Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:48 AM JST

PDB ID	:	5YRT
Title	:	Diol dehydratase, AdoCbl/substrate-free, anaerobically-prepared crystal
Authors	:	Shibata, N.
Deposited on	:	2017-11-10
Resolution	:	1.70 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:

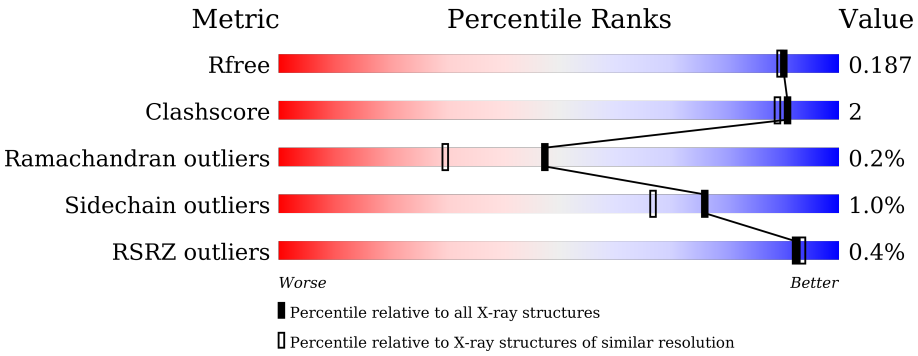
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	94% 5%
1	D	554	94% 5%
1	G	554	96%
1	J	554	% 96%
2	B	200	2% 86% 6% 9%
2	E	200	85% 11%

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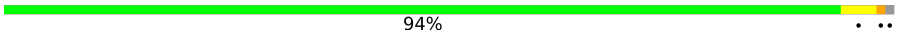
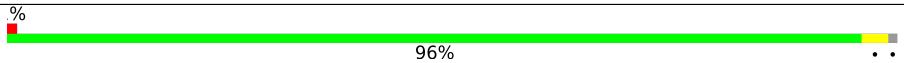
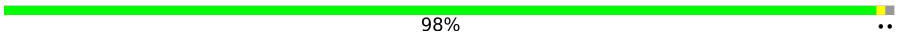
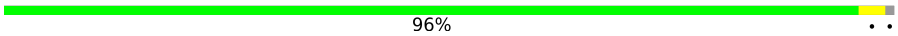
Mol	Chain	Length	Quality of chain
2	H	200	
2	K	200	
3	C	137	
3	F	137	
3	I	137	
3	L	137	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 30305 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	551	Total	C	N	O	S	0	6	0
			4227	2639	728	831	29			
1	D	551	Total	C	N	O	S	0	4	0
			4218	2632	729	828	29			
1	G	554	Total	C	N	O	S	0	5	0
			4251	2652	732	838	29			
1	J	554	Total	C	N	O	S	0	5	0
			4252	2651	734	838	29			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	2	0
			1391	880	249	260	2			
2	E	178	Total	C	N	O	S	0	2	0
			1372	869	244	257	2			
2	H	178	Total	C	N	O	S	0	5	0
			1392	882	253	255	2			
2	K	182	Total	C	N	O	S	0	2	0
			1391	881	249	259	2			

There are 84 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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
H	33	HIS	-	expression tag	UNP Q59471
H	34	SER	-	expression tag	UNP Q59471
H	35	ALA	-	expression tag	UNP Q59471
H	36	ALA	-	expression tag	UNP Q59471
H	37	LEU	-	expression tag	UNP Q59471
H	38	GLU	-	expression tag	UNP Q59471
H	39	VAL	-	expression tag	UNP Q59471
H	40	LEU	-	expression tag	UNP Q59471
H	41	PHE	-	expression tag	UNP Q59471
H	42	GLN	-	expression tag	UNP Q59471
H	43	GLY	-	expression tag	UNP Q59471
H	44	PRO	-	expression tag	UNP Q59471
H	45	GLY	-	expression tag	UNP Q59471
K	25	MET	-	expression tag	UNP Q59471
K	26	SER	-	expression tag	UNP Q59471
K	27	SER	-	expression tag	UNP Q59471
K	28	HIS	-	expression tag	UNP Q59471
K	29	HIS	-	expression tag	UNP Q59471
K	30	HIS	-	expression tag	UNP Q59471
K	31	HIS	-	expression tag	UNP Q59471
K	32	HIS	-	expression tag	UNP Q59471
K	33	HIS	-	expression tag	UNP Q59471
K	34	SER	-	expression tag	UNP Q59471
K	35	ALA	-	expression tag	UNP Q59471
K	36	ALA	-	expression tag	UNP Q59471
K	37	LEU	-	expression tag	UNP Q59471
K	38	GLU	-	expression tag	UNP Q59471
K	39	VAL	-	expression tag	UNP Q59471
K	40	LEU	-	expression tag	UNP Q59471
K	41	PHE	-	expression tag	UNP Q59471
K	42	GLN	-	expression tag	UNP Q59471
K	43	GLY	-	expression tag	UNP Q59471
K	44	PRO	-	expression tag	UNP Q59471
K	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	4	0
			1105	690	195	216	4			
3	F	136	Total	C	N	O	S	0	0	0
			1087	678	194	212	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	136	Total	C	N	O	S	0	4	0
			1106	690	198	215	3			
3	L	136	Total	C	N	O	S	0	3	0
			1103	688	195	217	3			

There are 4 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
I	37	MET	-	expression tag	UNP Q59472
L	37	MET	-	expression tag	UNP Q59472

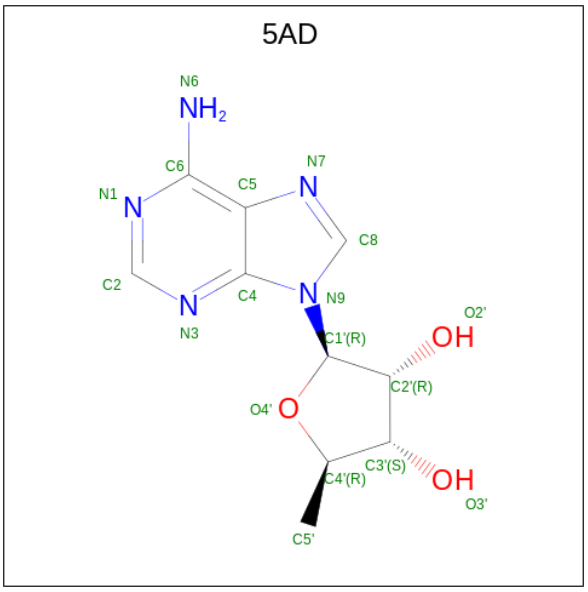
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	K	0	0
			2	2		
5	D	2	Total	K	0	0
			2	2		
5	G	2	Total	K	0	0
			2	2		
5	J	2	Total	K	0	0
			2	2		

- Molecule 6 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).

