Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 11:01 PM JST

PDB ID	:	7XRL
Title	:	Diol dehydratase complexed with AdoMeCbl and 1,2-propanediol
Authors	:	Shibata, N.; Toraya, T.
Deposited on	:	2022-05-10
Resolution	:	1.75 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

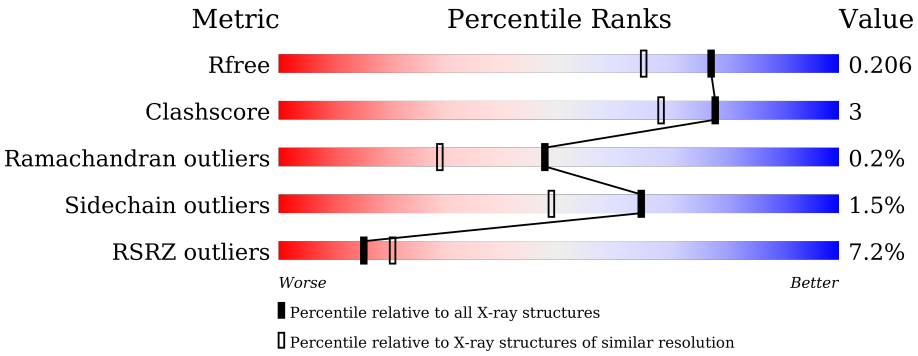
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	95%
1	D	554	2% 94% 6%
2	B	200	2% 84% 6% 10%
2	E	200	52% 77% 12% 11%
3	C	137	96%
3	F	137	4% 88% 10%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15201 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	C	N	O	S	0	3	0
			4224	2636	729	830	29			
1	D	554	Total	C	N	O	S	0	0	0
			4227	2635	730	833	29			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total	C	N	O	S	0	2	0
			1376	871	246	256	3			
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

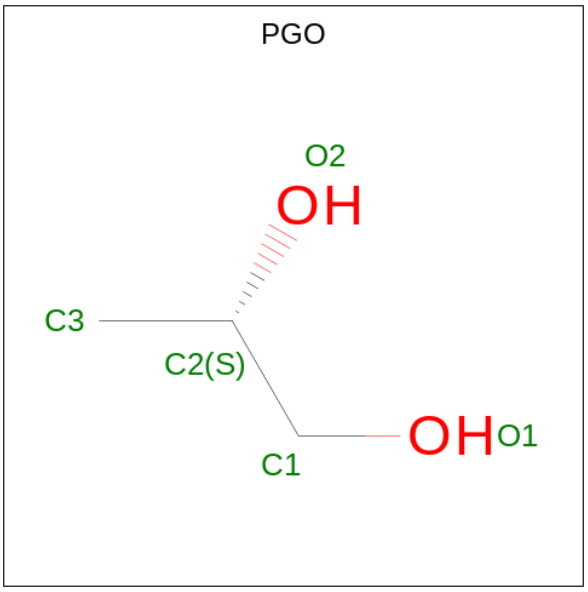
- Molecule 3 is a protein called Diol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	136	Total	C	N	O	S	0	6	0
			1117	700	197	216	4			
3	F	136	Total	C	N	O	S	0	2	0
			1095	684	194	213	4			

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 S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 3 2	0	0
4	D	1	Total C O 5 3 2	0	0

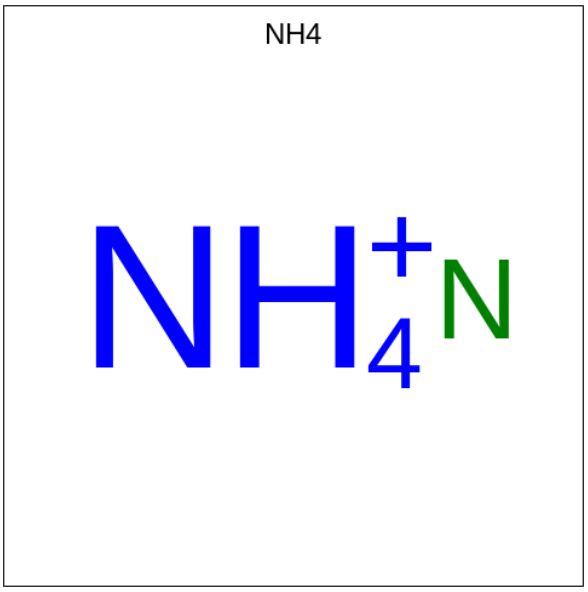
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

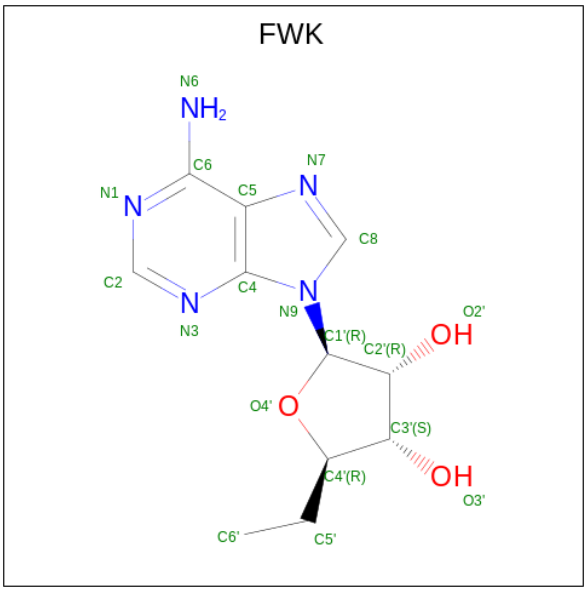
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N 1 1	0	0
7	D	1	Total N 1 1	0	0

- Molecule 8 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).



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

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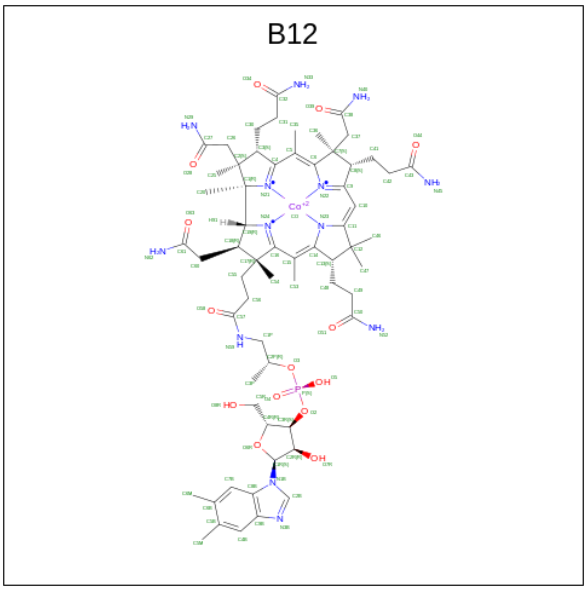
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			19	11	5	3		

- Molecule 9 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
9	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
9	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 10 is water.

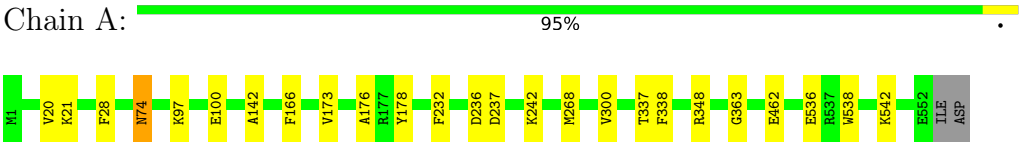
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	600	Total	O	0	0
			600	600		
10	B	173	Total	O	0	0
			173	173		
10	C	162	Total	O	0	0
			162	162		
10	D	455	Total	O	0	0
			455	455		
10	E	44	Total	O	0	0
			44	44		
10	F	135	Total	O	0	0
			135	135		

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.

