



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 03:28 PM JST

PDB ID : 7XRL / pdb_00007xrl
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

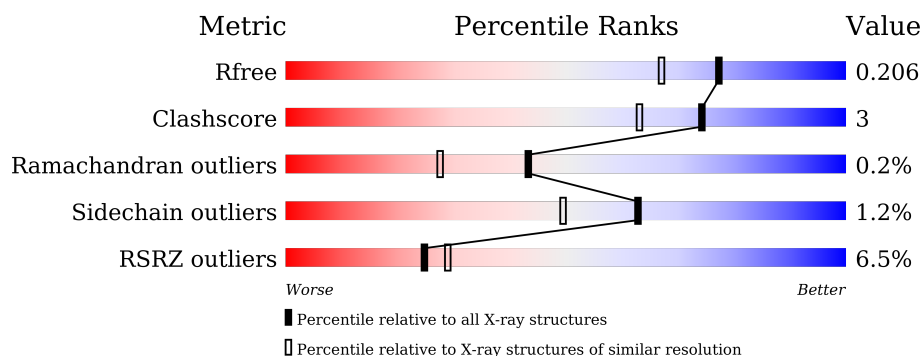
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 $\leq 5\%$. 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	
1	D	554	
2	B	200	
2	E	200	
3	C	137	
3	F	137	

2 Entry composition

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

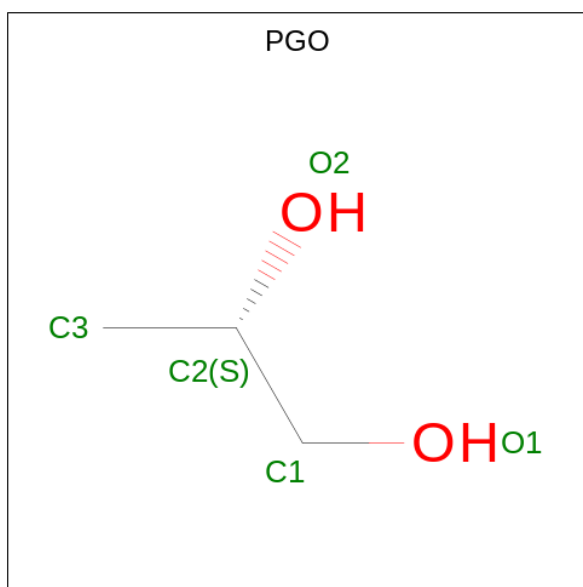
- Molecule 3 is a protein called Diol dehydrase gamma subunit.

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 (CCD ID: PGO) (formula: C₃H₈O₂).



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

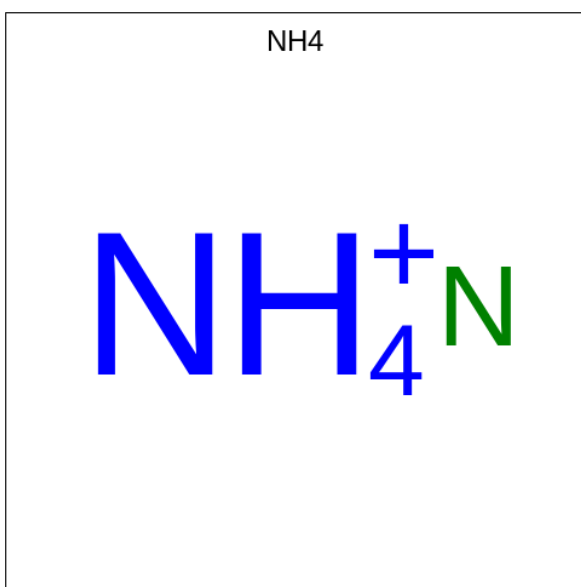
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

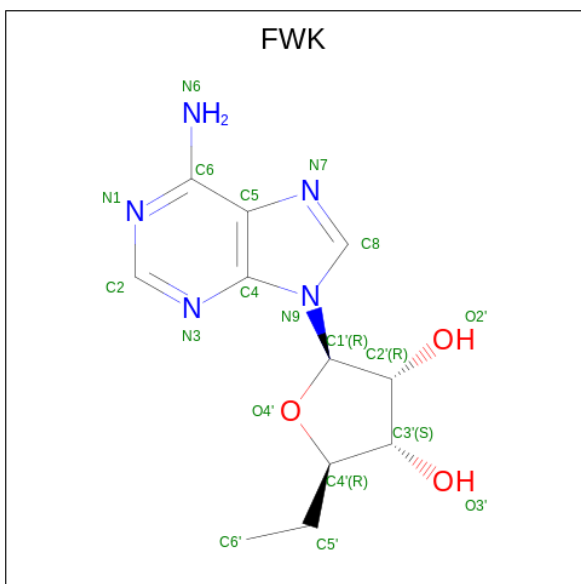
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	D	1	Total	K	0	0
			1	1		

- Molecule 7 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



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

- Molecule 8 is (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-ethyl-oxolane-3,4-diol (CCD ID: FWK) (formula: C₁₁H₁₅N₅O₃) (labeled as "Ligand of Interest" by depositor).



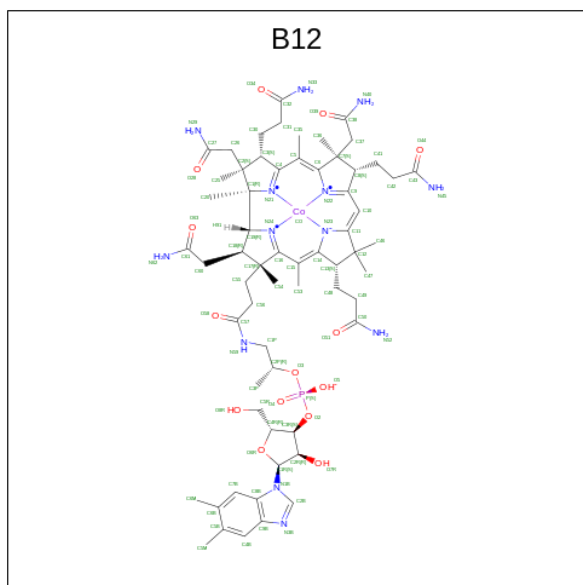
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	N	O	
			19	11	5	3	

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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 (CCD ID: 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		

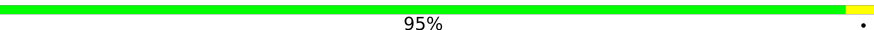
- Molecule 10 is water.

