WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 22, 2023 – 10:06 PM JST

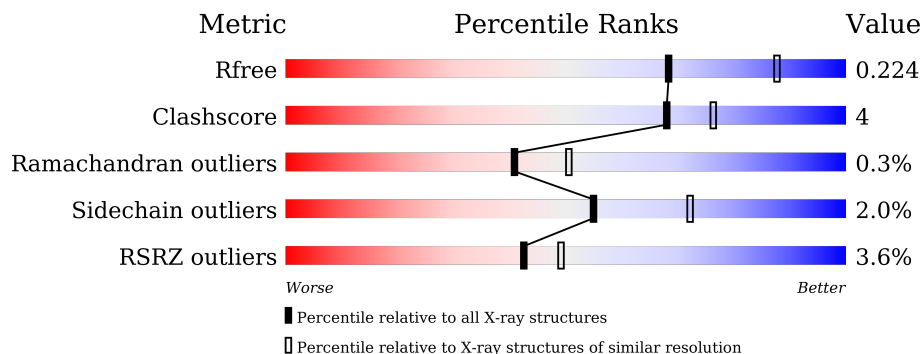|		
PDB ID	:	7XRK
Title	:	Diol dehydratase complexed with AdoMeCbl
Authors	:	Shibata, N.; Toraya, T.
Deposited on	:	2022-05-10
Resolution	:	2.30 Å(reported)

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	Percentile Ranks	Value
Rfree		0.224
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		2.0%
RSRZ outliers		3.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◧ Percentile relative to X-ray structures of similar resolution

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 >=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 <=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	3% / 90% 10% •
2	B	200	2% / 80% 9% 11%
2	E	200	11% / 80% 8% 11%
3	C	137	94% 5% •
3	F	137	12% / 88% 9% ••

2 Entry composition ⓘ

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
1	A	552	Total 4210	C 2624	N 728	O 830	S 28	0	0	0
1	D	553	Total 4218	C 2629	N 729	O 831	S 29	0	0	0

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
2	B	178	Total 1358	C 859	N 244	O 253	S 2	0	0	0
2	E	178	Total 1357	C 859	N 244	O 252	S 2	0	0	0

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
3	C	136	Total	C	N	O	S	0	0	0
			1087	678	194	212	3			
3	F	135	Total	C	N	O	S	0	0	0
			1078	674	193	208	3			

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: $C_{11}H_{15}N_5O_3$) (labeled as "Ligand of Interest" by depositor).
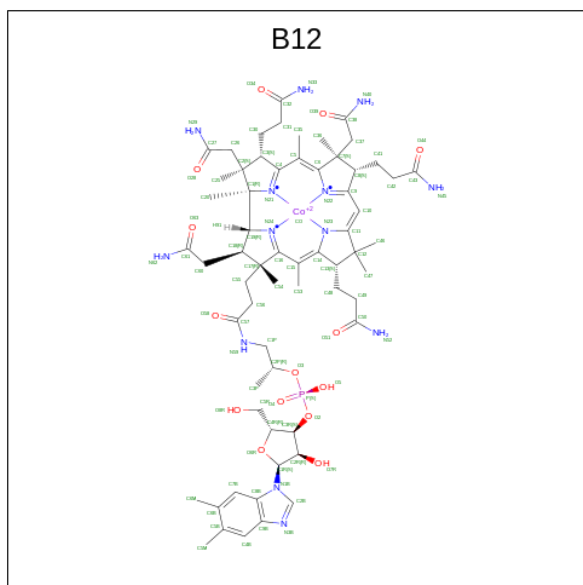
FWK
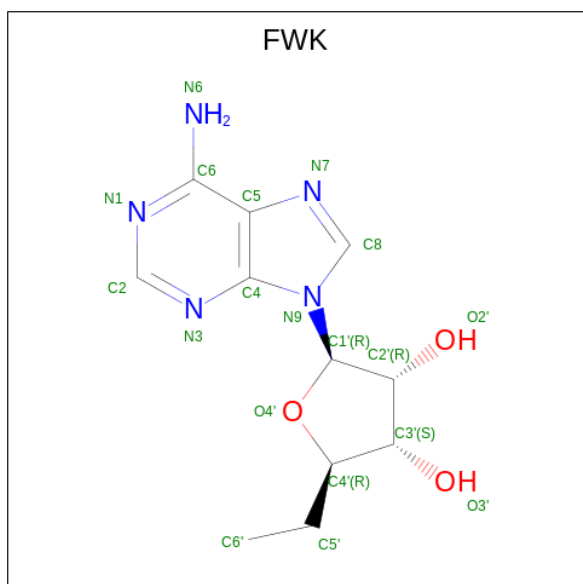
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 19	C 11	N 5	O 3	0	0

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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).