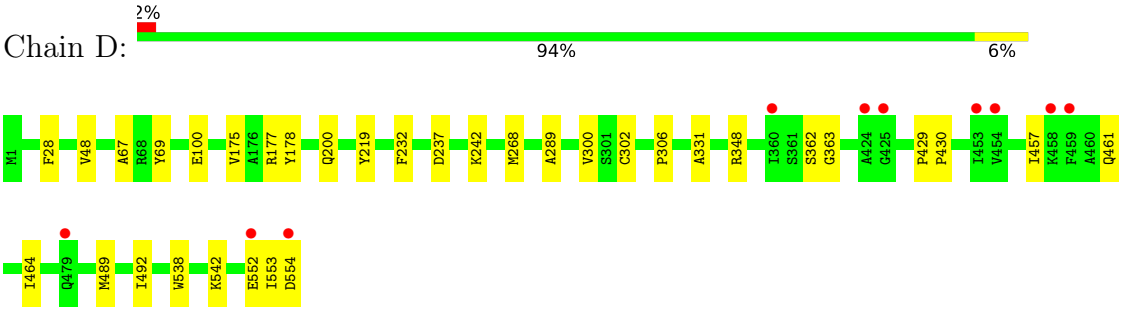
• Molecule 1: Diol dehydrase alpha subunit

Chain A:



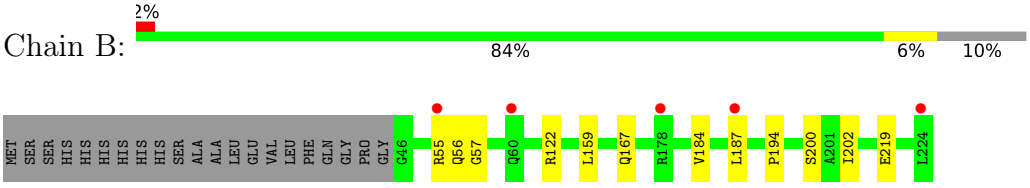
• Molecule 1: Diol dehydrase alpha subunit

Chain D:



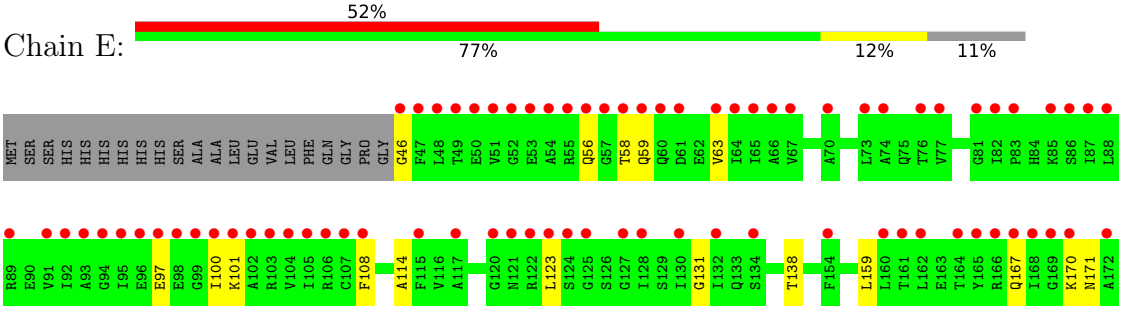
• Molecule 2: Diol dehydrase beta subunit

Chain B:



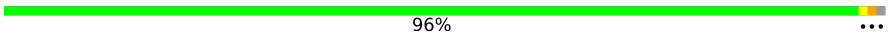
• Molecule 2: Diol dehydrase beta subunit

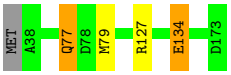
Chain E:



• Molecule 3: Diol dehydrase gamma subunit

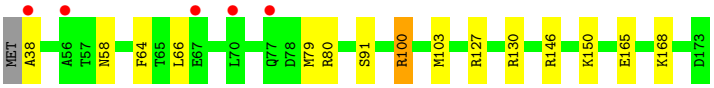
Chain C:





• Molecule 3: Diol dehydrase gamma subunit

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.72Å 117.25Å 201.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.72 – 1.75 45.72 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.72-1.75) 99.9 (45.72-1.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.167 , 0.206 0.167 , 0.206	Depositor DCC
R_{free} test set	4912 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15201	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FWK, CA, K, NH4, B12, PGO

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	0.38	0/4305	0.60	0/5831
1	D	0.36	0/4299	0.56	0/5821
2	B	0.33	0/1404	0.55	0/1899
2	E	0.27	0/1379	0.49	0/1867
3	C	0.32	0/1150	0.55	0/1553
3	F	0.30	0/1116	0.54	0/1507
All	All	0.35	0/13653	0.56	0/18478