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

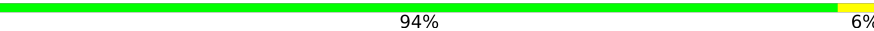
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

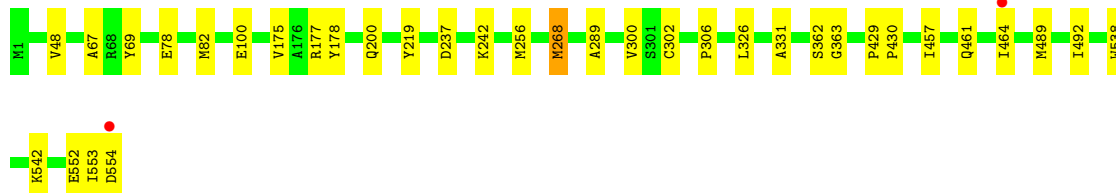
- Molecule 1: Diol dehydrase alpha subunit

Chain A:  95%



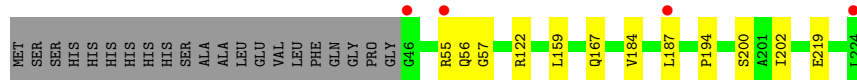
- Molecule 1: Diol dehydrase alpha subunit

Chain D:  94% 6%



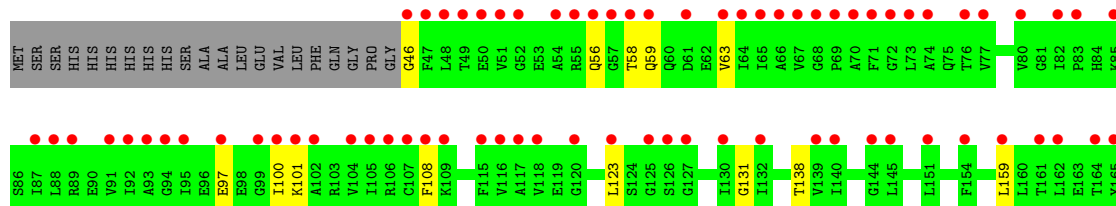
- Molecule 2: Diol dehydrase beta subunit

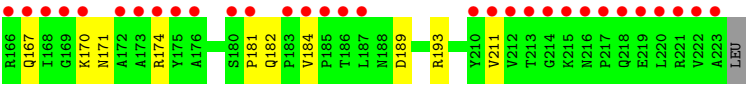
Chain B:  84% 6% 10%



- Molecule 2: Diol dehydrase beta subunit

Chain E:  52% 78% 12% 11%

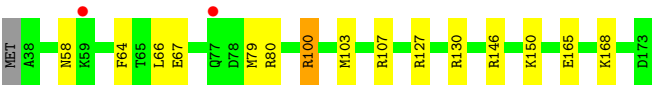
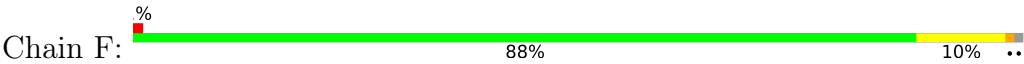




● Molecule 3: Diol dehydrase gamma subunit



● Molecule 3: Diol dehydrase gamma subunit



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGO, FWK, K, CA, NH4, B12

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	0.31	0/4305	0.51	0/5831
1	D	0.27	0/4299	0.46	0/5821
2	B	0.24	0/1404	0.44	0/1899
2	E	0.14	0/1379	0.31	0/1867
3	C	0.23	0/1150	0.40	0/1553
3	F	0.22	0/1116	0.38	0/1507
All	All	0.26	0/13653	0.45	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 [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	4224	0	4169	18	0
1	D	4227	0	4160	17	0
2	B	1376	0	1432	11	0
2	E	1357	0	1405	15	0
3	C	1117	0	1145	6	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	8	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	85	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 (85) 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
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
1:A:20[B]:VAL:HG12	1:A:21:LYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:78:GLU:HG2	1:D:82:MET:HE3	1.88	0.56
1:D:237:ASP:CG	1:D:242:LYS:HE2	2.30	0.55
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
1:A:69:TYR:CD1	3:C:103[A]:MET:HE1	2.42	0.54
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
1:A:237:ASP:CG	1:A:242:LYS:HE2	2.35	0.52
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: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
1:A:338:PHE:HA	2:B:194:PRO:CB	2.44	0.47
3:C:77:GLN:H	3:C:77:GLN:CD	2.23	0.47
9:E:301:B12:H362	9:E:301:B12:H351	1.96	0.47
1:D:268:MET:HE3	1:D:268:MET:HB3	1.82	0.47
1:D:48:VAL:HB	1:D:67:ALA:HB1	1.97	0.47
3:C:134:GLU:CD	3:C:134:GLU:H	2.24	0.46
9:B:301:B12:H602	9:B:301:B12:H541	1.70	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
3:F:103[A]:MET:HE3	3:F:107:ARG:NH1	2.31	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
3:C:100:ARG:HD3	3:C:103[A]:MET:HE2	1.97	0.44
1:D:175:VAL:HG11	1:D:457:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:168:LYS:NZ	10:F:215:HOH:O	2.50	0.44
2:E:58:THR:OG1	2:E:59:GLN:OE1	2.27	0.43
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
3:F:100:ARG:HH12	3:F:103[A]:MET:CE	2.32	0.43
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
1:A:174:ALA:HA	1:A:373:MET:HE2	2.01	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
2:E:97:GLU:OE1	2:E:170:LYS:NZ	2.34	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:D:256:MET:HE2	1:D:256:MET:HB2	1.99	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
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
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
9:E:301:B12:H253	9:E:301:B12:H301	1.77	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%)	30	15
1	D	552/554 (100%)	534 (97%)	16 (3%)	2 (0%)	30	15
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%)	43	27