B12

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

- Molecule 8 is water.

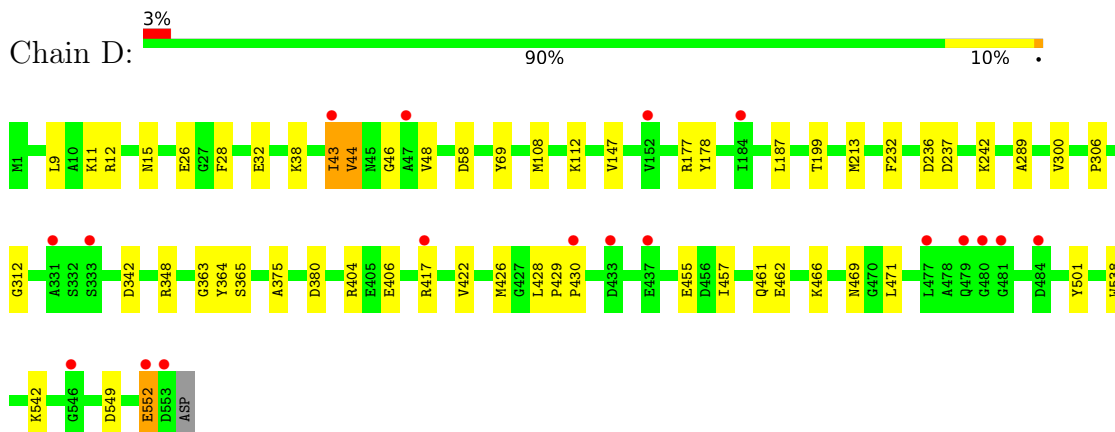| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	150	150	150	0	0
			Total	O		
8	B	36	36	36	0	0
			Total	O		
8	C	29	29	29	0	0
			Total	O		
8	D	140	140	140	0	0
			Total	O		
8	E	28	28	28	0	0
			Total	O		
8	F	25	25	25	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
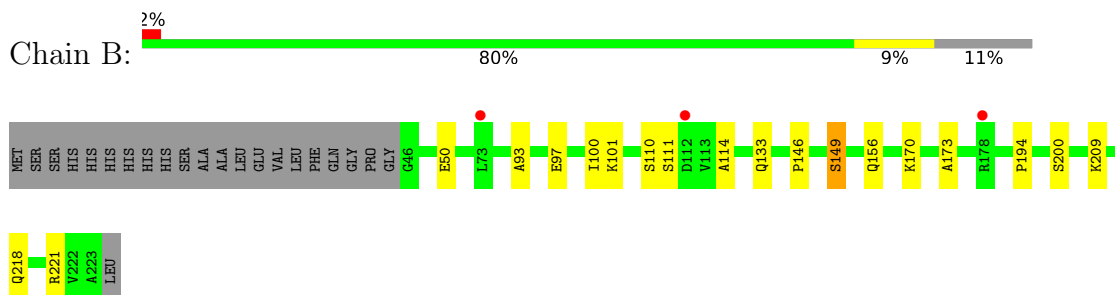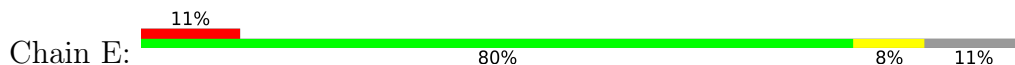
• Molecule 1: Diol dehydrase alpha subunit
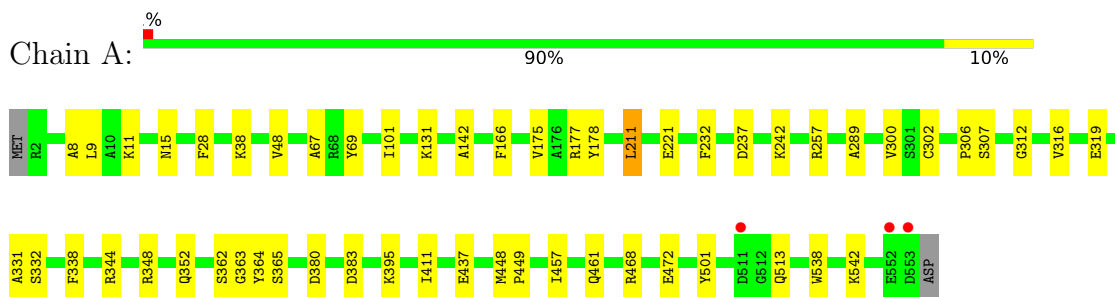
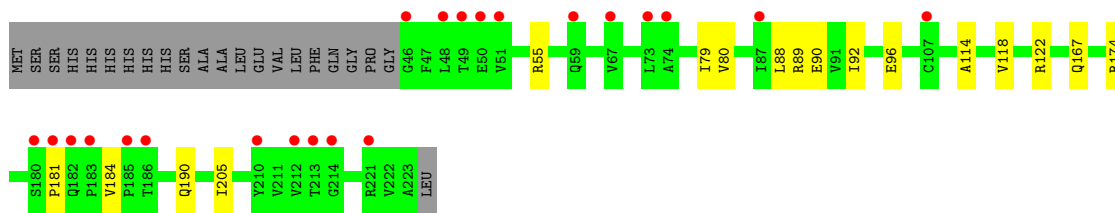• Molecule 1: Diol dehydrase alpha subunit