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4224	0	4169	16	0
1	D	4227	0	4160	14	0
2	B	1376	0	1432	11	0
2	E	1357	0	1405	16	0
3	C	1117	0	1145	4	0
3	F	1095	0	1110	12	0
4	A	5	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	6	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	19	0	0	0	0
8	D	19	0	0	0	0
9	B	91	0	88	7	0
9	E	91	0	88	9	0
10	A	600	0	0	4	0
10	B	173	0	0	1	0
10	C	162	0	0	1	0
10	D	455	0	0	2	0
10	E	44	0	0	3	0
10	F	135	0	0	6	0
All	All	15201	0	13609	80	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 (80) 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)
3:C:127[A]:ARG:NH2	10:C:201:HOH:O	2.10	0.84
3:F:100:ARG:HH12	3:F:103[A]:MET:HE1	1.47	0.78
9:E:301:B12:C2B	9:E:301:B12:H492	2.15	0.77
9:B:301:B12:C2B	9:B:301:B12:H492	2.18	0.73
9:B:301:B12:H601	9:B:301:B12:H262	1.74	0.69
9:E:301:B12:H601	9:E:301:B12:H262	1.72	0.68
1:D:69:TYR:O	3:F:100:ARG:HD3	1.94	0.67
9:E:301:B12:H552	9:E:301:B12:H531	1.77	0.66
2:E:193:ARG:NH2	10:E:402:HOH:O	2.28	0.65
1:A:20[B]:VAL:HG11	2:B:202:ILE:HD11	1.78	0.65
2:E:97:GLU:OE2	10:E:401:HOH:O	2.14	0.64
2:E:46:GLY:N	10:E:404:HOH:O	2.31	0.63
2:E:171:ASN:ND2	2:E:182:GLN:O	2.29	0.62
3:F:100:ARG:HG2	10:F:295:HOH:O	2.01	0.59
2:E:174:ARG:HD3	2:E:181:PRO:HB3	1.86	0.58
9:B:301:B12:H552	9:B:301:B12:H531	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20[B]:VAL:HG12	1:A:21:LYS:O	2.04	0.57
3:F:64:PHE:CE1	3:F:79:MET:HG2	2.39	0.57
3:F:146:ARG:NH1	10:F:202:HOH:O	2.39	0.56
2:B:55:ARG:NH2	10:B:403:HOH:O	2.38	0.55
2:E:159:LEU:HD21	2:E:189:ASP:HB3	1.89	0.55
9:B:301:B12:H362	9:B:301:B12:H351	1.88	0.54
1:A:538:TRP:NE1	1:A:542:LYS:HE3	2.22	0.54
1:D:553:ILE:O	1:D:554:ASP:HB2	2.07	0.54
1:A:20[B]:VAL:CG1	2:B:202:ILE:HD11	2.38	0.54
3:F:127:ARG:HB2	3:F:130:ARG:HG3	1.89	0.54
3:F:150:LYS:NZ	10:F:203:HOH:O	2.41	0.53
2:E:167:GLN:HG3	2:E:184:VAL:HG22	1.90	0.53
2:B:55:ARG:HH12	2:B:57:GLY:HA2	1.73	0.53
2:E:63:VAL:HG23	2:E:100:ILE:HG21	1.91	0.52
2:B:56[A]:GLN:NE2	2:B:122:ARG:O	2.43	0.52
1:A:97:LYS:HB2	1:A:100:GLU:HG3	1.93	0.51
1:A:236:ASP:O	3:C:127[B]:ARG:HD2	2.11	0.51
1:D:69:TYR:HB2	1:D:289:ALA:HB1	1.93	0.50
1:D:100:GLU:OE2	10:D:701:HOH:O	2.20	0.50
1:D:237:ASP:CG	1:D:242:LYS:HE2	2.30	0.50
1:A:536:GLU:OE1	10:A:701:HOH:O	2.19	0.50
1:D:538:TRP:NE1	1:D:542:LYS:HE3	2.27	0.49
2:E:97:GLU:OE1	2:E:170:LYS:NZ	2.34	0.48
1:A:237:ASP:CG	1:A:242:LYS:HE2	2.35	0.48
1:A:338:PHE:HA	2:B:194:PRO:CB	2.44	0.47
9:E:301:B12:H362	9:E:301:B12:H351	1.96	0.47
1:D:48:VAL:HB	1:D:67:ALA:HB1	1.97	0.47
9:B:301:B12:H602	9:B:301:B12:H541	1.70	0.46
3:F:38:ALA:N	3:F:91[A]:SER:HG	2.14	0.46
1:D:177:ARG:HD2	1:D:461:GLN:HG3	1.98	0.46
2:E:131:GLY:O	2:E:138:THR:HA	2.16	0.46
1:D:302:CYS:O	1:D:306:PRO:HD2	2.17	0.45
2:E:56:GLN:HG3	2:E:123:LEU:HA	1.98	0.45
10:D:943:HOH:O	3:F:100:ARG:HD2	2.16	0.45
1:A:74:ASN:HD22	1:A:74:ASN:N	2.15	0.45
2:B:200:SER:OG	9:B:301:B12:H3P1	2.17	0.44
1:D:175:VAL:HG11	1:D:457:ILE:HD11	2.00	0.44
3:F:168:LYS:NZ	10:F:215:HOH:O	2.50	0.44
2:E:108:PHE:O	2:E:211:VAL:HG13	2.18	0.43
1:A:97:LYS:NZ	10:A:712:HOH:O	2.47	0.43
1:D:200:GLN:HG2	1:D:219:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG21	1:A:176:ALA:HA	2.01	0.43
2:B:159:LEU:HD13	2:B:187:LEU:O	2.19	0.43
2:E:193:ARG:HG3	9:E:301:B12:O58	2.19	0.43
2:B:167:GLN:HG2	2:B:184:VAL:HG22	2.01	0.42
3:F:146:ARG:NE	10:F:216:HOH:O	2.50	0.42
9:E:301:B12:H473	9:E:301:B12:H491	2.00	0.42
1:D:429:PRO:HA	1:D:430:PRO:HD3	1.87	0.42
1:A:338:PHE:HA	2:B:194:PRO:HB3	2.01	0.42
1:A:462:GLU:OE1	10:A:702:HOH:O	2.22	0.42
9:B:301:B12:H491	9:B:301:B12:H473	2.01	0.42
2:E:58:THR:OG1	2:E:59:GLN:OE1	2.27	0.41
1:D:489:MET:O	1:D:492:ILE:HG22	2.20	0.41
1:A:142:ALA:HB2	1:A:166:PHE:CG	2.56	0.41
1:D:331:ALA:HB1	1:D:362:SER:HB3	2.03	0.41
2:E:114:ALA:HB2	9:E:301:B12:HM62	2.02	0.41
1:A:337[B]:THR:HG23	10:A:1082:HOH:O	2.21	0.41
2:B:55:ARG:NH1	2:B:57:GLY:HA2	2.36	0.41
3:C:77:GLN:CD	3:C:77:GLN:H	2.23	0.41
9:E:301:B12:H253	9:E:301:B12:H301	1.77	0.41
3:C:134:GLU:CD	3:C:134:GLU:H	2.24	0.41
2:E:101:LYS:HA	2:E:101:LYS:HD2	1.95	0.40
9:E:301:B12:C6	9:E:301:B12:H4B	2.51	0.40
3:F:80:ARG:HD2	10:F:230:HOH:O	2.21	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	553/554 (100%)	535 (97%)	16 (3%)	2 (0%)	34 17
1	D	552/554 (100%)	534 (97%)	16 (3%)	2 (0%)	34 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	179/200 (90%)	175 (98%)	4 (2%)	0	100	100
2	E	176/200 (88%)	169 (96%)	7 (4%)	0	100	100
3	C	140/137 (102%)	138 (99%)	2 (1%)	0	100	100
3	F	136/137 (99%)	135 (99%)	1 (1%)	0	100	100
All	All	1736/1782 (97%)	1686 (97%)	46 (3%)	4 (0%)	47	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	VAL
1	D	300	VAL
1	D	363	GLY
1	A	363	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	454/453 (100%)	448 (99%)	6 (1%)	69	54
1	D	453/453 (100%)	446 (98%)	7 (2%)	65	49
2	B	149/164 (91%)	148 (99%)	1 (1%)	84	75
2	E	146/164 (89%)	146 (100%)	0	100	100
3	C	121/116 (104%)	118 (98%)	3 (2%)	47	25
3	F	117/116 (101%)	113 (97%)	4 (3%)	37	14
All	All	1440/1466 (98%)	1419 (98%)	21 (2%)	65	49

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

Mol	Chain	Res	Type
1	A	28	PHE
1	A	74	ASN
1	A	178	TYR

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Mol	Chain	Res	Type
1	A	232	PHE
1	A	268	MET
1	A	348	ARG
2	B	219	GLU
3	C	77	GLN
3	C	79	MET
3	C	134	GLU
1	D	28	PHE
1	D	178	TYR
1	D	232	PHE
1	D	268	MET
1	D	348	ARG
1	D	464	ILE
1	D	552	GLU
3	F	58	ASN
3	F	66	LEU
3	F	100	ARG
3	F	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
3	C	148	GLN
1	D	461	GLN
1	D	513	GLN
2	E	167	GLN
3	F	47	ASN
3	F	58	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 12 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 6 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	$\#\|Z\| > 2$
4	PGO	D	601	5	3,4,4	0.20	0	1,4,4	0.16	0
4	PGO	A	601	5	3,4,4	0.28	0	1,4,4	0.08	0
8	FWK	D	605	-	18,21,21	1.02	1 (5%)	17,31,31	1.49	4 (23%)
9	B12	E	301	2	90,101,101	1.28	10 (11%)	137,166,166	1.17	13 (9%)
9	B12	B	301	-	90,101,101	1.26	8 (8%)	137,166,166	1.21	13 (9%)
8	FWK	A	605	-	18,21,21	1.08	1 (5%)	17,31,31	1.68	5 (29%)