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 ⓘ

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%)	451 (99%)	3 (1%)	76	67
1	D	453/453 (100%)	448 (99%)	5 (1%)	65	52
2	B	149/164 (91%)	148 (99%)	1 (1%)	76	67
2	E	146/164 (89%)	146 (100%)	0	100	100
3	C	121/116 (104%)	118 (98%)	3 (2%)	42	22
3	F	117/116 (101%)	112 (96%)	5 (4%)	26	8
All	All	1440/1466 (98%)	1423 (99%)	17 (1%)	63	49

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	178	TYR
1	A	268	MET
2	B	219	GLU
3	C	77	GLN
3	C	79	MET
3	C	134	GLU
1	D	178	TYR
1	D	268	MET
1	D	326	LEU
1	D	464	ILE
1	D	552	GLU
3	F	58	ASN
3	F	66	LEU
3	F	67	GLU
3	F	100	ARG
3	F	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	95	ASN
1	A	267	GLN
2	B	142	GLN
3	C	148	GLN
1	D	89	ASN
1	D	461	GLN
2	E	167	GLN
3	F	148	GLN

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 [i](#)

There are no oligosaccharides 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
8	FWK	A	605	-	21,21,21	1.54	4 (19%)	30,31,31	2.30	11 (36%)
8	FWK	D	605	-	21,21,21	1.53	4 (19%)	30,31,31	2.28	10 (33%)
4	PGO	A	601	5	3,4,4	0.28	0	1,4,4	0.08	0
9	B12	B	301	-	93,101,101	1.30	10 (10%)	146,166,166	1.41	18 (12%)
9	B12	E	301	2	93,101,101	1.34	10 (10%)	146,166,166	1.40	18 (12%)

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	-
8	FWK	A	605	-	-	2/6/22/22	0/3/3/3
8	FWK	D	605	-	-	2/6/22/22	0/3/3/3
4	PGO	A	601	5	-	0/2/2/2	-
9	B12	B	301	-	-	2/56/223/223	0/3/11/11
9	B12	E	301	2	-	6/56/223/223	0/3/11/11

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	301	B12	C8B-C9B	5.53	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	301	B12	C8B-C9B	5.32	1.49	1.40
8	A	605	FWK	C5-C4	4.97	1.48	1.39
8	D	605	FWK	C5-C4	4.96	1.48	1.39
9	E	301	B12	C14-N23	-4.81	1.28	1.35
9	B	301	B12	C14-N23	-4.76	1.29	1.35
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
9	E	301	B12	C9B-N3B	-2.80	1.34	1.39
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
8	A	605	FWK	C5-N7	-2.44	1.34	1.39
8	D	605	FWK	C5-C6	2.38	1.47	1.41
8	A	605	FWK	C5-C6	2.37	1.47	1.41
9	E	301	B12	C19-N24	-2.32	1.44	1.48
8	A	605	FWK	C8-N7	2.20	1.35	1.31
9	B	301	B12	C19-N24	-2.17	1.44	1.48
9	E	301	B12	C1-C2	-2.13	1.53	1.58
9	B	301	B12	C9B-N3B	-2.09	1.35	1.39
9	B	301	B12	C2B-N1B	-2.03	1.33	1.37
8	D	605	FWK	C5-N7	-2.02	1.35	1.39
8	D	605	FWK	C8-N7	2.02	1.35	1.31

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	605	FWK	C5-C4-N3	-6.66	118.06	126.75
8	A	605	FWK	C5-C4-N3	-6.32	118.50	126.75
9	E	301	B12	C8B-C9B-N3B	-5.83	103.54	109.97
9	B	301	B12	C8B-C9B-N3B	-5.73	103.65	109.97
8	D	605	FWK	N3-C4-N9	5.60	136.32	127.08
9	E	301	B12	C9B-N3B-C2B	5.57	111.07	104.44
8	A	605	FWK	N3-C4-N9	5.42	136.01	127.08
9	B	301	B12	C9B-N3B-C2B	5.40	110.88	104.44
8	D	605	FWK	C2-N3-C4	3.95	121.07	111.75
9	B	301	B12	C17-C16-C15	3.92	132.44	126.26
8	A	605	FWK	C2-N3-C4	3.86	120.86	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	B	301	B12	C4B-C9B-N3B	3.72	136.90	130.51
9	E	301	B12	C13-C14-N23	3.67	114.10	109.10
9	E	301	B12	C9-C10-C11	-3.54	120.85	125.97
9	E	301	B12	C4B-C9B-N3B	3.49	136.50	130.51
8	A	605	FWK	N1-C2-N3	-3.49	123.14	128.60
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	D	605	FWK	N1-C2-N3	-3.20	123.59	128.60
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	C8B-N1B-C2B	2.98	109.15	106.37
9	E	301	B12	C9B-C8B-N1B	2.93	106.59	105.35
8	D	605	FWK	C4-C5-N7	-2.92	107.06	110.62
9	B	301	B12	C55-C56-C57	-2.87	104.97	111.23
9	E	301	B12	C55-C56-C57	-2.77	105.17	111.23
8	A	605	FWK	C4-C5-N7	-2.76	107.26	110.62
9	E	301	B12	C20-C1-N21	2.76	114.79	110.27
8	D	605	FWK	C4-N9-C8	2.75	108.71	105.73
8	A	605	FWK	C4-N9-C8	2.75	108.71	105.73
9	B	301	B12	N1B-C2B-N3B	-2.75	110.15	113.91
9	B	301	B12	C48-C13-C14	2.71	115.25	108.49
9	E	301	B12	N1B-C2B-N3B	-2.65	110.30	113.91
8	A	605	FWK	C5-N7-C8	2.63	107.24	103.51
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
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	D	605	FWK	C5-N7-C8	2.38	106.89	103.51
8	A	605	FWK	C3'-C2'-C1'	2.36	105.92	101.43
9	E	301	B12	C53-C15-C16	2.36	124.44	120.38
8	A	605	FWK	C2-N1-C6	2.35	122.80	118.77
9	E	301	B12	C17-C16-N24	-2.34	107.54	111.15
9	E	301	B12	C8B-N1B-C2B	2.28	108.50	106.37
8	D	605	FWK	C6'-C5'-C4'	-2.26	107.03	113.27
9	B	301	B12	C1R-N1B-C2B	-2.23	122.11	127.14
8	A	605	FWK	O4'-C1'-N9	-2.22	103.68	108.06
9	B	301	B12	C12-C11-C10	2.19	126.21	123.37
9	B	301	B12	C60-C18-C17	-2.11	110.64	115.74
8	D	605	FWK	C1'-N9-C8	-2.08	122.44	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	301	B12	C48-C13-C14	2.08	113.67	108.49
8	D	605	FWK	O4'-C1'-N9	-2.01	104.10	108.06
9	B	301	B12	C18-C17-C16	2.00	103.10	100.67
9	E	301	B12	C8B-N1B-C1R	2.00	128.80	125.39

There are no chirality outliers.