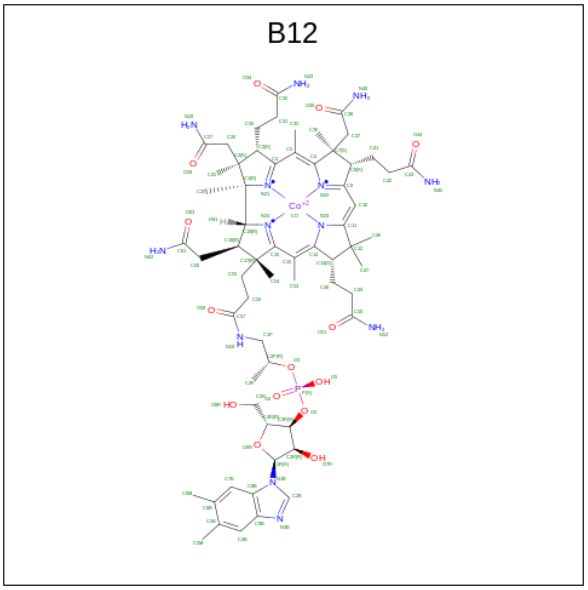


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 18 10 5 3	0	0
6	D	1	Total C N O 18 10 5 3	0	0
6	G	1	Total C N O 18 10 5 3	0	0
6	J	1	Total C N O 18 10 5 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0
7	C	1	Total Cl 1 1	0	0
7	D	2	Total Cl 2 2	0	0
7	F	1	Total Cl 1 1	0	0
7	G	2	Total Cl 2 2	0	0
7	I	1	Total Cl 1 1	0	0
7	J	2	Total Cl 2 2	0	0
7	L	1	Total Cl 1 1	0	0

- Molecule 8 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	436	Total	O	0	0
			436	436		
9	B	146	Total	O	0	0
			146	146		
9	C	148	Total	O	0	0
			148	148		
9	D	412	Total	O	0	0
			412	412		
9	E	176	Total	O	0	0
			176	176		
9	F	114	Total	O	0	0
			114	114		
9	G	442	Total	O	0	0
			442	442		

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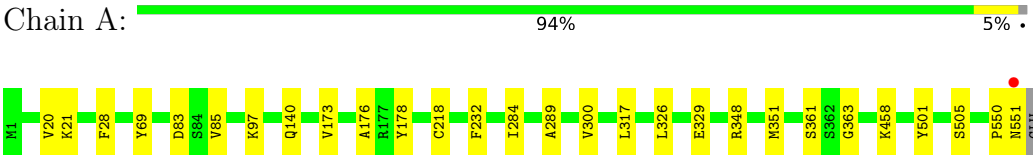
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	180	Total O 180 180	0	0
9	I	133	Total O 133 133	0	0
9	J	444	Total O 444 444	0	0
9	K	181	Total O 181 181	0	0
9	L	138	Total O 138 138	0	0

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.

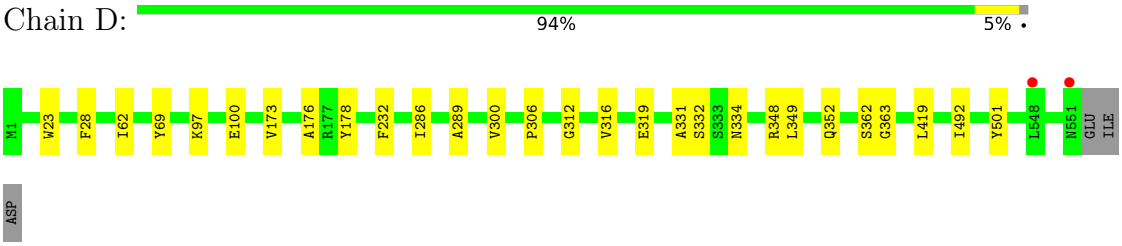
• Molecule 1: Diol dehydrase alpha subunit

Chain A:



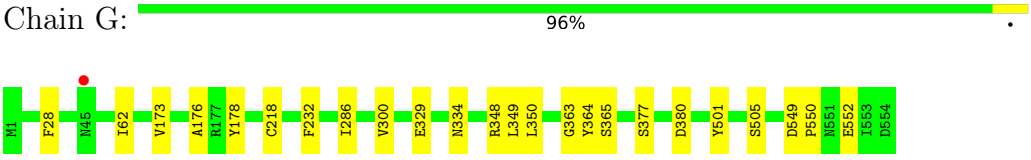
• Molecule 1: Diol dehydrase alpha subunit

Chain D:



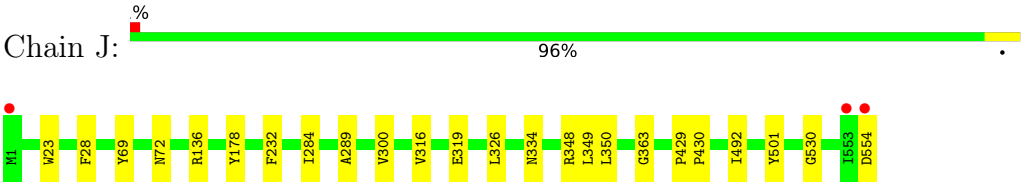
• Molecule 1: Diol dehydrase alpha subunit

Chain G:



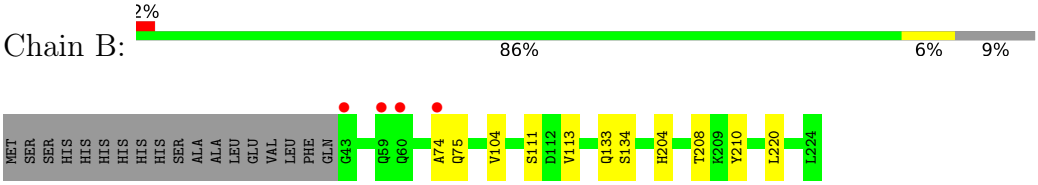
• Molecule 1: Diol dehydrase alpha subunit

Chain J:



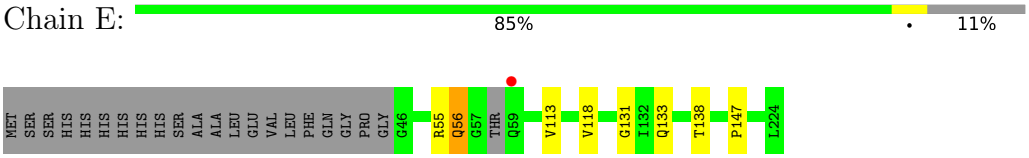
• Molecule 2: Diol dehydrase beta subunit

Chain B:



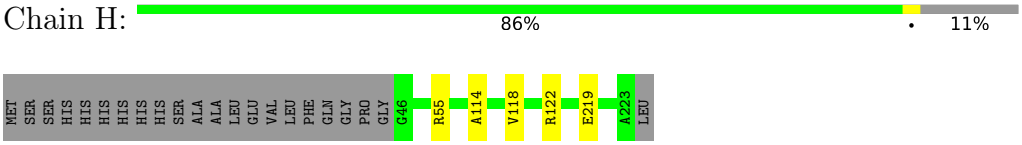
• Molecule 2: Diol dehydrase beta subunit