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
4	PGO	D	601	5	-	0/2/2/2	-
4	PGO	A	601	5	-	0/2/2/2	-
8	FWK	D	605	-	-	0/2/22/22	0/3/3/3
9	B12	E	301	2	-	6/52/223/223	0/3/11/11
9	B12	B	301	-	-	2/52/223/223	0/3/11/11
8	FWK	A	605	-	-	0/2/22/22	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	301	B12	C14-N23	-4.81	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	301	B12	C14-N23	-4.76	1.29	1.35
9	E	301	B12	C8B-C9B	4.48	1.49	1.40
9	B	301	B12	C8B-C9B	4.31	1.49	1.40
9	B	301	B12	C11-N23	4.13	1.44	1.37
9	E	301	B12	C16-C15	-3.97	1.33	1.44
9	E	301	B12	C11-N23	3.92	1.44	1.37
9	B	301	B12	C16-C15	-3.85	1.33	1.44
9	E	301	B12	C6B-C5B	3.30	1.49	1.40
9	B	301	B12	C6B-C5B	3.29	1.49	1.40
8	A	605	FWK	C5-C4	2.78	1.48	1.40
8	D	605	FWK	C5-C4	2.78	1.48	1.40
9	B	301	B12	C10-C9	2.70	1.46	1.39
9	E	301	B12	C10-C9	2.68	1.46	1.39
9	B	301	B12	C14-C15	2.66	1.49	1.38
9	E	301	B12	C14-C15	2.62	1.49	1.38
9	E	301	B12	C19-N24	-2.32	1.44	1.48
9	E	301	B12	O6R-C1R	2.19	1.44	1.41
9	B	301	B12	C19-N24	-2.17	1.44	1.48
9	E	301	B12	C1-C2	-2.13	1.53	1.58

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	301	B12	C17-C16-C15	3.92	132.44	126.26
9	B	301	B12	C13-C14-N23	3.75	114.21	109.10
9	B	301	B12	C9-C10-C11	-3.73	120.57	125.97
9	E	301	B12	C13-C14-N23	3.67	114.10	109.10
8	A	605	FWK	N3-C2-N1	-3.54	123.14	128.68
9	E	301	B12	C9-C10-C11	-3.54	120.85	125.97
9	E	301	B12	C13-C14-C15	-3.36	119.18	124.32
9	B	301	B12	C13-C14-C15	-3.32	119.25	124.32
8	A	605	FWK	C3'-C2'-C1'	3.28	105.92	100.98
8	D	605	FWK	N3-C2-N1	-3.25	123.59	128.68
9	E	301	B12	C17-C16-C15	3.01	131.00	126.26
9	B	301	B12	C17-C16-N24	-3.00	106.52	111.15
9	B	301	B12	C55-C56-C57	-2.86	104.98	111.23
9	E	301	B12	C55-C56-C57	-2.77	105.17	111.23
9	E	301	B12	C20-C1-N21	2.76	114.79	110.27
9	B	301	B12	C48-C13-C14	2.71	115.25	108.49
9	E	301	B12	C30-C3-C2	-2.59	113.61	119.09
9	E	301	B12	C2P-C1P-N59	-2.59	109.12	112.93
8	D	605	FWK	C3'-C2'-C1'	2.54	104.81	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	301	B12	C30-C3-C2	-2.49	113.82	119.09
9	B	301	B12	C53-C15-C16	2.49	124.66	120.38
8	A	605	FWK	C6'-C5'-C4'	-2.46	106.48	113.27
8	A	605	FWK	C2-N1-C6	2.36	122.80	118.75
9	E	301	B12	C53-C15-C16	2.36	124.44	120.38
9	E	301	B12	C17-C16-N24	-2.34	107.54	111.15
8	D	605	FWK	C6'-C5'-C4'	-2.26	107.03	113.27
9	B	301	B12	C4B-C9B-N3B	2.25	136.90	130.88
8	D	605	FWK	C4-C5-N7	-2.24	107.06	109.40
9	B	301	B12	C12-C11-C10	2.19	126.22	123.37
9	B	301	B12	C60-C18-C17	-2.11	110.64	115.74
9	E	301	B12	C4B-C9B-N3B	2.10	136.50	130.88
9	E	301	B12	C48-C13-C14	2.08	113.67	108.49
8	A	605	FWK	C4-C5-N7	-2.06	107.26	109.40
9	E	301	B12	C8B-C9B-N3B	-2.04	103.54	107.83
9	B	301	B12	C18-C17-C16	2.00	103.10	100.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	301	B12	C2-C3-C30-C31
9	E	301	B12	C17-C18-C60-C61
9	B	301	B12	C19-C18-C60-C61
9	E	301	B12	C19-C18-C60-C61
9	E	301	B12	C42-C41-C8-C9
9	E	301	B12	C4-C3-C30-C31
9	B	301	B12	C17-C18-C60-C61
9	E	301	B12	C12-C13-C48-C49

There are no ring outliers.

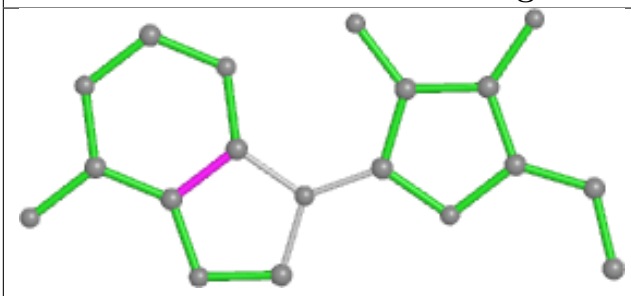
2 monomers are involved in 16 short contacts:

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

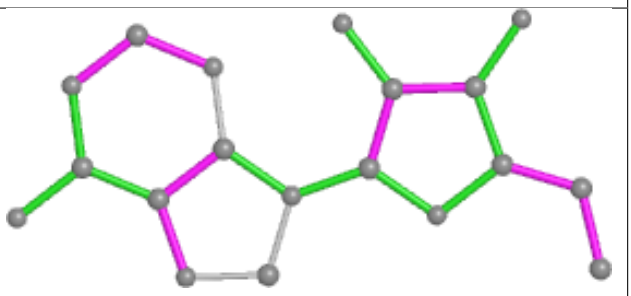
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