All (12) torsion outliers are listed below:

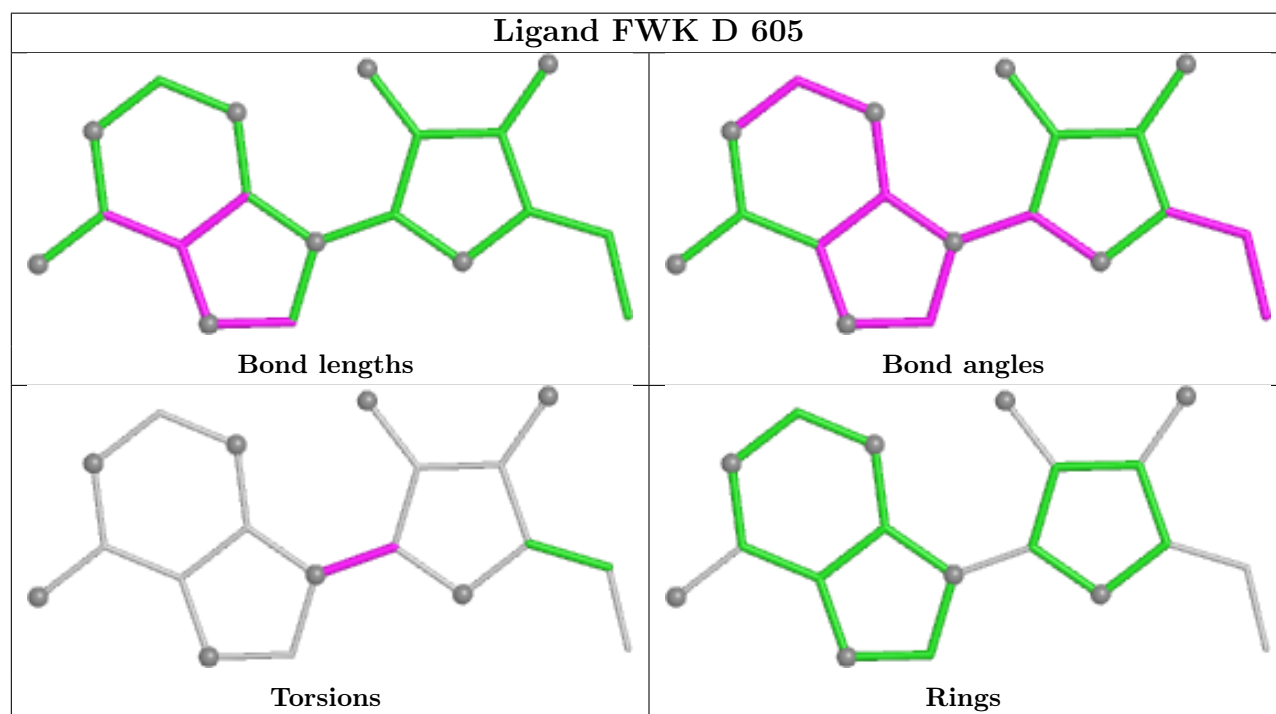
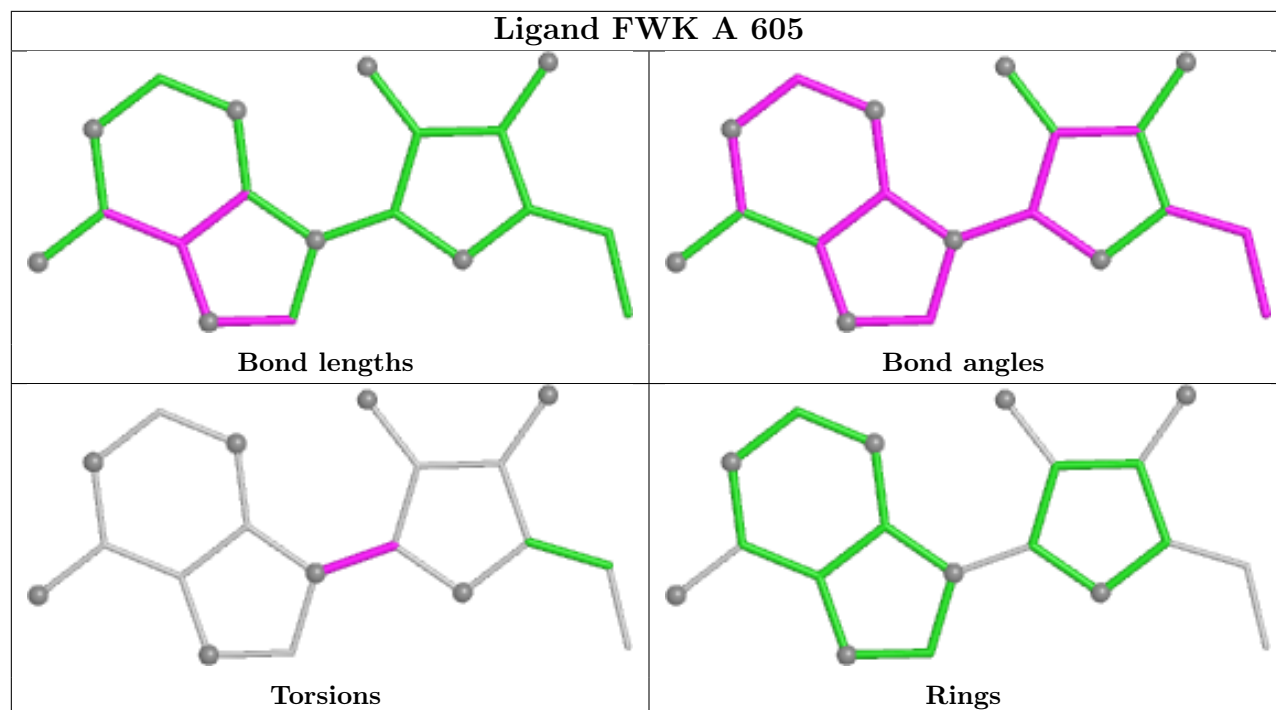
Mol	Chain	Res	Type	Atoms
8	A	605	FWK	C2'-C1'-N9-C4
8	D	605	FWK	C2'-C1'-N9-C4
8	A	605	FWK	C2'-C1'-N9-C8
8	D	605	FWK	C2'-C1'-N9-C8
9	E	301	B12	C2-C3-C30-C31
9	E	301	B12	C17-C18-C60-C61
9	B	301	B12	C19-C18-C60-C61
9	E	301	B12	C19-C18-C60-C61
9	E	301	B12	C42-C41-C8-C9
9	E	301	B12	C4-C3-C30-C31
9	B	301	B12	C17-C18-C60-C61
9	E	301	B12	C12-C13-C48-C49

