	301	B12	O6R-C4R-C5R-O8R
7	E	301	B12	C4-C3-C30-C31
7	E	301	B12	C17-C18-C60-C61
7	B	301	B12	C42-C41-C8-C9
7	E	301	B12	C19-C18-C60-C61
7	B	301	B12	C2-C3-C30-C31

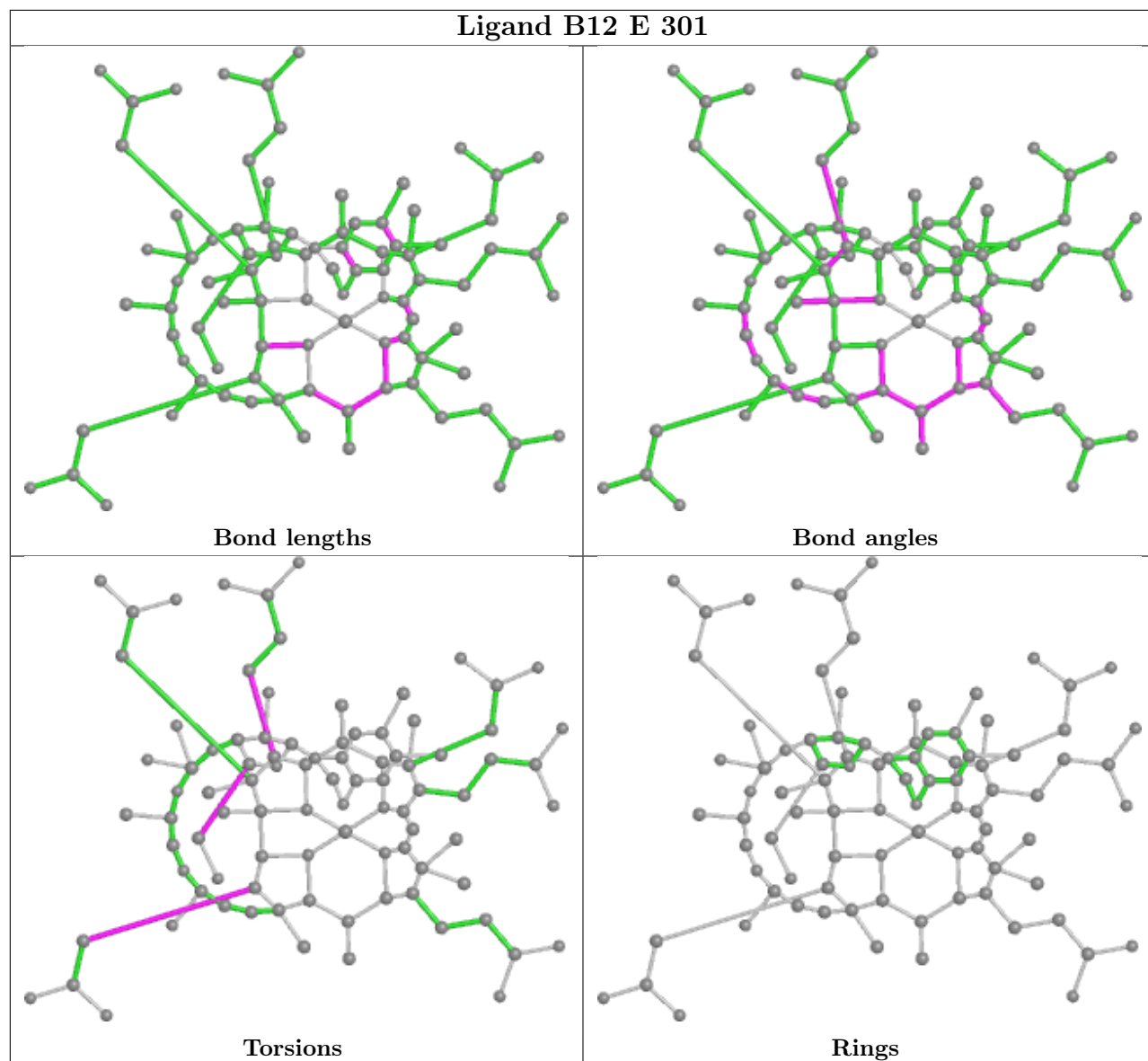
There are no ring outliers.