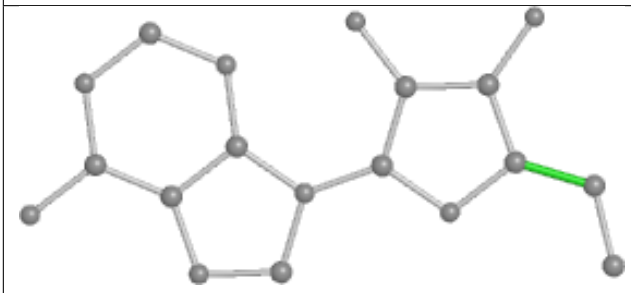
Ligand FWK D 605



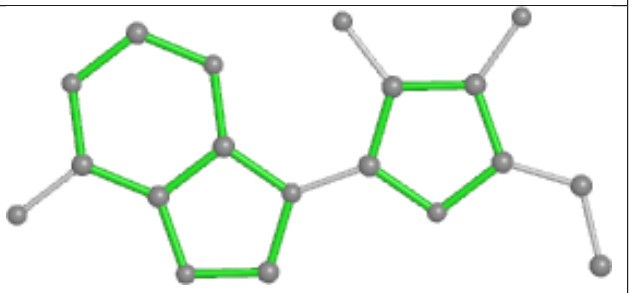
Bond lengths



Bond angles

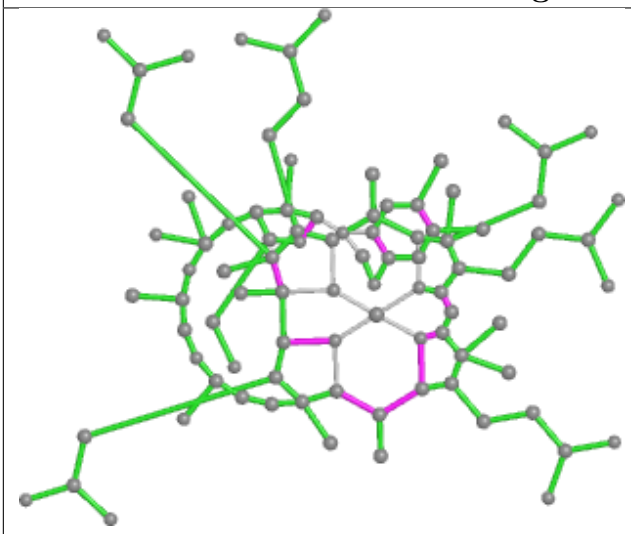


Torsions



Rings

Ligand B12 E 301



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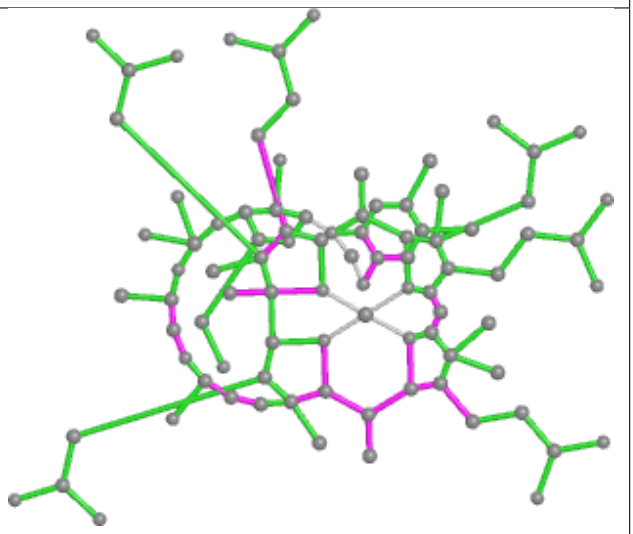
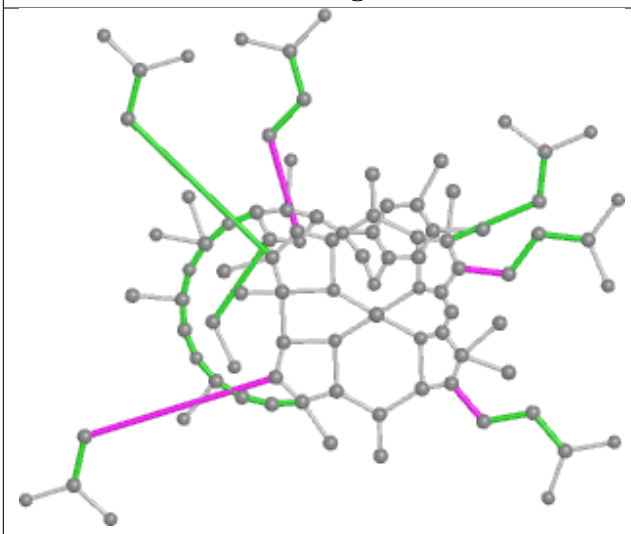


Bond angles



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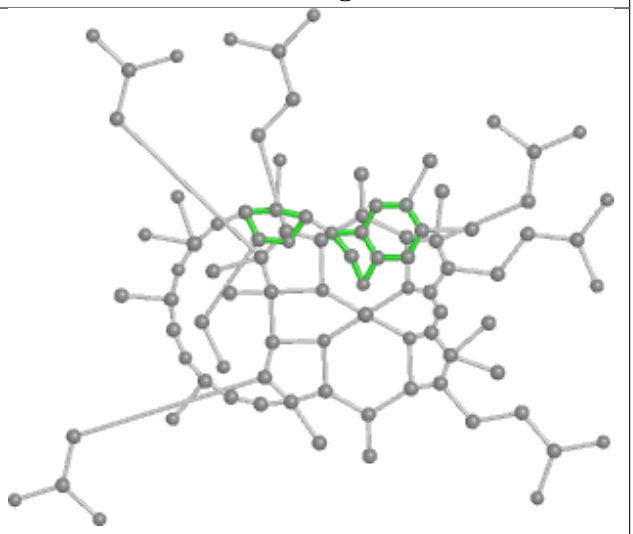
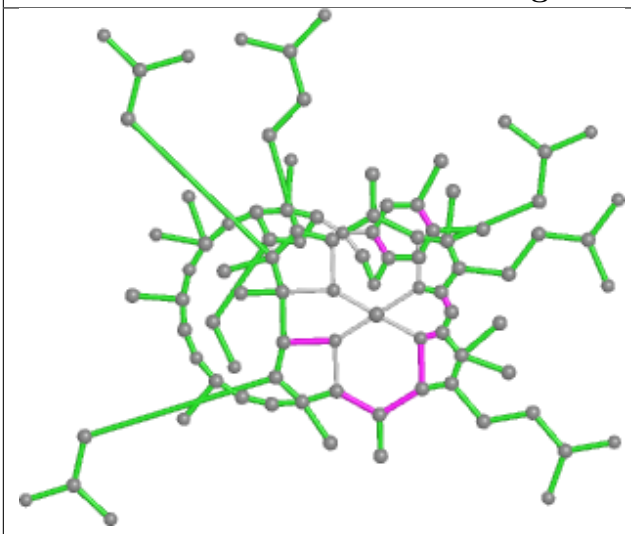
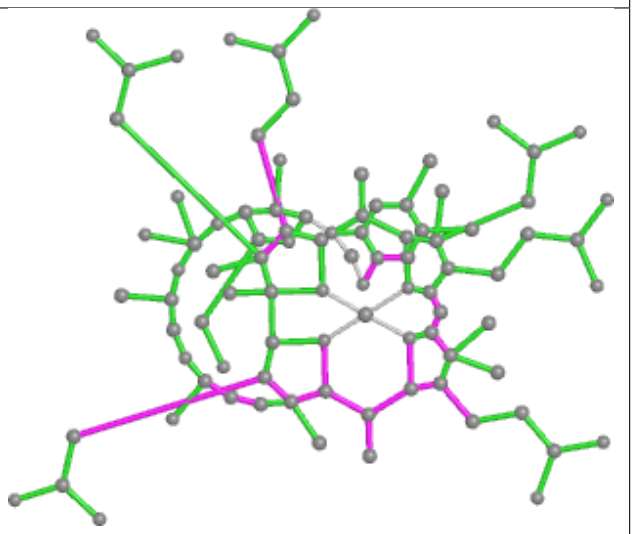