There are no ring outliers.

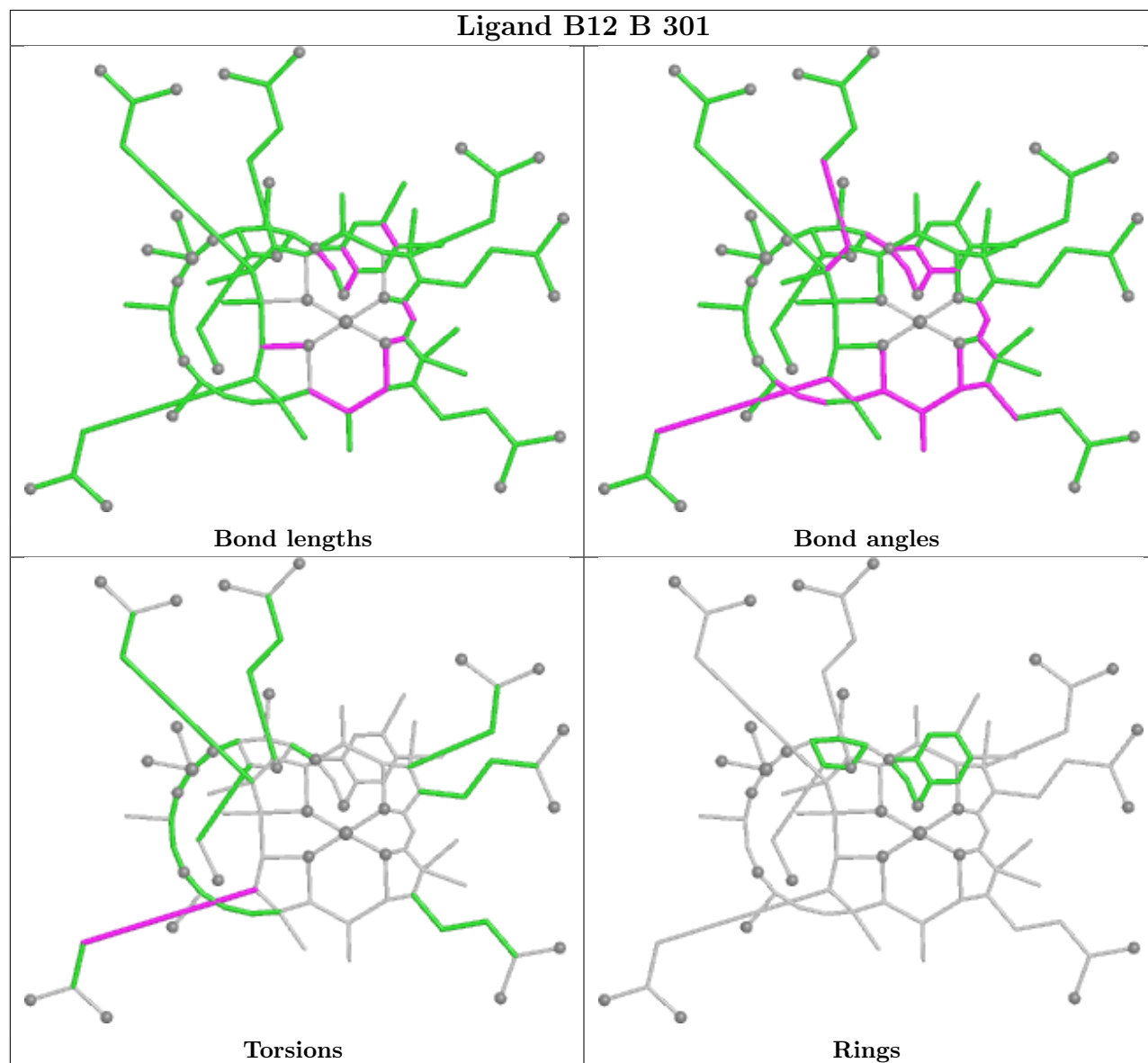
2 monomers are involved in 15 short contacts:

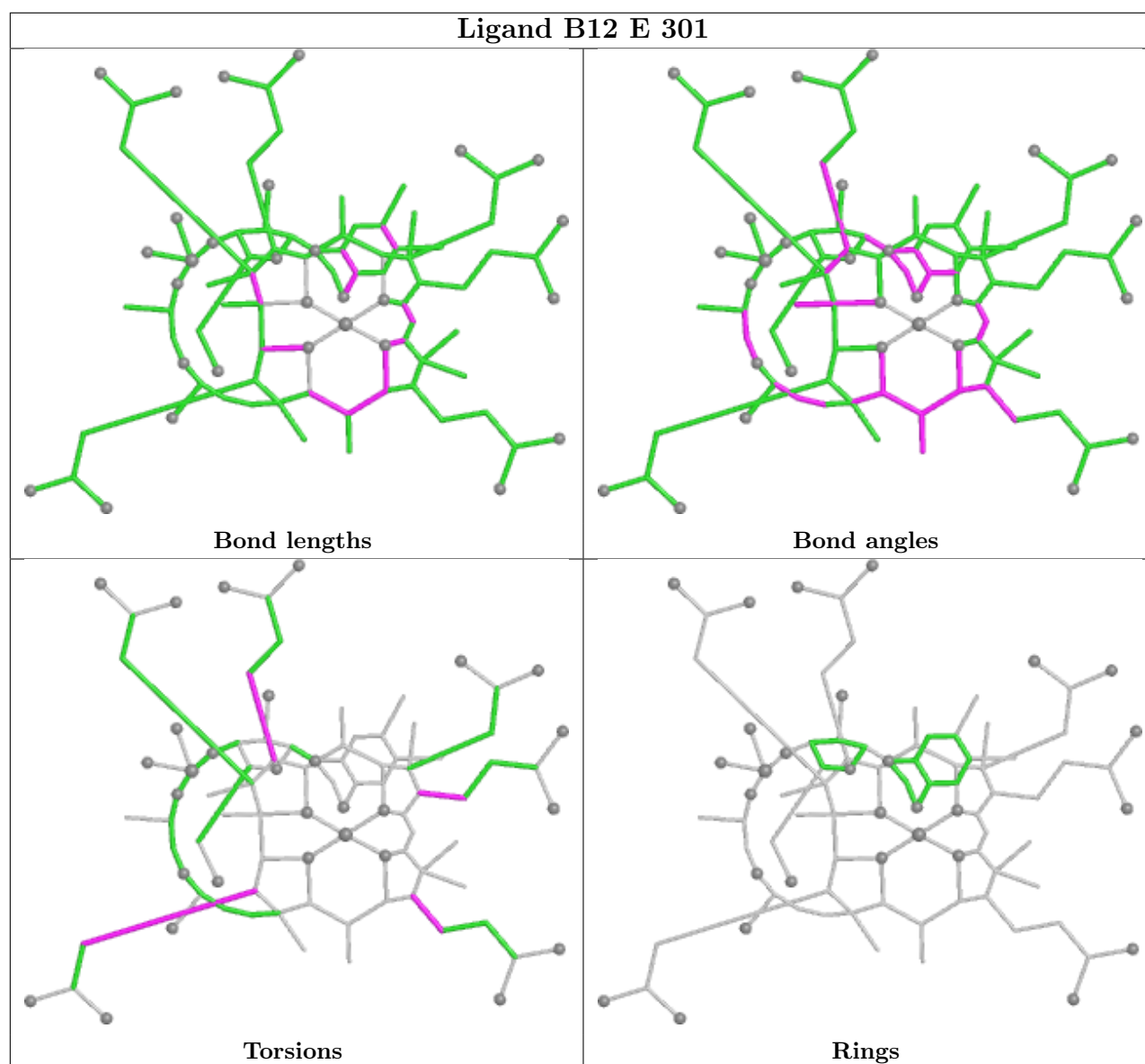
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	301	B12	7	0
9	E	301	B12	8	0

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.



Ligand B12 B 301





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, 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(Å ²)	Q<0.9
1	A	552/554 (99%)	-0.83	1 (0%) 91 93	8, 12, 22, 67	4 (0%)
1	D	554/554 (100%)	-0.51	2 (0%) 88 91	8, 18, 42, 70	1 (0%)
2	B	179/200 (89%)	-0.27	4 (2%) 62 69	12, 22, 40, 69	2 (1%)
2	E	178/200 (89%)	2.42	104 (58%) 0 0	29, 75, 121, 141	0
3	C	136/137 (99%)	-0.37	0 100 100	11, 20, 37, 44	6 (4%)
3	F	136/137 (99%)	-0.06	2 (1%) 72 78	15, 26, 48, 68	4 (2%)
All	All	1735/1782 (97%)	-0.24	113 (6%) 25 29	8, 18, 75, 141	17 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	223	ALA	7.6
2	E	187	LEU	6.2
2	E	92	ILE	5.4
2	E	220	LEU	5.4
2	E	47	PHE	5.3
2	E	212	VAL	5.1
2	E	54	ALA	5.0
2	E	107	CYS	5.0
2	E	222	VAL	4.8
2	E	73	LEU	4.7
2	E	51	VAL	4.7
2	E	213	THR	4.7
2	E	99	GLY	4.6
2	E	64	ILE	4.5
2	E	123	LEU	4.3
2	E	91	VAL	4.3
2	E	63	VAL	4.2
2	E	173	ALA	4.2
2	E	48	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	95	ILE	4.1
2	E	172	ALA	3.9
2	E	214	GLY	3.9
2	E	105	ILE	3.9
2	E	65	ILE	3.8
2	E	166	ARG	3.8
2	E	100	ILE	3.8
2	E	120	GLY	3.7
2	E	168	ILE	3.7
2	E	49	THR	3.6
2	E	70	ALA	3.5
2	E	108	PHE	3.5
2	E	46	GLY	3.5
2	E	58	THR	3.5
2	E	183	PRO	3.4
2	B	46	GLY	3.4
2	E	94	GLY	3.4
2	E	102	ALA	3.4
2	B	55	ARG	3.4
2	B	224	LEU	3.3
2	E	66	ALA	3.3
2	E	117	ALA	3.3
2	E	104	VAL	3.2
2	E	162	LEU	3.2
2	E	165	TYR	3.1
2	E	167	GLN	3.1
3	F	59	LYS	3.1
2	E	154	PHE	3.1
2	E	210	TYR	3.1
2	E	116	VAL	3.0
2	E	93	ALA	3.0
2	B	187	LEU	3.0
2	E	221	ARG	2.9
2	E	170	LYS	2.9
2	E	88	LEU	2.9
2	E	82	ILE	2.9
2	E	87	ILE	2.9
2	E	69	PRO	2.9
2	E	67	VAL	2.9
2	E	72	GLY	2.9
2	E	125	GLY	2.9
2	E	101	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	57	GLY	2.8
2	E	139	VAL	2.8
2	E	85	LYS	2.8
2	E	74	ALA	2.8
2	E	175	TYR	2.8
2	E	132	ILE	2.7
2	E	211	VAL	2.7
2	E	50	GLU	2.7
2	E	97	GLU	2.7
1	D	464	ILE	2.7
2	E	215	LYS	2.7
2	E	217	PRO	2.6
2	E	151	LEU	2.6
2	E	184	VAL	2.6
2	E	176	ALA	2.6
2	E	59	GLN	2.6
2	E	52	GLY	2.5
2	E	61	ASP	2.5
2	E	83	PRO	2.5
2	E	80	VAL	2.5
2	E	118	VAL	2.5
2	E	140	ILE	2.5
2	E	161	THR	2.4
2	E	174	ARG	2.4
2	E	127	GLY	2.4
2	E	159	LEU	2.4
2	E	56	GLN	2.4
2	E	130	ILE	2.4
2	E	55	ARG	2.4
2	E	180	SER	2.3
2	E	109	LYS	2.3
2	E	181	PRO	2.3
2	E	115	PHE	2.3
2	E	145	LEU	2.3
2	E	89	ARG	2.3
2	E	169	GLY	2.3
2	E	77	VAL	2.3
2	E	76	THR	2.2
1	D	554	ASP	2.2
2	E	218	GLN	2.2
2	E	106	ARG	2.1
2	E	71	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	185	PRO	2.1
2	E	186	THR	2.1
2	E	68	GLY	2.1
2	E	126	SER	2.1
3	F	77	GLN	2.1
2	E	216	ASN	2.1
2	E	144	GLY	2.0
1	A	551	ASN	2.0
2	E	219	GLU	2.0
2	E	164	THR	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](#)