Chain E:



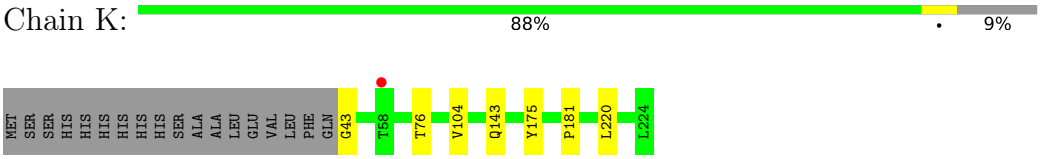
• Molecule 2: Diol dehydrase beta subunit

Chain H:



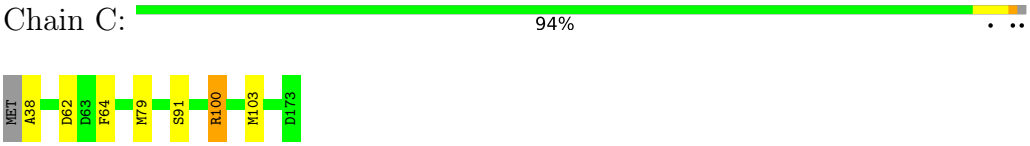
• Molecule 2: Diol dehydrase beta subunit

Chain K:



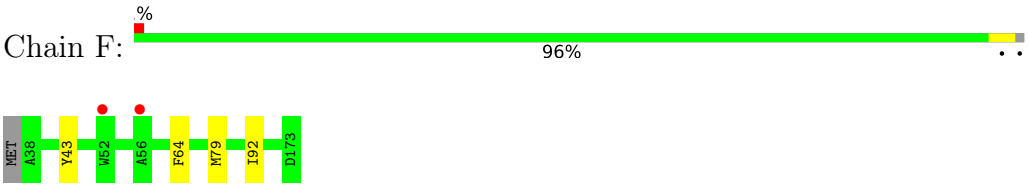
• Molecule 3: Diol dehydrase gamma subunit

Chain C:



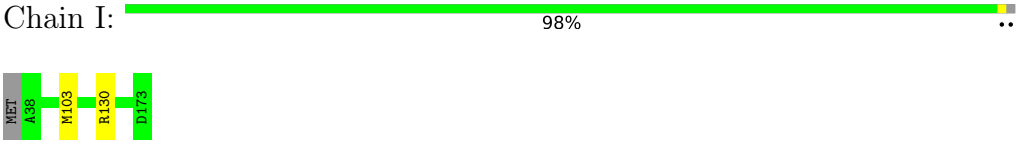
• Molecule 3: Diol dehydrase gamma subunit

Chain F:



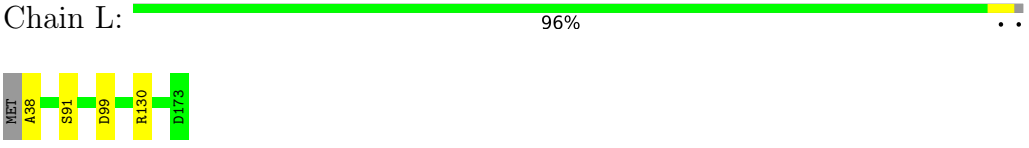
• Molecule 3: Diol dehydrase gamma subunit

Chain I:



• Molecule 3: Diol dehydrase gamma subunit

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.69Å 95.46Å 114.57Å 80.78° 87.58° 81.10°	Depositor
Resolution (Å)	47.00 – 1.70 46.58 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (47.00-1.70) 85.6 (46.58-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.149 , 0.187 0.149 , 0.187	Depositor DCC
R_{free} test set	3095 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	30305	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: 5AD, CA, B12, K, CL

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	0.37	1/4317 (0.0%)	0.57	0/5847
1	D	0.36	0/4302	0.56	0/5825
1	G	0.37	1/4338 (0.0%)	0.57	0/5872
1	J	0.38	0/4339	0.56	0/5874
2	B	0.34	0/1420	0.53	0/1921
2	E	0.36	0/1399	0.53	0/1890
2	H	0.35	0/1429	0.53	0/1931
2	K	0.35	0/1420	0.54	0/1921
3	C	0.34	0/1132	0.52	0/1529
3	F	0.30	0/1102	0.50	0/1489
3	I	0.34	0/1133	0.49	0/1530
3	L	0.33	0/1127	0.52	0/1523
All	All	0.36	2/27458 (0.0%)	0.55	0/37152

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	CYS	CB-SG	-6.36	1.71	1.82
1	G	218	CYS	CB-SG	-5.64	1.72	1.81

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	4227	0	4179	14	0
1	D	4218	0	4168	13	0
1	G	4251	0	4197	10	0
1	J	4252	0	4195	9	0
2	B	1391	0	1445	7	0
2	E	1372	0	1423	4	0
2	H	1392	0	1463	3	0
2	K	1391	0	1450	3	0
3	C	1105	0	1120	4	0
3	F	1087	0	1096	2	0
3	I	1106	0	1125	2	0
3	L	1103	0	1112	3	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	2	0	0	0	0
5	D	2	0	0	0	0
5	G	2	0	0	0	0
5	J	2	0	0	0	0
6	A	18	0	13	0	0
6	D	18	0	13	0	0
6	G	18	0	13	0	0
6	J	18	0	13	0	0
7	A	2	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
7	F	1	0	0	0	0
7	G	2	0	0	0	0
7	I	1	0	0	0	0
7	J	2	0	0	0	0
7	L	1	0	0	1	0
8	B	91	0	88	5	0
8	E	91	0	88	5	0
8	H	91	0	88	7	0
8	K	91	0	88	6	0
9	A	436	0	0	2	0
9	B	146	0	0	0	0
9	C	148	0	0	0	0
9	D	412	0	0	0	0
9	E	176	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	114	0	0	0	0
9	G	442	0	0	0	0
9	H	180	0	0	1	0
9	I	133	0	0	1	0
9	J	444	0	0	1	0
9	K	181	0	0	0	0
9	L	138	0	0	0	0
All	All	30305	0	27377	91	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 2.