Rings

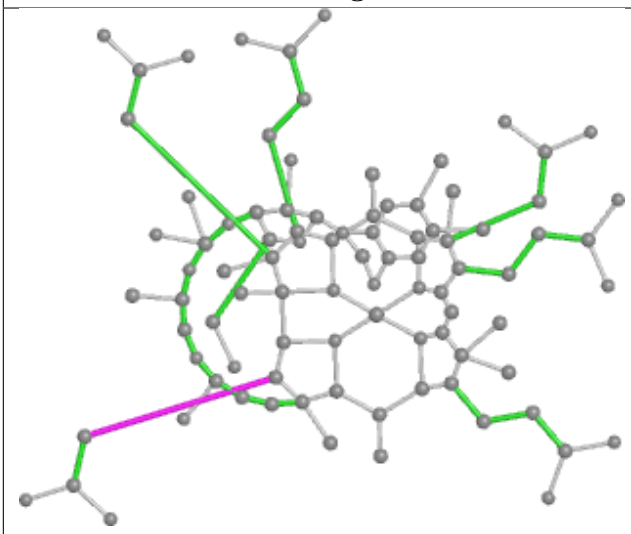
Ligand B12 B 301



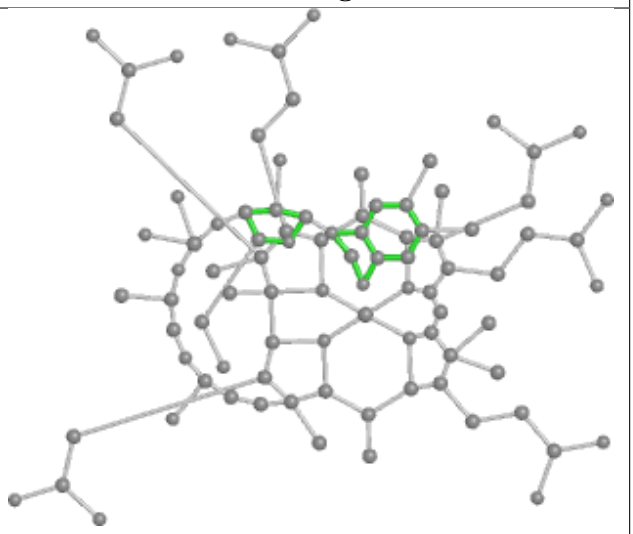
Bond lengths



Bond angles

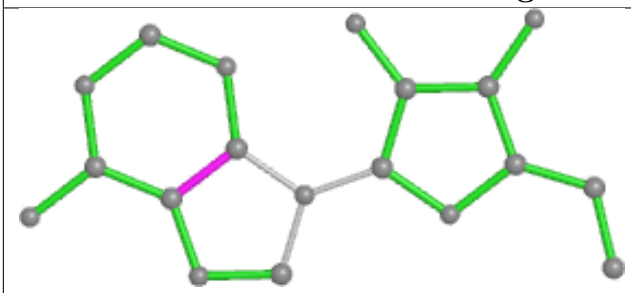


Torsions

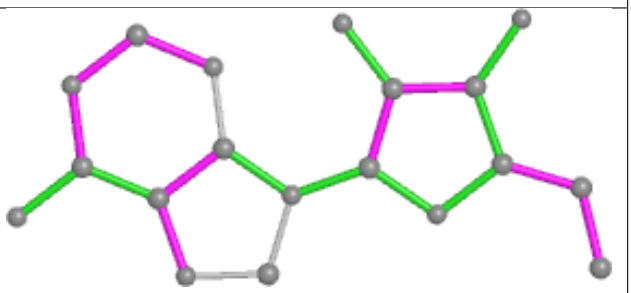


Rings

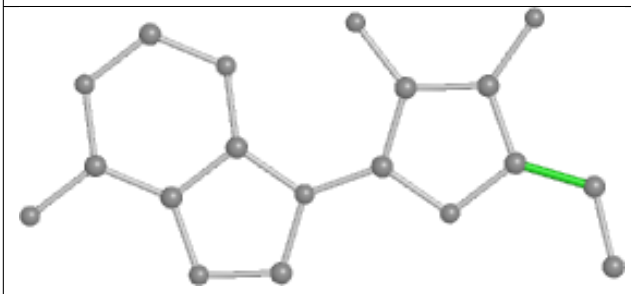
Ligand FWK A 605



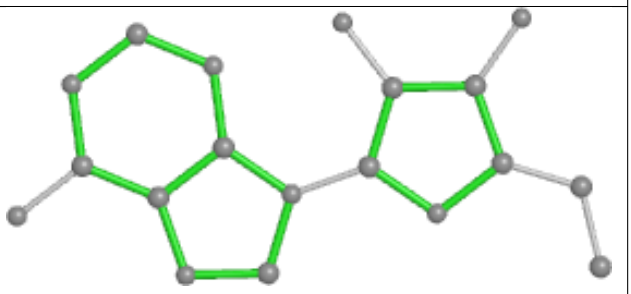
Bond lengths



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, 95^{th} 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^2)	Q<0.9
1	A	552/554 (99%)	-0.48	0 100 100	8, 12, 22, 67	1 (0%)
1	D	554/554 (100%)	-0.16	10 (1%) 68 76	8, 18, 42, 70	1 (0%)
2	B	179/200 (89%)	-0.39	5 (2%) 53 58	13, 22, 40, 69	0
2	E	178/200 (89%)	3.03	105 (58%) 0 0	29, 75, 121, 141	0
3	C	136/137 (99%)	-0.43	0 100 100	11, 20, 37, 44	0
3	F	136/137 (99%)	-0.01	5 (3%) 41 48	15, 26, 48, 68	2 (1%)
All	All	1735/1782 (97%)	0.03	125 (7%) 15 20	8, 18, 75, 141	4 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	51	VAL	16.2
2	E	58	THR	12.9
2	E	220	LEU	11.4
2	E	222	VAL	11.3
2	E	49	THR	10.5
2	E	57	GLY	8.9
2	E	95	ILE	8.4
2	E	47	PHE	8.3
2	E	92	ILE	8.3
2	E	213	THR	8.2
2	E	214	GLY	8.0
2	B	224	LEU	7.9
2	E	54	ALA	7.7
2	E	173	ALA	6.9
2	E	59	GLN	6.8
2	E	172	ALA	6.7
2	E	187	LEU	6.6
2	E	221	ARG	6.5
2	E	125	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
2	E	73	LEU	6.4
2	E	212	VAL	6.3
2	E	55	ARG	6.1
2	E	166	ARG	5.9
2	E	64	ILE	5.7
2	E	168	ILE	5.7
2	E	99	GLY	5.4
2	E	46	GLY	5.3
2	E	105	ILE	5.2
2	E	162	LEU	5.2
2	E	48	LEU	5.1
2	E	61	ASP	5.1
2	E	91	VAL	5.0
2	E	66	ALA	5.0
2	E	60	GLN	4.9
2	E	120	GLY	4.9
2	E	63	VAL	4.9
2	E	104	VAL	4.8
2	E	101	LYS	4.8
2	E	174	ARG	4.6
2	E	223	ALA	4.6
2	E	81	GLY	4.5
2	E	50	GLU	4.4
2	E	65	ILE	4.4
2	E	107	CYS	4.4
2	E	185	PRO	4.4
2	E	123	LEU	4.2
2	E	167	GLN	4.1
2	E	100	ILE	4.1
2	E	178	ARG	4.0
2	E	70	ALA	4.0
2	E	182	GLN	3.9
2	E	52	GLY	3.9
1	D	454	VAL	3.9
2	E	102	ALA	3.9
2	E	85	LYS	3.9
2	E	93	ALA	3.8
2	E	89	ARG	3.7
2	E	179	GLU	3.7
2	E	210	TYR	3.6
1	D	424	ALA	3.6
2	E	170	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	211	VAL	3.6
2	E	108	PHE	3.5
2	E	74	ALA	3.5
2	E	97	GLU	3.5
2	E	88	LEU	3.4
2	B	187	LEU	3.3
2	E	76	THR	3.3
2	E	181	PRO	3.3
2	E	56	GLN	3.2
2	E	161	THR	3.2
1	D	554	ASP	3.1
2	E	215	LYS	3.1
3	F	70	LEU	3.1
2	E	127	GLY	3.0
2	E	183	PRO	3.0
2	E	175	TYR	3.0
2	E	219	GLU	3.0
2	E	106	ARG	3.0
1	D	459	PHE	3.0
2	E	169	GLY	3.0
2	E	218	GLN	2.9
2	E	176	ALA	2.9
2	E	217	PRO	2.9
2	E	165	TYR	2.9
2	E	67	VAL	2.8
2	E	177	LYS	2.8
2	E	53	GLU	2.8
2	E	154	PHE	2.8
2	E	86	SER	2.7
2	E	83	PRO	2.7
2	B	55	ARG	2.7
2	E	87	ILE	2.6
2	E	103	ARG	2.6
2	E	96	GLU	2.6
2	E	121	ASN	2.6
2	E	184	VAL	2.6
3	F	56	ALA	2.6
3	F	67	GLU	2.5
3	F	38	ALA	2.5
3	F	77	GLN	2.5
2	E	128	ILE	2.5
2	E	124	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	453	ILE	2.5
1	D	479	GLN	2.5
2	E	186	THR	2.4
2	E	77	VAL	2.4
2	E	216	ASN	2.4
2	E	130	ILE	2.3
1	D	458	LYS	2.3
2	E	98	GLU	2.3
2	E	82	ILE	2.3
2	E	117	ALA	2.3
1	D	360	ILE	2.2
2	E	115	PHE	2.2
2	E	122	ARG	2.2
2	B	60	GLN	2.2
2	E	132	ILE	2.2
2	B	178	ARG	2.1
2	E	160	LEU	2.1
2	E	164	THR	2.1
1	D	425	GLY	2.1
1	D	552	GLU	2.0
2	E	134	SER	2.0
2	E	94	GLY	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^{th} 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
9	B12	E	301	91/91	0.94	0.13	25,35,49,59	0