• Molecule 2: Diol dehydrase beta subunit

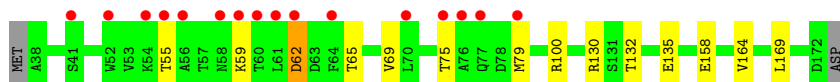• Molecule 2: Diol dehydrase beta subunit

MET SER HIS HIS HIS HIS HIS SER ALA ALA LEU GLU VAL LEU PHE GLN GLY PRO GLY G46 F47 L48 T49 E50 V51 R55 Q59 V67 L73 A74 I79 V80 I87 L88 R89 E90 V91 I92 E96 C107 A114 V118 R122 Q167 R174

S180 P181 Q182 P183 V184 P185 I186 Q190 I205 Y210 V211 V212 T213 G214 R221 V222 A223 LEU

• Molecule 3: Diol dehydrase gamma subunit

Chain C: 94%   5% •

MET A38 M47 T55 F64 E67 R146 V164 L169 D173

• Molecule 3: Diol dehydrase gamma subunit

Chain F: 88%   9% ••

MET A38 S41 W52 V53 K54 T55 A56 T57 N58 K59 T60 L61 D62 D63 F64 T65 V69 L70 T75 A76 Q77 D78 M79 R100 R130 S131 T132 E135 E158 V164 L169 D172 ASP

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.06 (at 2.29Å)	Xtriage
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^2)	21.3	Xtriage
Anisotropy	1.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.6	EDS
L-test for twinning [2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13940	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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 ⓘ

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

5 of 6 Ramachandran outliers are listed below:

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

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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	28	PHE
3	F	79	MET
1	D	147	VAL
1	D	552	GLU
1	D	58	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	56	GLN
2	E	190	GLN
3	F	124	ASN
1	A	543	ASN
3	C	68	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