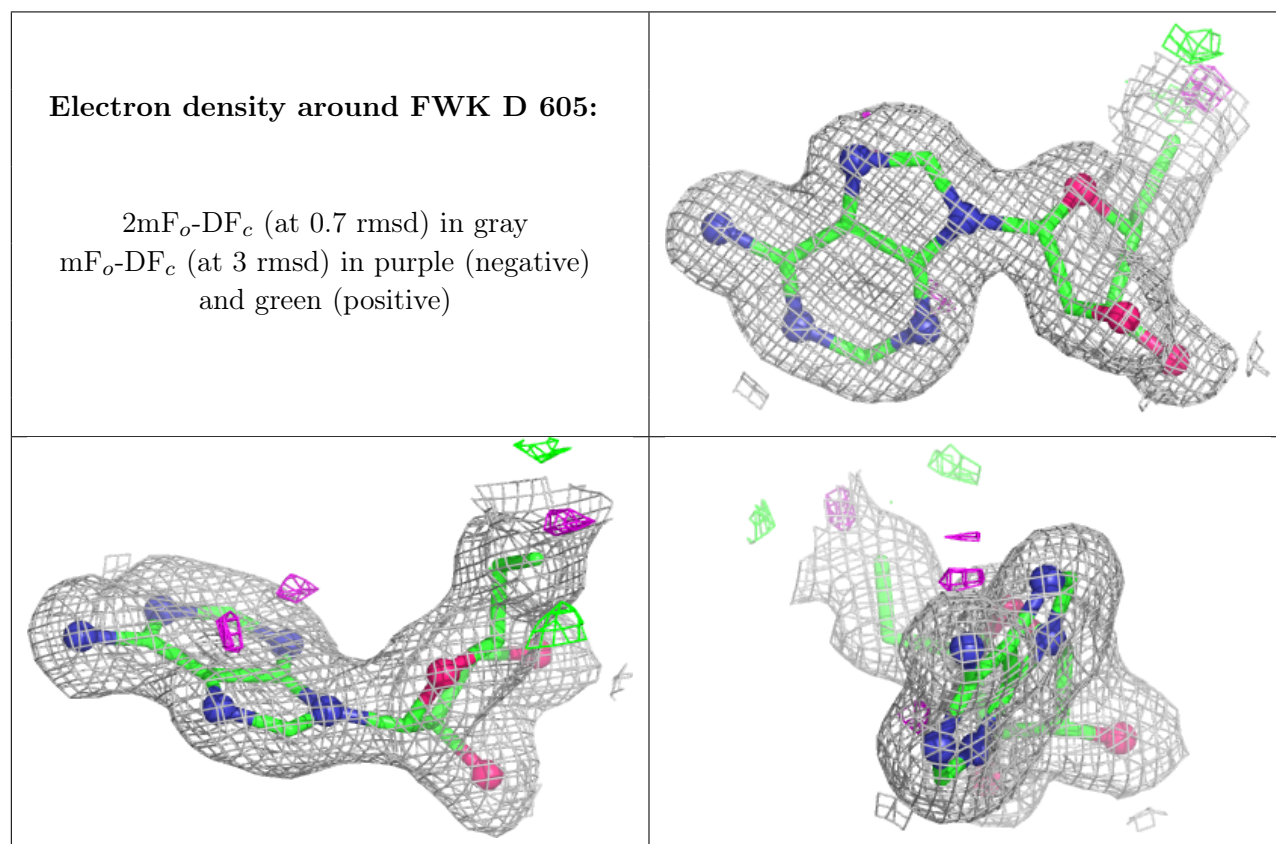
There are no oligosaccharides in this entry.

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, 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.