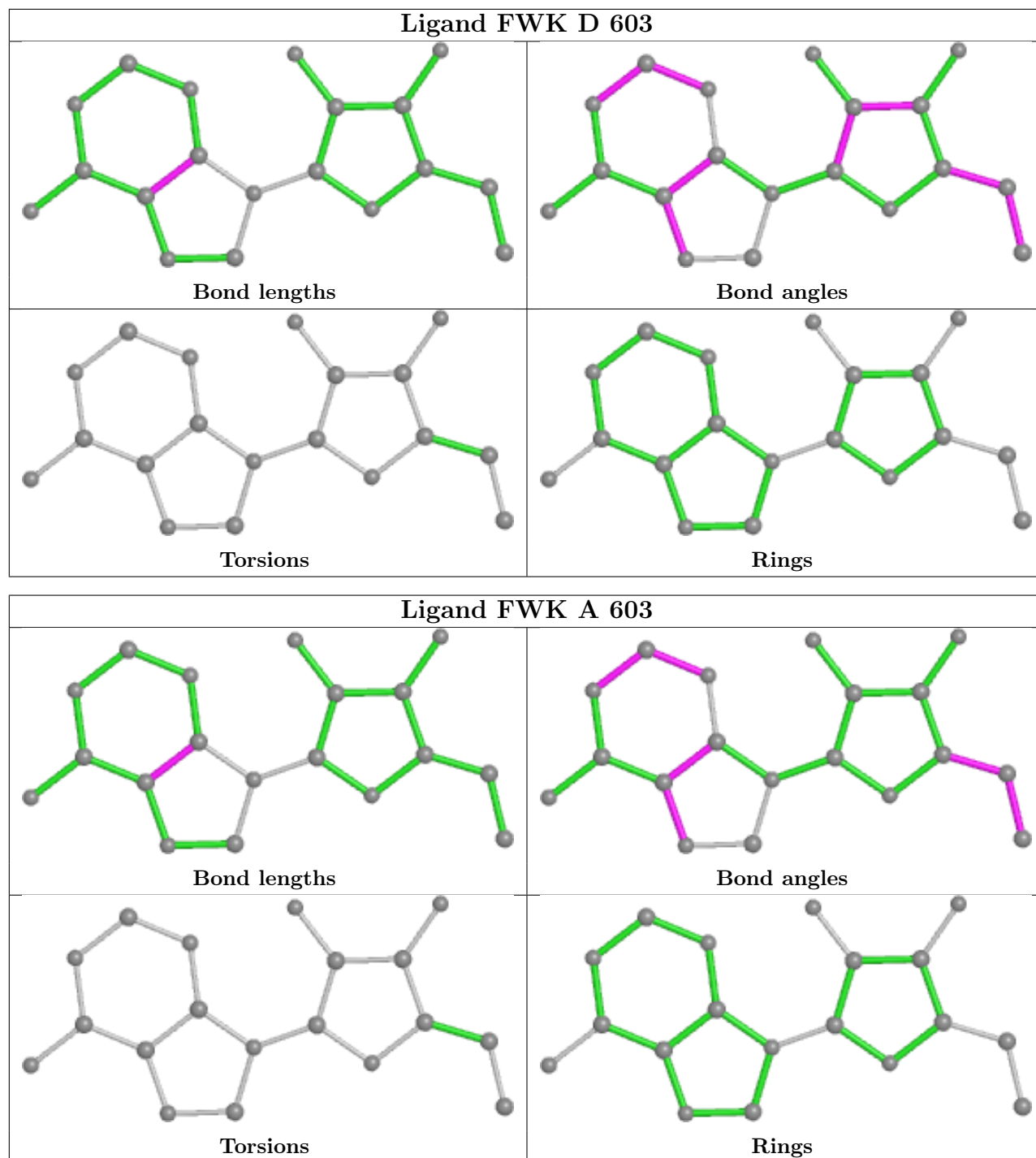
2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	301	B12	7	0
7	E	301	B12	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	552/554 (99%)	-0.24	3 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">94</span>	10, 20, 37, 75	1 (0%)
1	D	553/554 (99%)	0.13	18 (3%) <span style="border: 1px solid gray; padding: 2px;">46</span> <span style="border: 1px solid gray; padding: 2px;">53</span>	12, 25, 50, 74	1 (0%)
2	B	178/200 (89%)	0.01	3 (1%) <span style="border: 1px solid blue; padding: 2px;">70</span> <span style="border: 1px solid blue; padding: 2px;">76</span>	17, 28, 44, 62	0
2	E	178/200 (89%)	0.65	22 (12%) <span style="border: 1px solid red; padding: 2px;">4</span> <span style="border: 1px solid red; padding: 2px;">5</span>	25, 39, 60, 70	0
3	C	136/137 (99%)	-0.23	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	14, 28, 44, 70	1 (0%)