The worst 5 of 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

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.
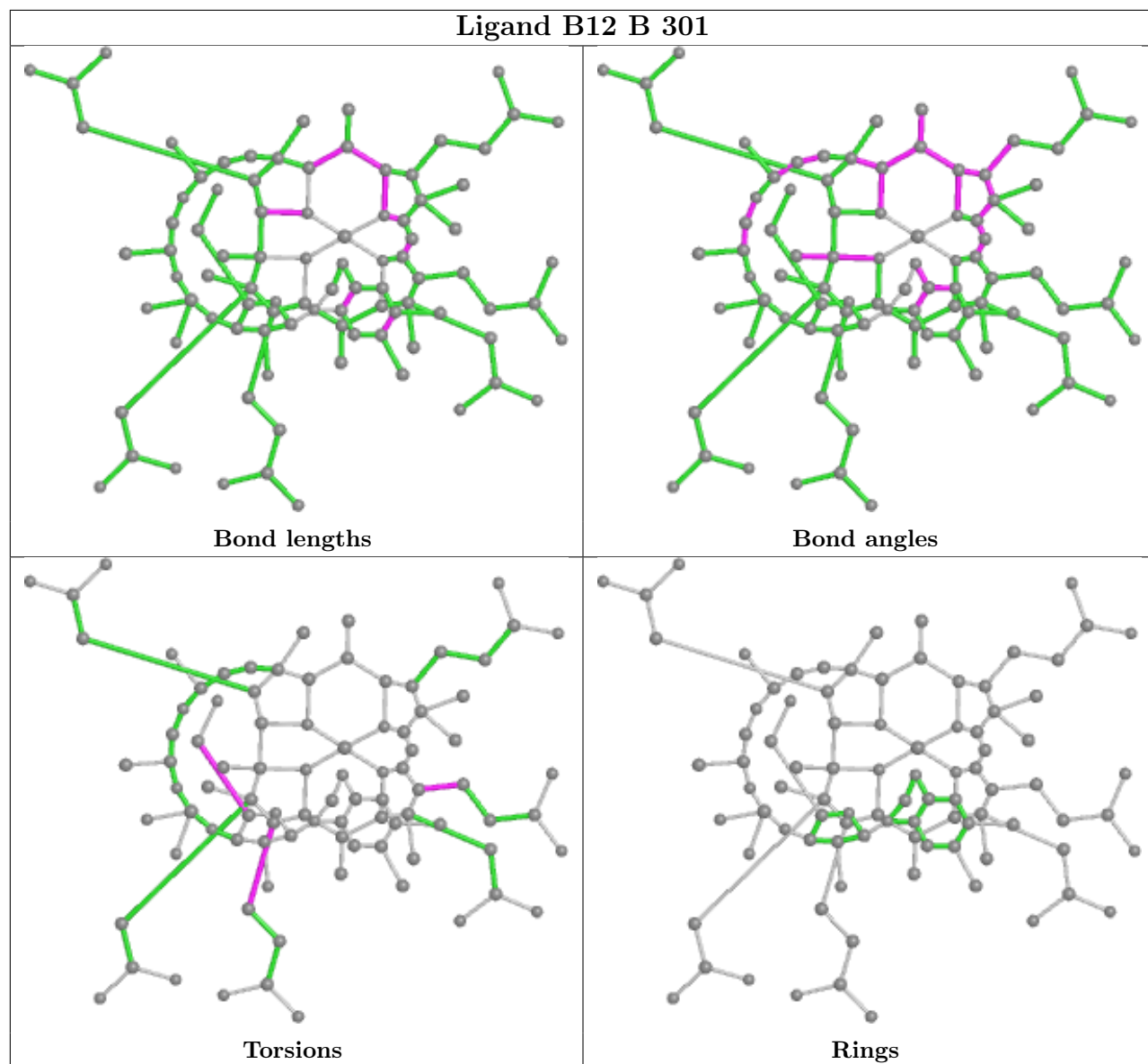
5 of 9 torsion outliers are listed below:

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

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand B12 B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FWK D 603