All (91) 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:J:72[A]:ASN:ND2	9:J:701:HOH:O	2.22	0.67
3:F:64:PHE:CE1	3:F:79:MET:HG2	2.30	0.67
3:C:64:PHE:CE2	3:C:79:MET:HG2	2.30	0.65
8:H:1601:B12:H552	8:H:1601:B12:H531	1.77	0.65
8:B:1601:B12:H552	8:B:1601:B12:H531	1.80	0.62
8:E:1601:B12:H552	8:E:1601:B12:H531	1.81	0.62
2:B:204:HIS:O	2:B:208:THR:HG23	2.00	0.61
1:G:350:LEU:HD12	1:J:350:LEU:HD12	1.82	0.61
3:L:38:ALA:N	3:L:91:SER:HG	1.99	0.60
8:E:1601:B12:C2B	8:E:1601:B12:H492	2.32	0.59
8:K:1601:B12:H552	8:K:1601:B12:H531	1.85	0.57
8:H:1601:B12:H362	8:H:1601:B12:H351	1.86	0.56
8:K:1601:B12:H362	8:K:1601:B12:H351	1.86	0.56
2:B:113:VAL:HB	2:B:133:GLN:HG3	1.88	0.56
1:A:20[B]:VAL:HG12	1:A:21:LYS:O	2.07	0.55
2:B:75:GLN:HB2	2:B:134[B]:SER:OG	2.06	0.54
1:A:284:ILE:HG22	1:A:326:LEU:HD12	1.90	0.54
8:H:1601:B12:H492	8:H:1601:B12:C2B	2.38	0.54
8:E:1601:B12:H351	8:E:1601:B12:H362	1.90	0.53
1:G:549:ASP:O	1:G:552[A]:GLU:HG2	2.10	0.52
8:K:1601:B12:C2B	8:K:1601:B12:H492	2.40	0.51
8:B:1601:B12:C2B	8:B:1601:B12:H492	2.40	0.51
8:H:1601:B12:H531	8:H:1601:B12:C55	2.41	0.50
8:B:1601:B12:H531	8:B:1601:B12:C55	2.40	0.50
2:E:113:VAL:HB	2:E:133:GLN:HG3	1.93	0.50
1:A:550:PRO:HG2	1:D:23:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:55:ARG:HG3	2:E:56:GLN:N	2.26	0.50
1:A:69:TYR:HB2	1:A:289:ALA:HB1	1.94	0.49
1:A:317:LEU:HD22	1:A:351:MET:HB3	1.94	0.49
8:B:1601:B12:H362	8:B:1601:B12:H351	1.94	0.49
3:L:99[A]:ASP:OD1	7:L:201:CL:CL	2.68	0.48
1:D:62:ILE:HG23	1:D:286:ILE:HD11	1.96	0.48
1:D:173:VAL:HG21	1:D:176:ALA:HA	1.96	0.48
8:K:1601:B12:H531	8:K:1601:B12:C55	2.43	0.47
1:J:69:TYR:HB2	1:J:289:ALA:HB1	1.96	0.47
1:A:551:ASN:HB3	1:D:23:TRP:CZ2	2.50	0.47
2:B:104:VAL:HG12	2:B:220:LEU:HD12	1.97	0.47
1:G:62:ILE:HG23	1:G:286:ILE:HD11	1.97	0.46
8:H:1601:B12:H253	8:H:1601:B12:H301	1.74	0.46
1:G:550:PRO:HG3	1:J:23:TRP:HB2	1.98	0.45
1:G:173:VAL:HG21	1:G:176:ALA:HA	1.97	0.45
2:K:43:GLY:N	2:K:76:THR:HG1	2.14	0.45
8:E:1601:B12:H531	8:E:1601:B12:C55	2.45	0.45
1:G:549:ASP:O	1:G:552[B]:GLU:HG2	2.16	0.45
1:J:429:PRO:HA	1:J:430:PRO:HD3	1.87	0.45
3:C:100:ARG:N	3:C:100:ARG:HD2	2.30	0.44
2:H:118:VAL:O	2:H:122[A]:ARG:HG2	2.16	0.44
1:D:69:TYR:HB2	1:D:289:ALA:HB1	1.99	0.44
2:B:111:SER:OG	2:B:208:THR:HG22	2.18	0.44
2:B:74:ALA:HB2	2:B:210:TYR:CZ	2.53	0.44
3:C:100:ARG:NH1	3:C:103[A]:MET:SD	2.91	0.44
2:K:175:TYR:CE1	2:K:181:PRO:HD2	2.53	0.43
1:A:329:GLU:OE2	1:A:505:SER:HA	2.18	0.43
2:H:219:GLU:OE1	9:H:1701:HOH:O	2.21	0.43
2:E:118:VAL:HG21	2:E:147:PRO:HA	2.00	0.43
1:D:334:ASN:OD1	1:D:349:LEU:HA	2.18	0.43
1:G:334:ASN:OD1	1:G:349:LEU:HA	2.19	0.43
8:H:1601:B12:H261	8:H:1601:B12:H91	1.85	0.43
1:J:284:ILE:HG22	1:J:326:LEU:HD12	2.01	0.43
1:G:329:GLU:OE2	1:G:505:SER:HA	2.19	0.42
1:A:140:GLN:OE1	1:A:361[B]:SER:HB3	2.20	0.42
1:A:550:PRO:HB2	1:D:23:TRP:CE3	2.55	0.42
1:D:97:LYS:HB2	1:D:100:GLU:HG3	2.01	0.42
3:F:43:TYR:HB2	3:F:92:ILE:HD13	2.01	0.42
1:A:458:LYS:HE3	9:A:1076:HOH:O	2.19	0.42
1:J:136[A]:ARG:NH2	1:J:530:GLY:O	2.53	0.42
1:D:306:PRO:O	1:D:312:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:SER:HB2	1:D:352:GLN:HG2	2.02	0.42
2:E:131:GLY:O	2:E:138:THR:HA	2.20	0.41
1:D:331:ALA:HB1	1:D:362:SER:HB3	2.01	0.41
8:K:1601:B12:H253	8:K:1601:B12:H301	1.82	0.41
3:C:38:ALA:N	3:C:91[A]:SER:HG	2.17	0.41
1:A:83:ASP:OD2	1:A:85:VAL:HB	2.20	0.41
8:K:1601:B12:C4	8:K:1601:B12:C27	2.99	0.41
1:A:140:GLN:OE1	1:A:361[A]:SER:HB2	2.21	0.41
1:A:173:VAL:HG21	1:A:176:ALA:HA	2.02	0.41
1:G:365:SER:HB2	1:G:377:SER:HB3	2.02	0.41
1:J:316:VAL:O	1:J:319:GLU:HG2	2.20	0.41
2:K:104:VAL:HG12	2:K:220:LEU:HD12	2.03	0.41
2:B:75:GLN:HB2	2:B:134[B]:SER:HG	1.85	0.41
2:H:114:ALA:HB2	8:H:1601:B12:HM62	2.02	0.41
1:D:419:LEU:HD12	1:D:419:LEU:HA	1.95	0.40
3:I:103:MET:HG3	9:I:386:HOH:O	2.21	0.40
1:A:97:LYS:HE2	9:A:1063:HOH:O	2.21	0.40
1:J:334:ASN:OD1	1:J:349:LEU:HA	2.21	0.40
8:E:1601:B12:H253	8:E:1601:B12:H301	1.85	0.40
1:G:365:SER:HB3	1:G:380:ASP:HA	2.03	0.40
8:B:1601:B12:H301	8:B:1601:B12:H253	1.90	0.40
1:D:316:VAL:O	1:D:319:GLU:HG2	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	555/554 (100%)	535 (96%)	18 (3%)	2 (0%)	34	18
1	D	553/554 (100%)	537 (97%)	14 (2%)	2 (0%)	34	18
1	G	557/554 (100%)	539 (97%)	16 (3%)	2 (0%)	34	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	557/554 (100%)	541 (97%)	14 (2%)	2 (0%)	34 18
2	B	182/200 (91%)	178 (98%)	4 (2%)	0	100 100
2	E	176/200 (88%)	172 (98%)	4 (2%)	0	100 100
2	H	181/200 (90%)	177 (98%)	4 (2%)	0	100 100
2	K	182/200 (91%)	179 (98%)	3 (2%)	0	100 100
3	C	138/137 (101%)	137 (99%)	1 (1%)	0	100 100
3	F	134/137 (98%)	133 (99%)	1 (1%)	0	100 100
3	I	138/137 (101%)	136 (99%)	2 (1%)	0	100 100
3	L	137/137 (100%)	135 (98%)	2 (2%)	0	100 100
All	All	3490/3564 (98%)	3399 (97%)	83 (2%)	8 (0%)	47 30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	GLY
1	G	363	GLY
1	A	300	VAL
1	D	300	VAL
1	D	363	GLY
1	G	300	VAL
1	J	300	VAL
1	J	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	456/453 (101%)	451 (99%)	5 (1%)	73 63
1	D	454/453 (100%)	448 (99%)	6 (1%)	69 56
1	G	458/453 (101%)	452 (99%)	6 (1%)	69 56
1	J	458/453 (101%)	451 (98%)	7 (2%)	65 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	150/164 (92%)	150 (100%)	0	100 100
2	E	148/164 (90%)	147 (99%)	1 (1%)	84 77
2	H	151/164 (92%)	149 (99%)	2 (1%)	69 56
2	K	150/164 (92%)	149 (99%)	1 (1%)	84 77
3	C	119/116 (103%)	116 (98%)	3 (2%)	47 29
3	F	115/116 (99%)	115 (100%)	0	100 100
3	I	119/116 (103%)	119 (100%)	0	100 100
3	L	118/116 (102%)	118 (100%)	0	100 100
All	All	2896/2932 (99%)	2865 (99%)	31 (1%)	76 63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	178	TYR
1	A	232	PHE
1	A	348	ARG
1	A	501	TYR
3	C	62[A]	ASP
3	C	62[B]	ASP
3	C	100	ARG
1	D	28	PHE
1	D	178	TYR
1	D	232	PHE
1	D	348	ARG
1	D	492	ILE
1	D	501	TYR
2	E	56	GLN
1	G	28	PHE
1	G	178	TYR
1	G	232	PHE
1	G	348	ARG
1	G	364	TYR
1	G	501	TYR
2	H	55[A]	ARG
2	H	55[B]	ARG
1	J	28	PHE
1	J	178	TYR
1	J	232	PHE