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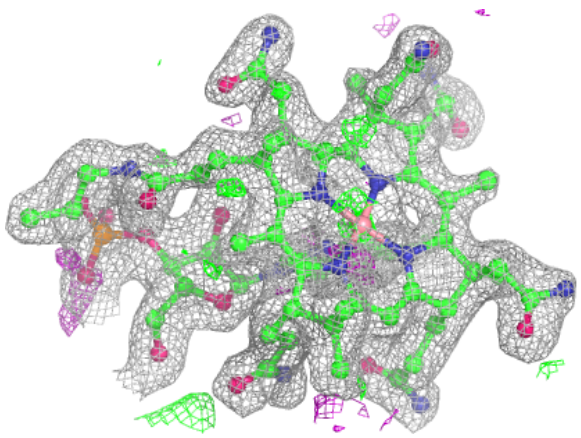
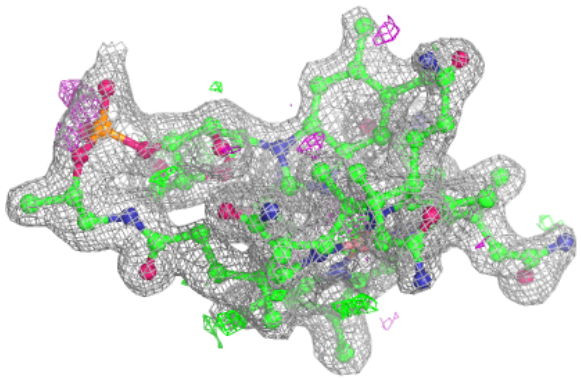
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FWK	D	605	19/19	0.95	0.15	18,22,28,30	0
6	K	D	603	1/1	0.96	0.09	15,15,15,15	0
4	PGO	D	601	5/5	0.97	0.13	16,17,20,20	0
8	FWK	A	605	19/19	0.97	0.14	14,16,16,17	0
9	B12	B	301	91/91	0.98	0.08	12,18,29,39	0
6	K	A	603	1/1	0.98	0.09	12,12,12,12	0
4	PGO	A	601	5/5	0.99	0.14	9,10,12,16	0
5	CA	D	602	1/1	0.99	0.06	13,13,13,13	0
7	NH4	A	604	1/1	0.99	0.15	7,7,7,7	0
7	NH4	D	604	1/1	0.99	0.24	16,16,16,16	0
5	CA	A	602	1/1	1.00	0.07	7,7,7,7	0

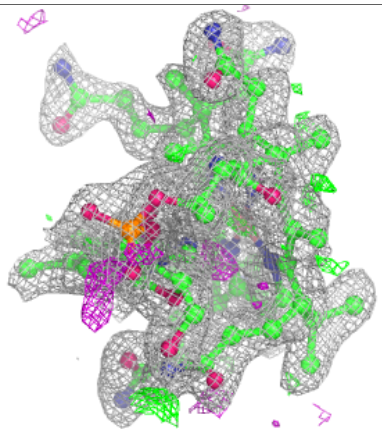
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