Bond lengths

Bond angles

Torsions

Rings

Ligand FWK A 603

Bond lengths

Bond angles

Torsions

Rings
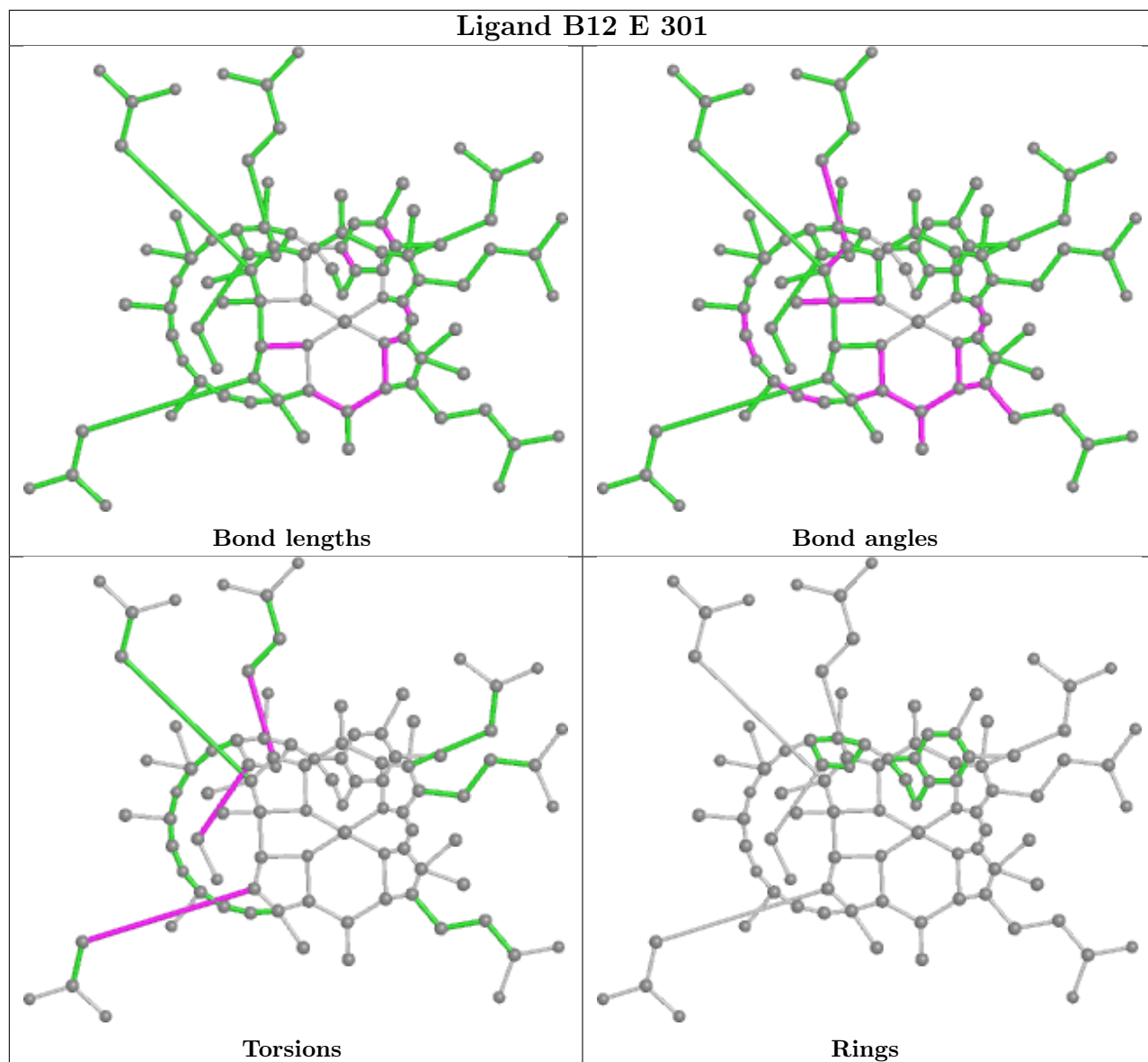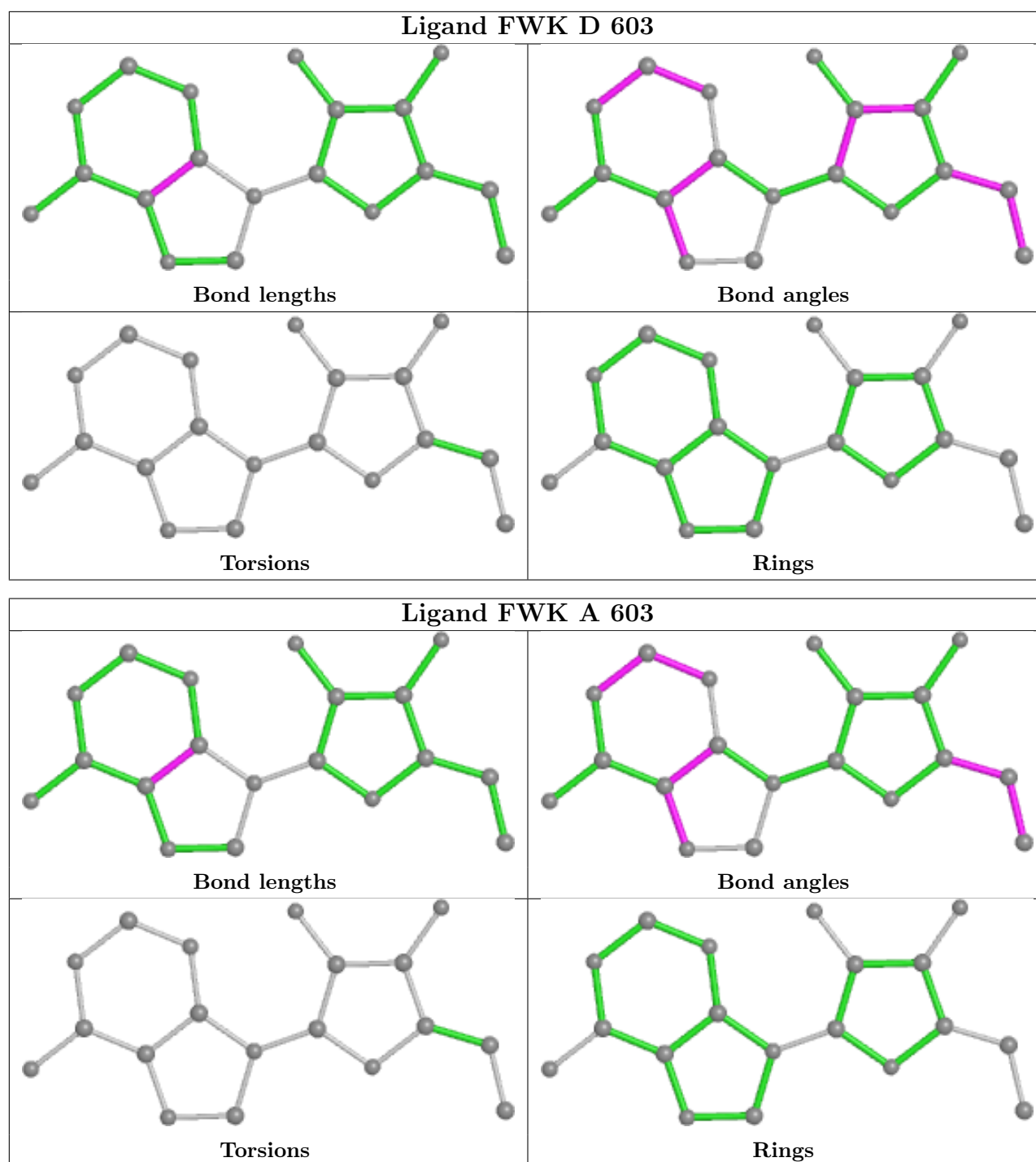
5.7 Other polymers ⓘ