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Mol	Chain	Res	Type
1	J	348	ARG
1	J	492	ILE
1	J	501	TYR
1	J	554	ASP
2	K	143	GLN

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

Mol	Chain	Res	Type
2	B	56	GLN
2	B	60	GLN
1	D	74	ASN
2	E	56	GLN
2	E	218	GLN
3	I	47	ASN
1	J	16	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 24 are monoatomic - leaving 8 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	$\#\|Z\|>2$
6	5AD	D	604	-	17,20,20	1.11	1 (5%)	15,30,30	1.44	3 (20%)
8	B12	B	1601	-	90,101,101	1.63	9 (10%)	137,166,166	1.43	16 (11%)
8	B12	H	1601	-	90,101,101	1.56	9 (10%)	137,166,166	1.25	12 (8%)
6	5AD	J	604	-	17,20,20	1.01	1 (5%)	15,30,30	1.84	4 (26%)
8	B12	K	1601	-	90,101,101	1.56	8 (8%)	137,166,166	1.24	17 (12%)
6	5AD	A	604	-	17,20,20	1.13	1 (5%)	15,30,30	1.64	3 (20%)
6	5AD	G	604	-	17,20,20	1.15	1 (5%)	15,30,30	1.67	3 (20%)
8	B12	E	1601	-	90,101,101	1.63	9 (10%)	137,166,166	1.34	16 (11%)

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
6	5AD	D	604	-	-	0/0/20/20	0/3/3/3
8	B12	B	1601	-	-	7/52/223/223	0/3/11/11
8	B12	H	1601	-	-	8/52/223/223	0/3/11/11
6	5AD	J	604	-	-	0/0/20/20	0/3/3/3
8	B12	K	1601	-	-	7/52/223/223	0/3/11/11
6	5AD	A	604	-	-	0/0/20/20	0/3/3/3
6	5AD	G	604	-	-	0/0/20/20	0/3/3/3
8	B12	E	1601	-	-	5/52/223/223	0/3/11/11

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1601	B12	C19-N24	-10.45	1.29	1.48
8	E	1601	B12	C19-N24	-9.88	1.30	1.48
8	K	1601	B12	C19-N24	-9.88	1.30	1.48
8	H	1601	B12	C19-N24	-9.43	1.31	1.48
8	E	1601	B12	C14-N23	-5.29	1.28	1.35
8	E	1601	B12	C11-N23	4.58	1.45	1.37
8	H	1601	B12	C8B-C9B	4.48	1.49	1.40
8	E	1601	B12	C8B-C9B	4.35	1.49	1.40
8	K	1601	B12	C8B-C9B	4.30	1.49	1.40
8	B	1601	B12	C8B-C9B	4.26	1.49	1.40
8	H	1601	B12	C14-N23	-4.21	1.29	1.35
8	B	1601	B12	C14-N23	-4.20	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1601	B12	C11-N23	4.16	1.44	1.37
8	K	1601	B12	C14-N23	-4.08	1.29	1.35
8	H	1601	B12	C11-N23	4.04	1.44	1.37
8	K	1601	B12	C11-N23	3.72	1.44	1.37
8	B	1601	B12	C6B-C5B	3.53	1.49	1.40
8	H	1601	B12	C16-C15	-3.38	1.35	1.44
8	E	1601	B12	C6B-C5B	3.34	1.49	1.40
8	K	1601	B12	C16-C15	-3.31	1.35	1.44
8	H	1601	B12	C6B-C5B	3.23	1.48	1.40
8	B	1601	B12	C16-C15	-3.23	1.35	1.44
8	K	1601	B12	C6B-C5B	3.18	1.48	1.40
8	E	1601	B12	C16-C15	-2.92	1.36	1.44
8	K	1601	B12	C10-C9	2.87	1.47	1.39
8	H	1601	B12	C10-C9	2.86	1.47	1.39
8	B	1601	B12	C14-C15	2.83	1.50	1.38
8	E	1601	B12	C14-C15	2.77	1.50	1.38
8	H	1601	B12	C14-C15	2.75	1.50	1.38
6	G	604	5AD	C5-C4	2.72	1.48	1.40
8	K	1601	B12	C14-C15	2.71	1.49	1.38
8	B	1601	B12	C10-C9	2.68	1.46	1.39
8	E	1601	B12	C10-C9	2.67	1.46	1.39
6	D	604	5AD	C5-C4	2.63	1.47	1.40
6	J	604	5AD	C5-C4	2.42	1.47	1.40
6	A	604	5AD	C5-C4	2.41	1.47	1.40
8	H	1601	B12	O6R-C1R	2.06	1.44	1.41
8	E	1601	B12	O6R-C1R	2.03	1.43	1.41
8	B	1601	B12	O6R-C1R	2.02	1.43	1.41