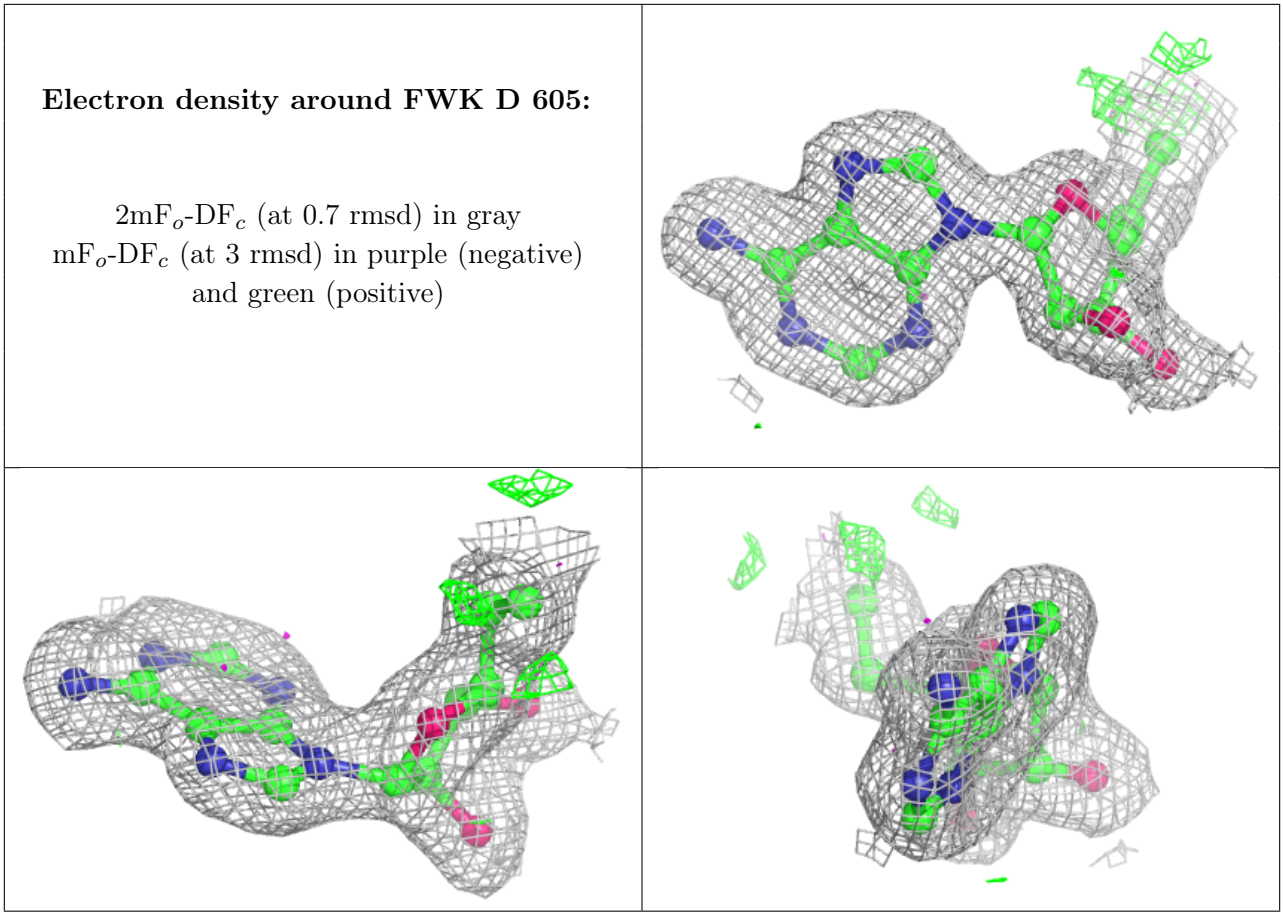






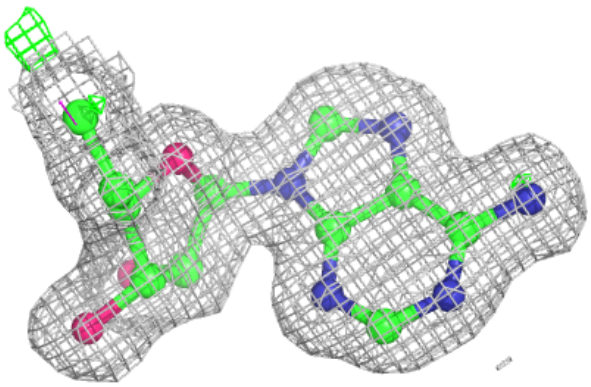
Electron density around FWK D 605:

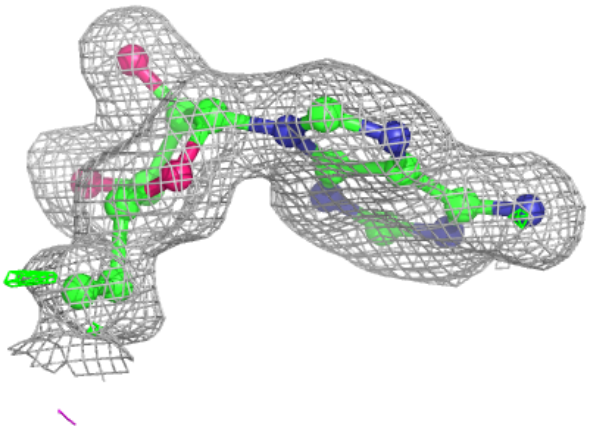
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

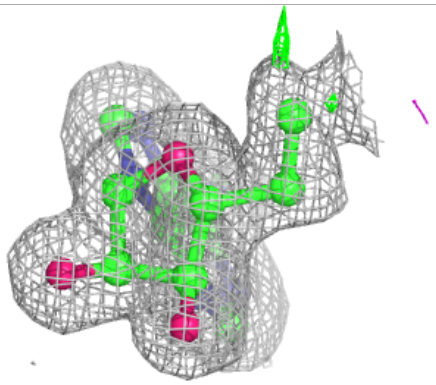


Electron density around FWK A 605:

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

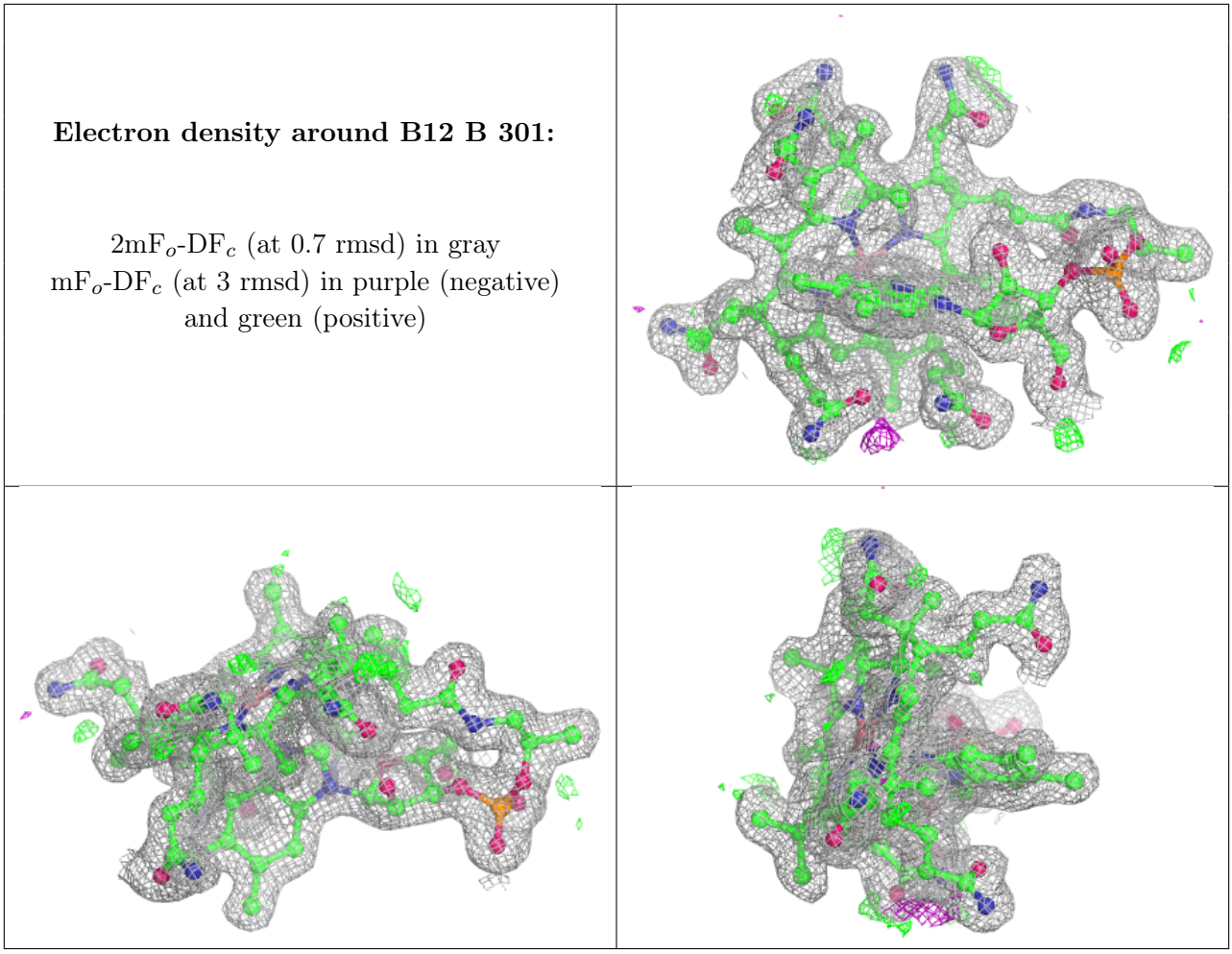






Electron density around B12 B 301:

$2mF_o$-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.