3	F	135/137 (98%)	0.47	16 (11%) <span style="border: 1px solid red; padding: 2px;">4</span> <span style="border: 1px solid red; padding: 2px;">6</span>	20, 33, 73, 95	3 (2%)
All	All	1732/1782 (97%)	0.05	62 (3%) <span style="border: 1px solid gray; padding: 2px;">42</span> <span style="border: 1px solid gray; padding: 2px;">49</span>	10, 26, 53, 95	6 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	553	ASP	8.4
1	A	553	ASP	7.5
3	F	56	ALA	6.0
3	F	60	THR	6.0
3	F	77	GLN	5.2
3	F	70	LEU	4.4
3	F	79	MET	4.3
3	F	59	LYS	4.2
2	E	49	THR	4.1
1	D	152	VAL	3.8
2	E	51	VAL	3.8
1	D	480	GLY	3.7
1	D	43	ILE	3.7
2	E	180	SER	3.6
1	A	552	GLU	3.5
3	F	61	LEU	3.4
2	E	74	ALA	3.3
1	D	481	GLY	3.2
2	E	87	ILE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	47	ALA	3.2
3	F	64	PHE	3.1
2	E	73	LEU	3.1
2	E	186	THR	3.1
3	F	76	ALA	3.1
2	E	182	GLN	3.0