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1601	B12	C20-C1-C19	-6.88	102.72	109.36
8	E	1601	B12	C20-C1-C19	-5.53	104.03	109.36
8	H	1601	B12	C9-C10-C11	-4.09	120.05	125.97
8	K	1601	B12	C20-C1-C19	-4.09	105.42	109.36
8	B	1601	B12	C18-C19-N24	4.08	108.52	102.31
8	E	1601	B12	C9-C10-C11	-3.86	120.39	125.97
8	B	1601	B12	C9-C10-C11	-3.77	120.51	125.97
8	H	1601	B12	C18-C19-N24	3.64	107.85	102.31
8	E	1601	B12	C18-C19-N24	3.59	107.78	102.31
8	E	1601	B12	C17-C16-C15	3.58	131.90	126.26
6	J	604	5AD	C5'-C4'-C3'	-3.52	112.00	115.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	1601	B12	C20-C1-C19	-3.49	105.99	109.36
6	J	604	5AD	N3-C2-N1	-3.46	123.27	128.68
8	K	1601	B12	C18-C19-N24	3.46	107.57	102.31
8	B	1601	B12	C13-C14-N23	3.44	113.79	109.10
8	H	1601	B12	C17-C16-C15	3.40	131.61	126.26
6	G	604	5AD	C5'-C4'-C3'	-3.39	112.14	115.70
8	K	1601	B12	C13-C14-N23	3.38	113.70	109.10
6	A	604	5AD	N3-C2-N1	-3.37	123.41	128.68
8	H	1601	B12	C17-C16-N24	-3.33	106.01	111.15
8	H	1601	B12	C13-C14-N23	3.32	113.62	109.10
8	B	1601	B12	C17-C16-C15	3.29	131.45	126.26
6	G	604	5AD	N3-C2-N1	-3.24	123.62	128.68
8	E	1601	B12	C26-C2-C1	3.23	115.04	110.01
6	D	604	5AD	N3-C2-N1	-3.17	123.73	128.68
8	E	1601	B12	C17-C16-N24	-3.14	106.30	111.15
8	H	1601	B12	C4B-C9B-C8B	-3.13	117.90	121.10
8	B	1601	B12	C17-C16-N24	-3.10	106.38	111.15
8	K	1601	B12	C9-C10-C11	-3.06	121.54	125.97
8	E	1601	B12	C13-C14-N23	3.04	113.23	109.10
8	K	1601	B12	C13-C14-C15	-3.01	119.72	124.32
8	B	1601	B12	C26-C2-C1	2.98	114.65	110.01
8	K	1601	B12	C17-C16-N24	-2.94	106.62	111.15
6	A	604	5AD	C4-C5-N7	-2.87	106.41	109.40
8	E	1601	B12	C1-C19-N24	2.86	109.46	106.24
8	K	1601	B12	C48-C13-C14	2.86	115.61	108.49
8	B	1601	B12	C48-C13-C14	2.80	115.47	108.49
8	K	1601	B12	C17-C16-C15	2.79	130.65	126.26
8	H	1601	B12	C13-C14-C15	-2.78	120.07	124.32
8	E	1601	B12	C53-C15-C16	2.76	125.14	120.38
8	H	1601	B12	C2P-C1P-N59	-2.73	108.91	112.93
8	E	1601	B12	C48-C13-C14	2.68	115.17	108.49
6	G	604	5AD	C4-C5-N7	-2.65	106.64	109.40
8	B	1601	B12	C13-C14-C15	-2.61	120.33	124.32
8	K	1601	B12	C41-C8-C9	-2.61	106.60	111.19
8	H	1601	B12	C4B-C9B-N3B	2.59	137.83	130.88
8	E	1601	B12	C25-C2-C26	-2.59	104.47	109.71
8	K	1601	B12	C26-C2-C1	2.58	114.03	110.01
6	D	604	5AD	C4-C5-N7	-2.57	106.72	109.40
8	E	1601	B12	C4B-C9B-N3B	2.55	137.72	130.88
6	J	604	5AD	C2-N1-C6	2.55	123.12	118.75
8	B	1601	B12	C1-C19-N24	2.53	109.08	106.24
8	B	1601	B12	C4B-C9B-N3B	2.49	137.54	130.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	1601	B12	C4B-C9B-N3B	2.48	137.53	130.88
8	K	1601	B12	C53-C15-C16	2.46	124.62	120.38
8	B	1601	B12	C19-C1-N21	2.45	104.67	102.16
8	B	1601	B12	C2P-C1P-N59	-2.44	109.33	112.93
6	A	604	5AD	C2-N1-C6	2.44	122.93	118.75
6	J	604	5AD	C4-C5-N7	-2.44	106.86	109.40
8	H	1601	B12	C53-C15-C16	2.43	124.57	120.38
8	E	1601	B12	C2P-C1P-N59	-2.42	109.37	112.93
8	E	1601	B12	C4B-C9B-C8B	-2.41	118.63	121.10
8	E	1601	B12	C53-C15-C14	-2.38	113.65	118.43
8	B	1601	B12	C12-C11-C10	2.33	126.41	123.37
8	H	1601	B12	C48-C13-C14	2.33	114.30	108.49
8	E	1601	B12	C13-C14-C15	-2.32	120.78	124.32
8	B	1601	B12	C4B-C9B-C8B	-2.27	118.78	121.10
8	K	1601	B12	C8B-C9B-N3B	-2.18	103.23	107.83
6	D	604	5AD	C2-N1-C6	2.14	122.41	118.75
8	K	1601	B12	C30-C3-C2	-2.09	114.67	119.09
8	B	1601	B12	C1-C19-C18	2.08	125.29	121.88
8	K	1601	B12	C12-C11-C10	2.03	126.01	123.37
8	K	1601	B12	C1-C19-N24	2.02	108.51	106.24
8	K	1601	B12	C25-C2-C26	-2.01	105.64	109.71

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1601	B12	C2-C3-C30-C31
8	B	1601	B12	C1-C2-C26-C27
8	B	1601	B12	C25-C2-C26-C27
8	E	1601	B12	C1-C2-C26-C27
8	E	1601	B12	C25-C2-C26-C27
8	H	1601	B12	C1-C2-C26-C27
8	H	1601	B12	C25-C2-C26-C27
8	K	1601	B12	C1-C2-C26-C27
8	K	1601	B12	C25-C2-C26-C27
8	K	1601	B12	C2-C3-C30-C31
8	H	1601	B12	C42-C41-C8-C9
8	K	1601	B12	C4-C3-C30-C31
8	E	1601	B12	C42-C41-C8-C9
8	K	1601	B12	C42-C41-C8-C9
8	H	1601	B12	C3-C2-C26-C27
8	E	1601	B12	C17-C18-C60-C61