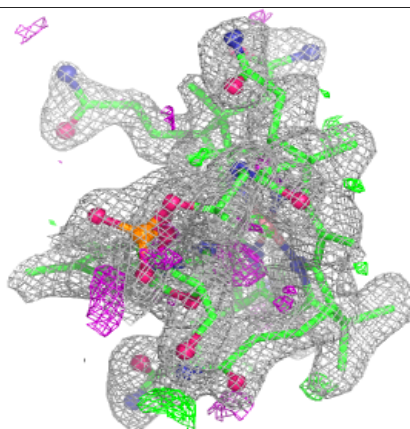
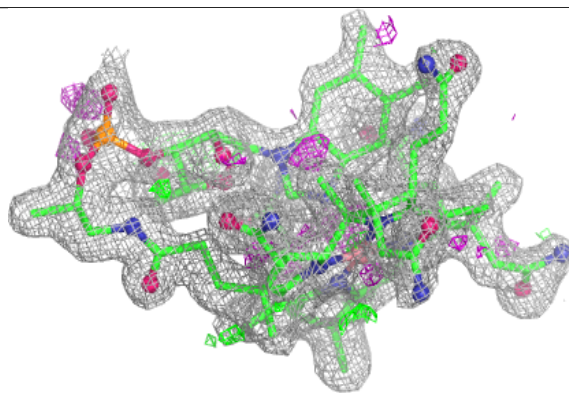
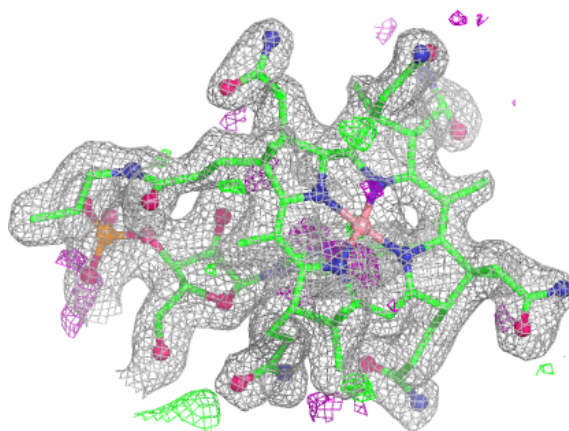
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	K	D	603	1/1	0.94	0.06	15,15,15,15	0
8	FWK	D	605	19/19	0.94	0.07	18,22,28,30	0
9	B12	E	301	91/91	0.94	0.10	25,35,49,59	0
6	K	A	603	1/1	0.95	0.05	12,12,12,12	0
4	PGO	D	601	5/5	0.97	0.06	16,17,20,20	0
8	FWK	A	605	19/19	0.97	0.05	14,16,16,17	0
9	B12	B	301	91/91	0.98	0.06	12,18,29,39	0
4	PGO	A	601	5/5	0.99	0.03	9,10,12,16	0
5	CA	D	602	1/1	0.99	0.03	13,13,13,13	0
7	NH4	A	604	1/1	0.99	0.05	7,7,7,7	0
7	NH4	D	604	1/1	0.99	0.07	16,16,16,16	0
5	CA	A	602	1/1	1.00	0.01	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.

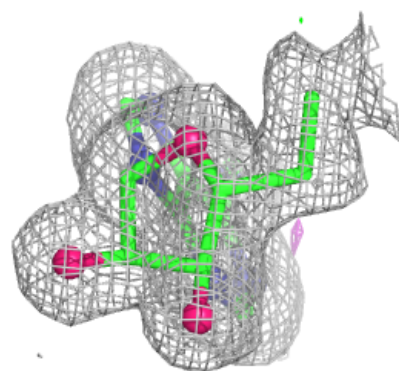
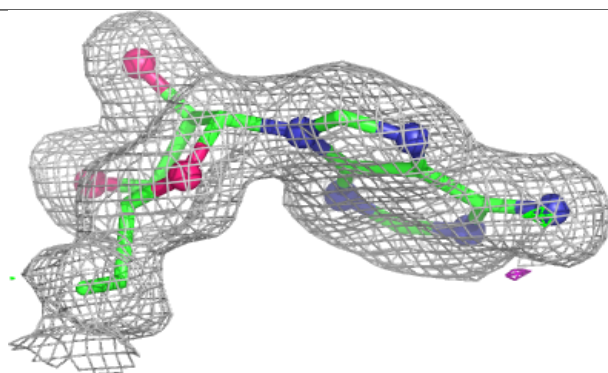
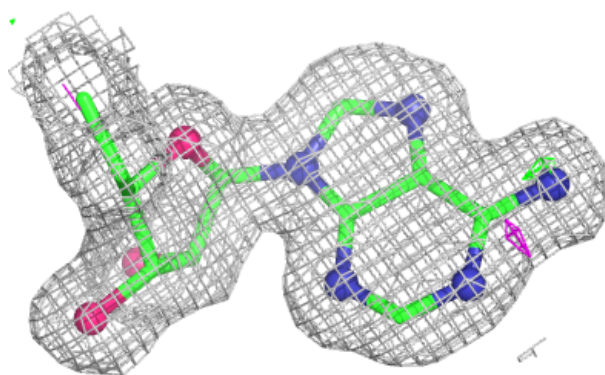


Electron density around B12 E 301:

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

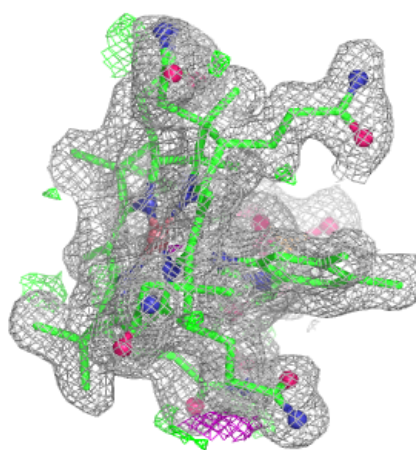
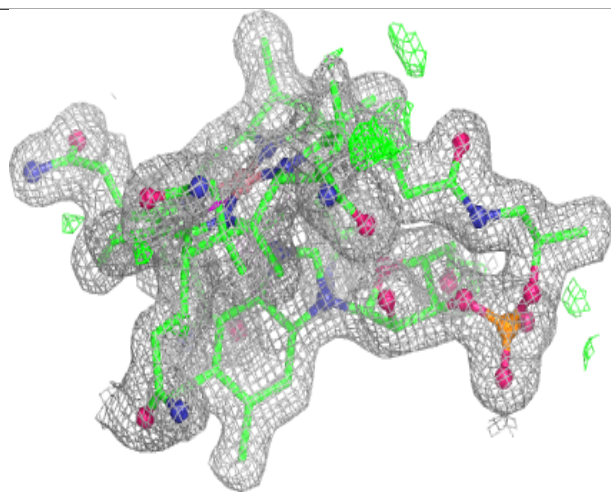
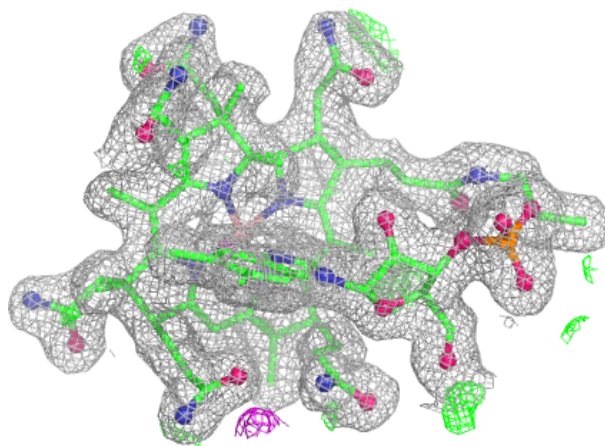
**Electron density around FWK A 605:**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.