2	E	213	THR	3.0
1	D	552	GLU	2.9
3	F	54	LYS	2.9
2	E	46	GLY	2.8
2	E	214	GLY	2.8
2	E	212	VAL	2.7
2	B	73	LEU	2.7
1	D	433	ASP	2.6
2	E	107	CYS	2.6
3	F	62	ASP	2.5
1	D	546	GLY	2.5
3	F	75	THR	2.5
1	A	511	ASP	2.5
1	D	333	SER	2.5
2	E	48	LEU	2.4
3	F	52	TRP	2.4
2	E	221	ARG	2.4
2	E	67	VAL	2.4
1	D	479	GLN	2.4
3	F	58	ASN	2.4
2	E	210	TYR	2.3
1	D	430	PRO	2.3
3	F	41	SER	2.3
2	B	178	ARG	2.2
2	E	59	GLN	2.2
2	E	181	PRO	2.2
3	F	55	THR	2.2
2	E	185	PRO	2.2
1	D	417	ARG	2.2
1	D	477	LEU	2.2
2	E	50	GLU	2.1
2	B	112	ASP	2.1
1	D	331	ALA	2.1
2	E	183	PRO	2.1
1	D	484	ASP	2.1
1	D	437	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	184	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

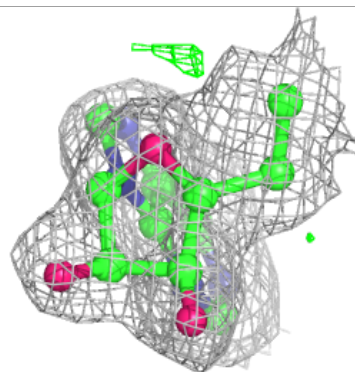
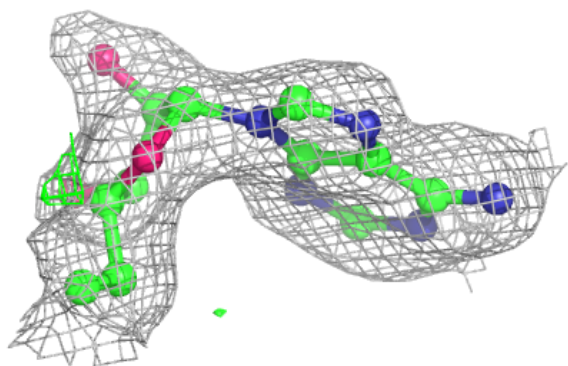
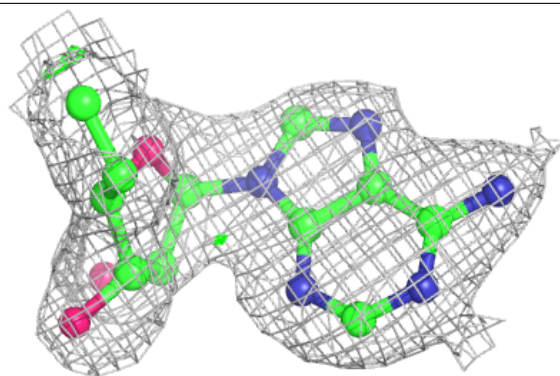
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	FWK	D	603	19/19	0.94	0.16	20,25,32,32	0