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Mol	Chain	Res	Type	Atoms
8	H	1601	B12	C17-C18-C60-C61
8	K	1601	B12	C17-C18-C60-C61
8	H	1601	B12	C4-C3-C30-C31
8	B	1601	B12	C42-C41-C8-C9
8	B	1601	B12	C19-C18-C60-C61
8	E	1601	B12	C19-C18-C60-C61
8	H	1601	B12	C19-C18-C60-C61
8	K	1601	B12	C19-C18-C60-C61
8	B	1601	B12	C12-C13-C48-C49
8	B	1601	B12	C3-C2-C26-C27
8	B	1601	B12	C17-C18-C60-C61

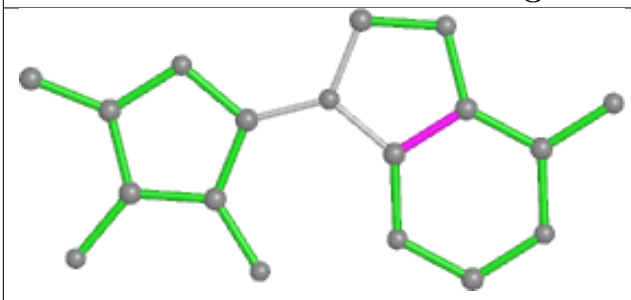
There are no ring outliers.

4 monomers are involved in 23 short contacts:

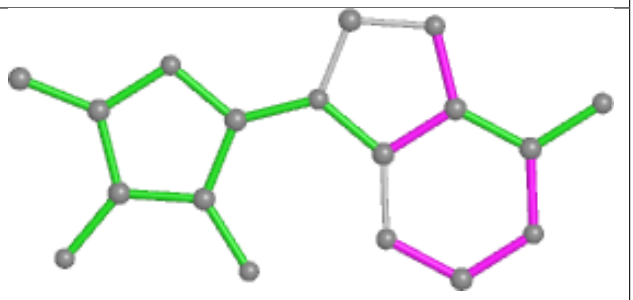
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1601	B12	5	0
8	H	1601	B12	7	0
8	K	1601	B12	6	0
8	E	1601	B12	5	0

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.

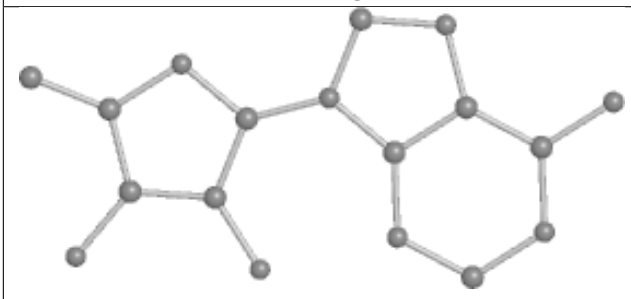
Ligand 5AD D 604



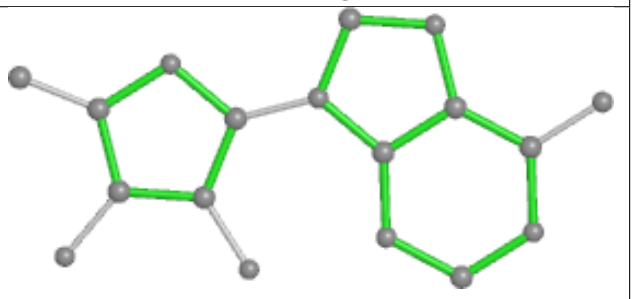
Bond lengths



Bond angles

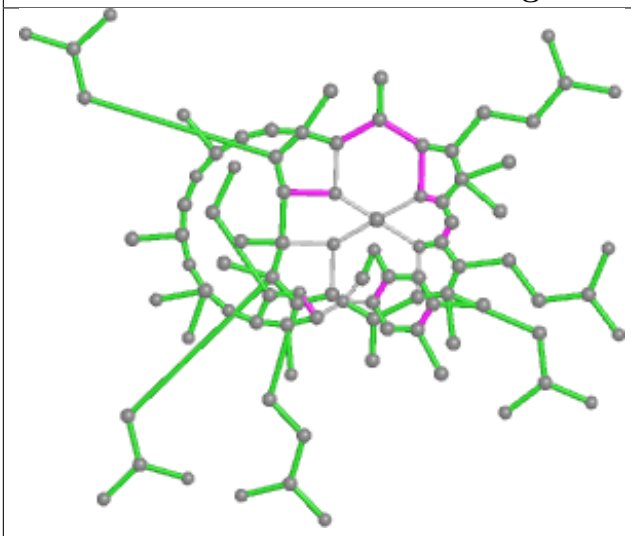


Torsions



Rings

Ligand B12 B 1601



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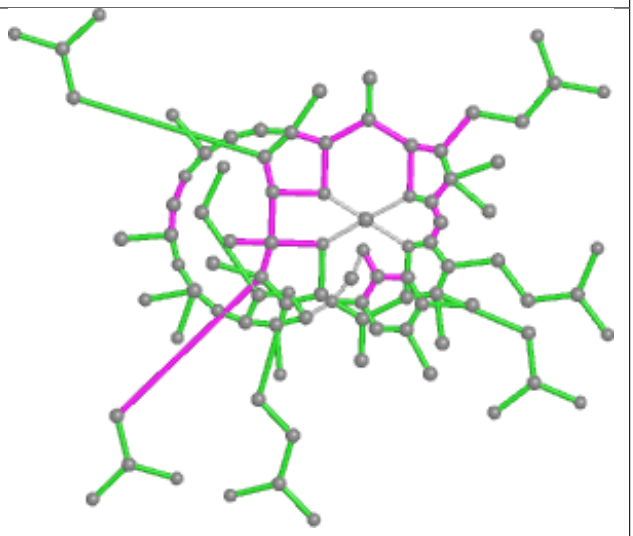

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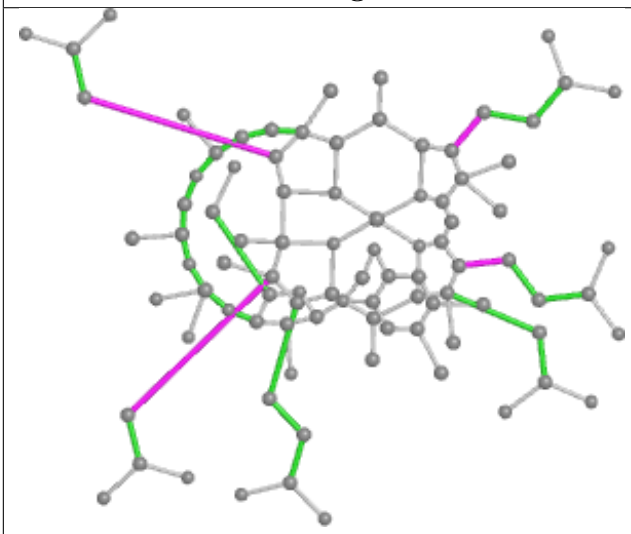