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, 95th 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(Å²)	Q<0.9
1	A	552/554 (99%)	-0.24	3 (0%)	91	94	10, 20, 37, 75	1 (0%)
1	D	553/554 (99%)	0.13	18 (3%)	46	53	12, 25, 50, 74	1 (0%)
2	B	178/200 (89%)	0.01	3 (1%)	70	76	17, 28, 44, 62	0
2	E	178/200 (89%)	0.65	22 (12%)	4	5	25, 39, 60, 70	0
3	C	136/137 (99%)	-0.23	0	100	100	14, 28, 44, 70	1 (0%)
3	F	135/137 (98%)	0.47	16 (11%)	4	6	20, 33, 73, 95	3 (2%)
All	All	1732/1782 (97%)	0.05	62 (3%)	42	49	10, 26, 53, 95	6 (0%)

The worst 5 of 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

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

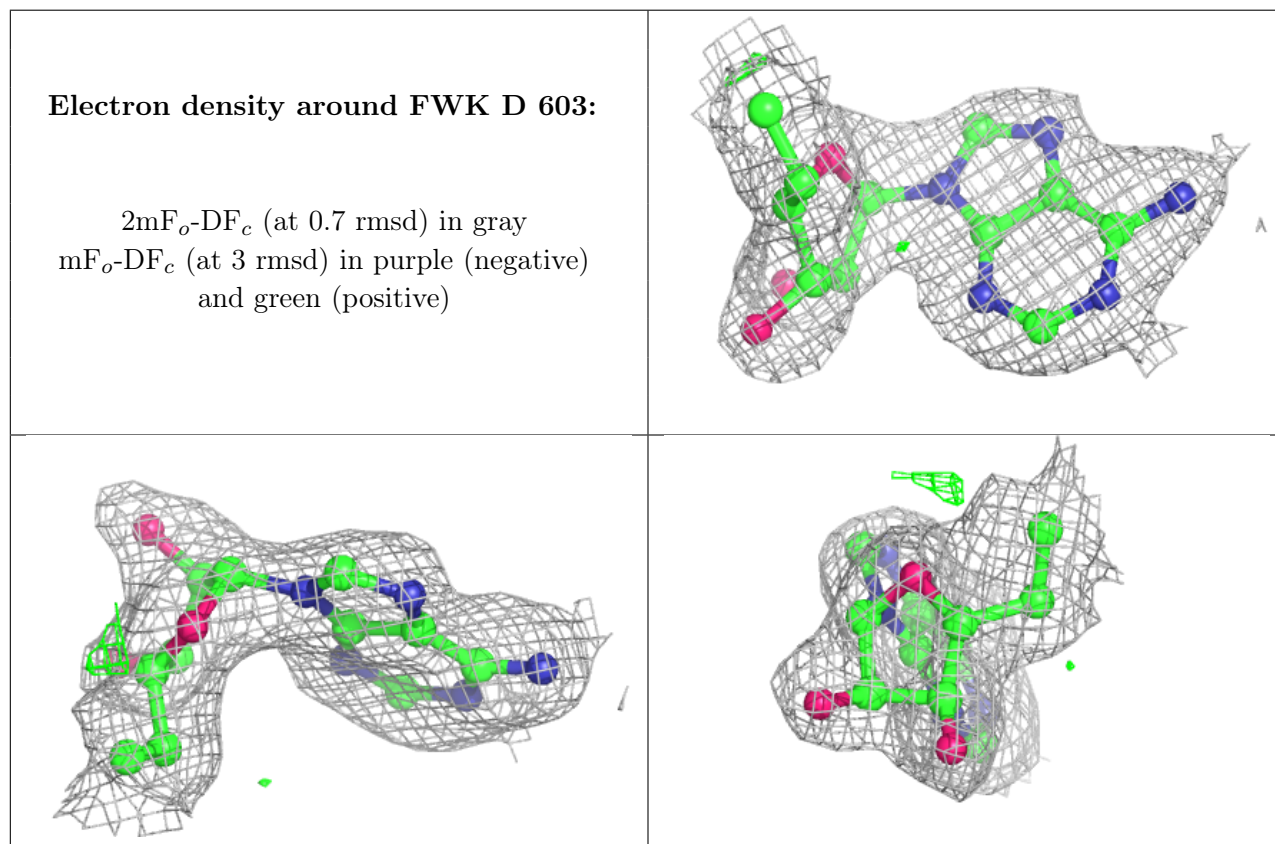There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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($Å^2$)	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.
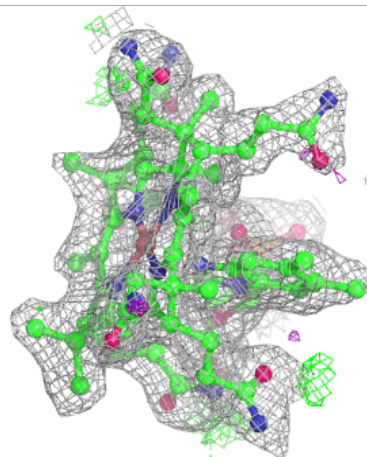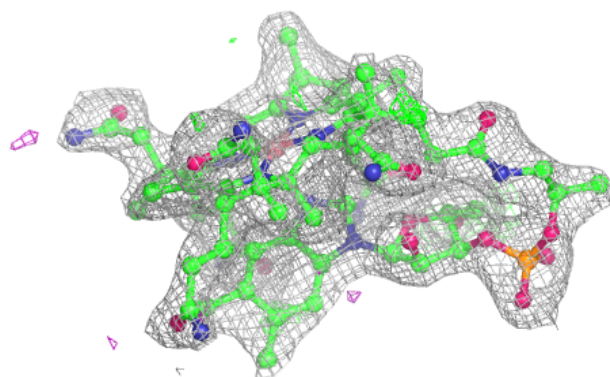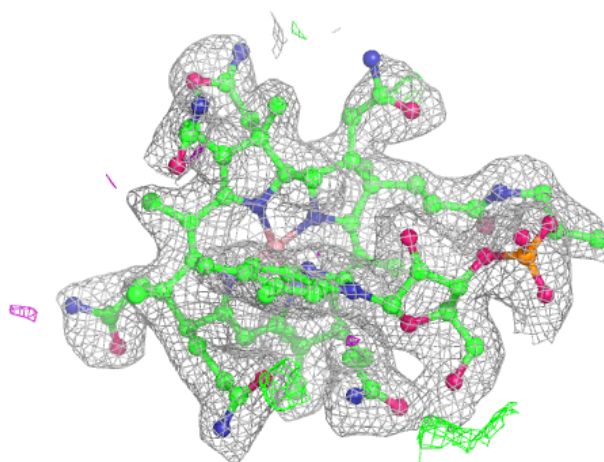

Electron density around FWK D 603:

$2mF_o$-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)
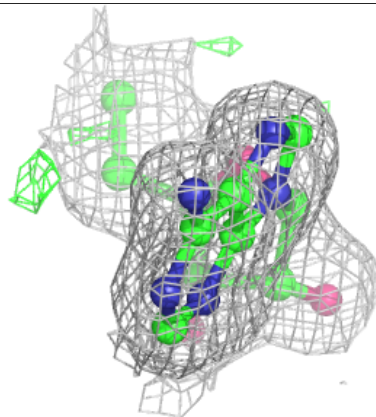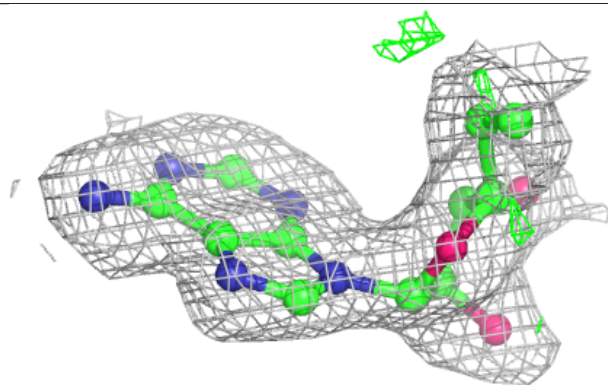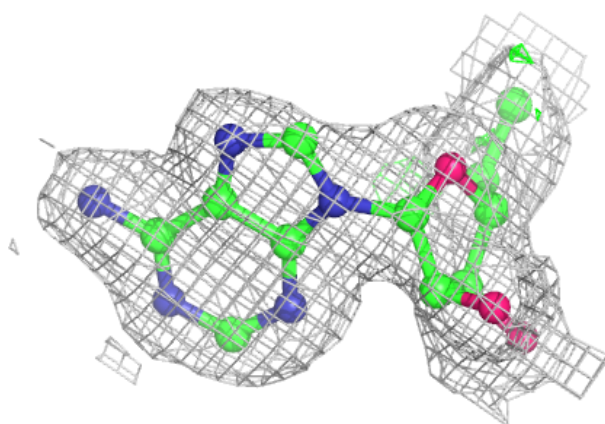
Electron density around B12 E 301:

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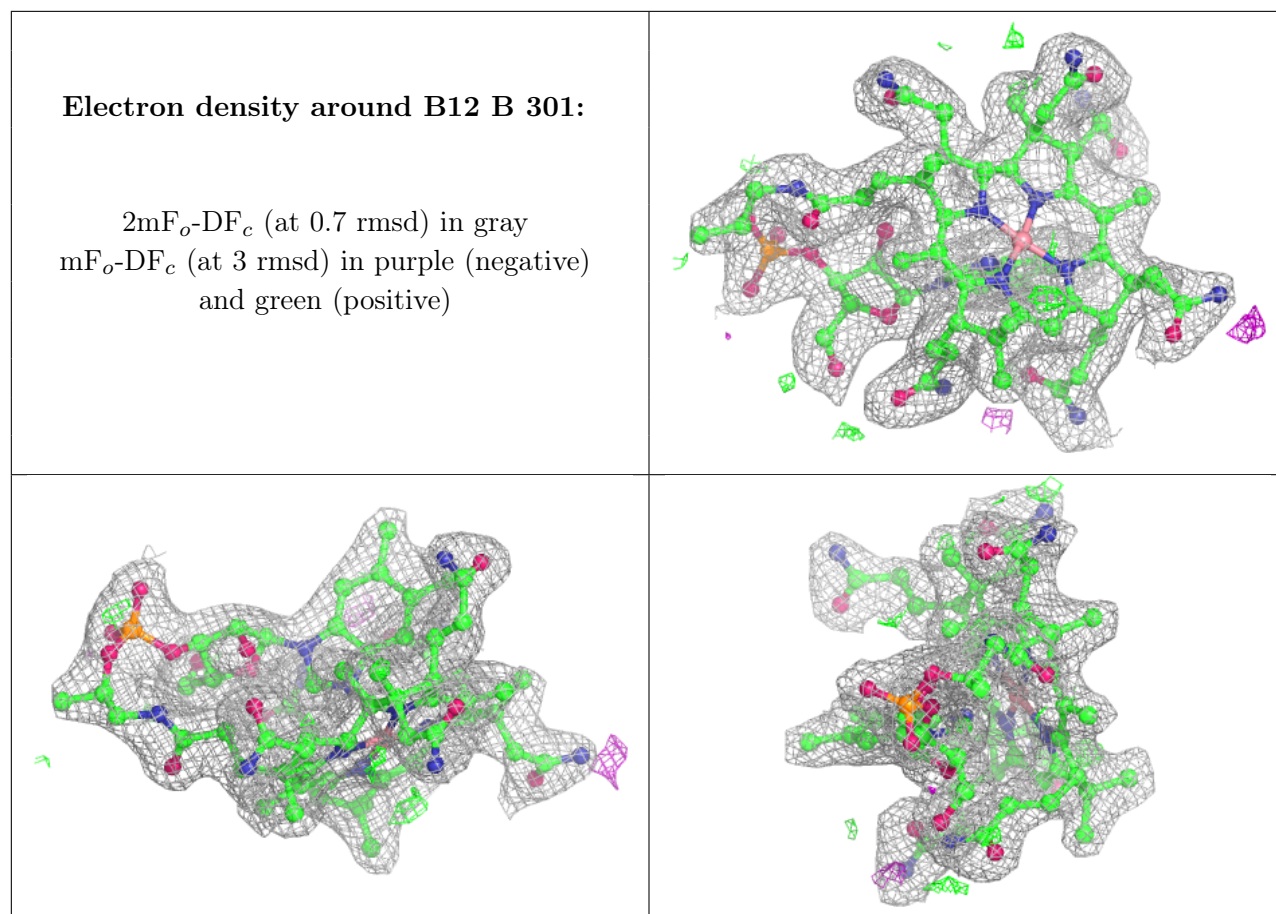and green (positive)

Electron density around B12 B 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 ⓘ

There are no such residues in this entry.