6	FWK	A	603	19/19	0.95	0.13	17,21,24,25	0
7	B12	E	301	91/91	0.95	0.12	21,27,37,51	0
7	B12	B	301	91/91	0.96	0.12	15,21,28,31	0
5	K	A	602	1/1	0.96	0.14	23,23,23,23	0
4	CA	D	601	1/1	0.98	0.08	21,21,21,21	0
4	CA	A	601	1/1	0.99	0.05	17,17,17,17	0
5	K	D	602	1/1	0.99	0.12	22,22,22,22	0

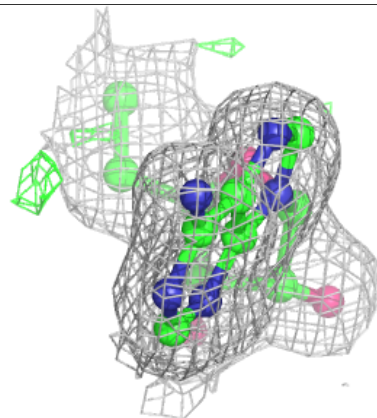
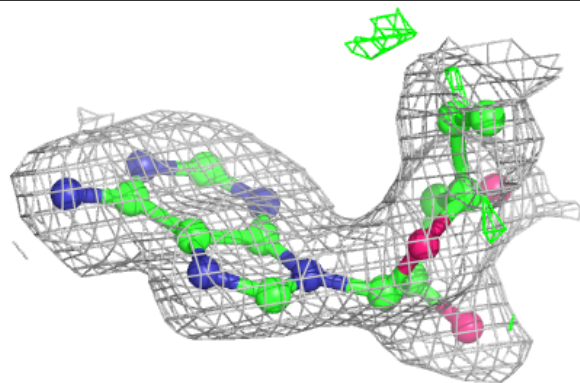
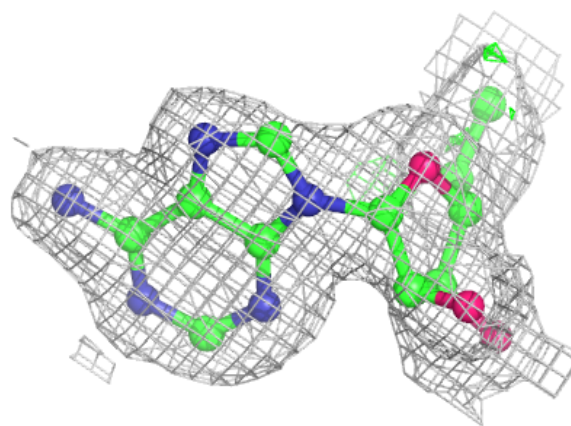
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FWK D 603:**

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

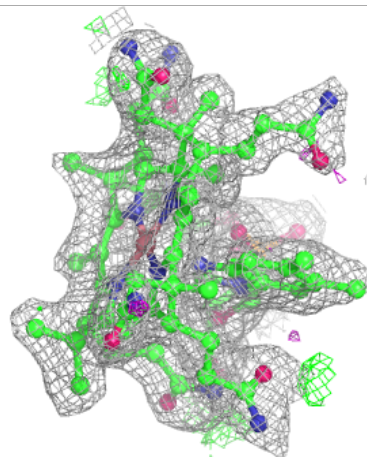
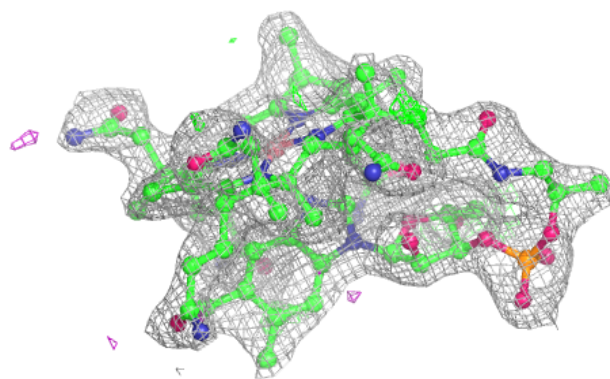
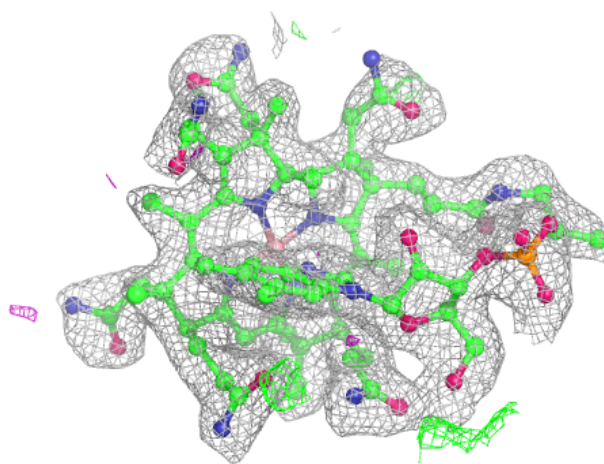
**Electron density around FWK A 603:**

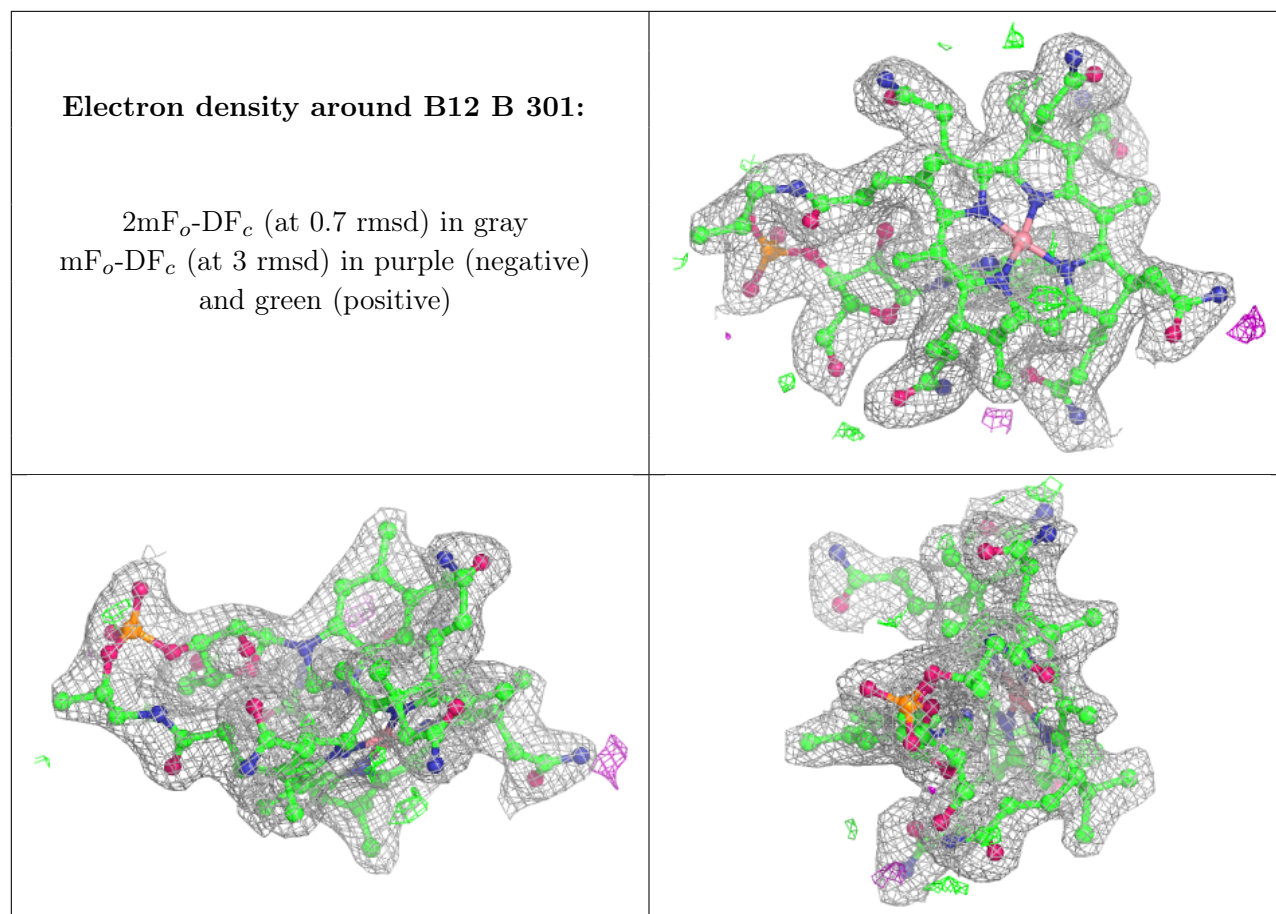
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around B12 E 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.