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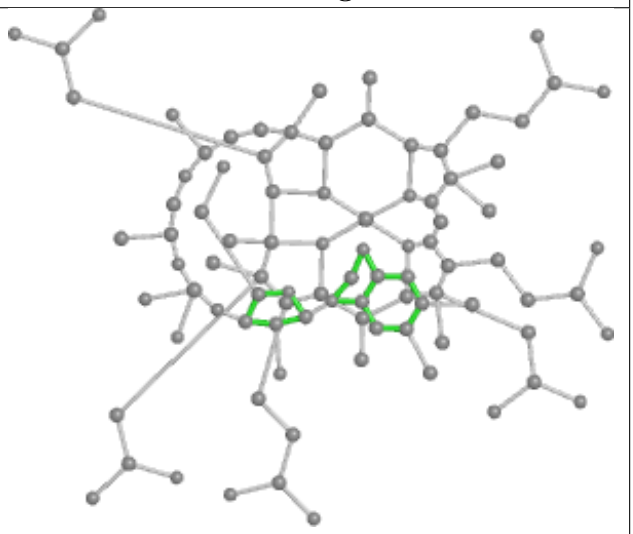
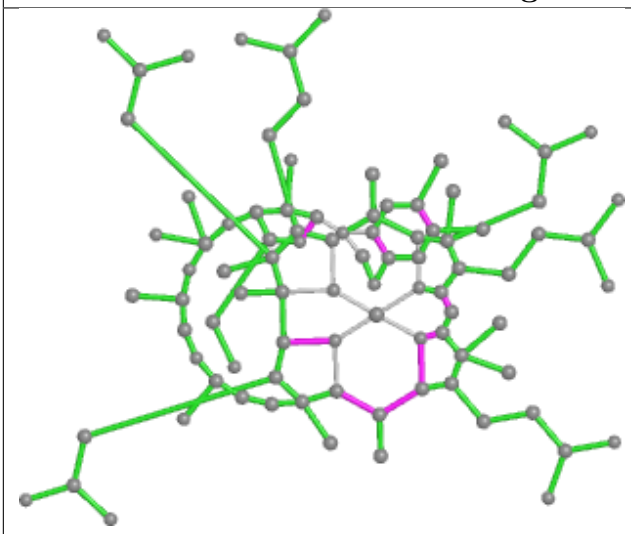


Rings

Ligand B12 H 1601



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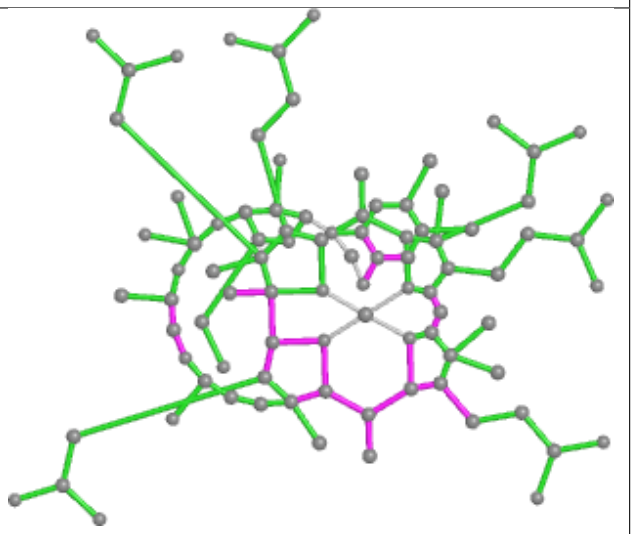
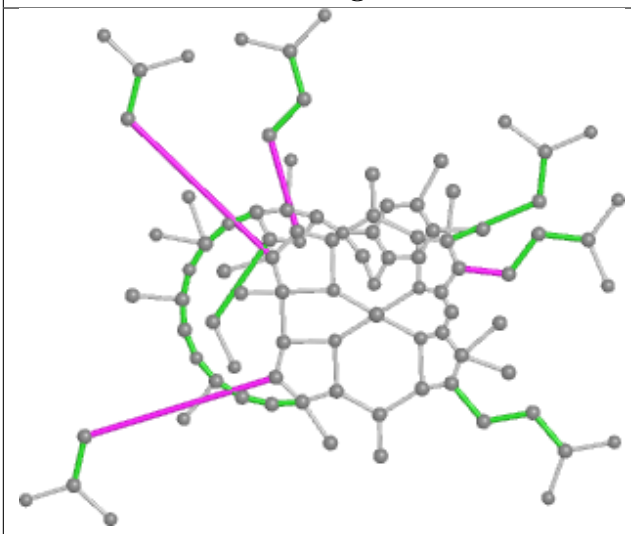


Bond angles



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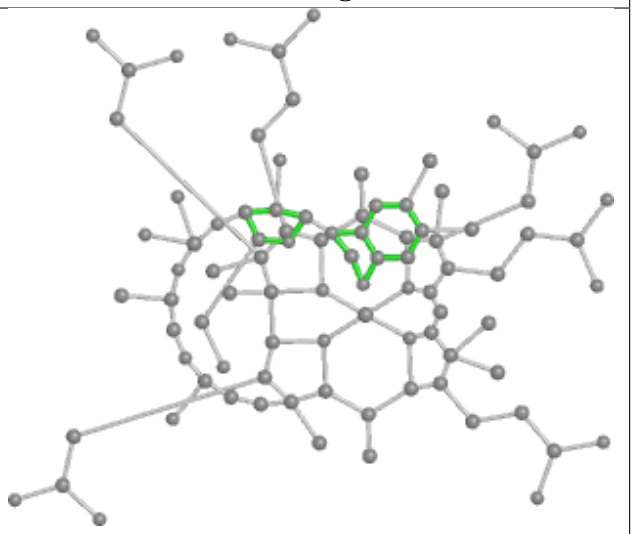
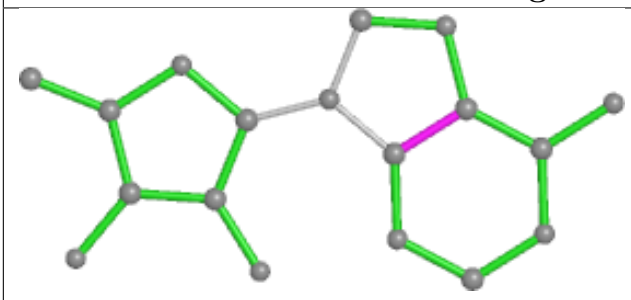


Rings

Ligand 5AD J 604



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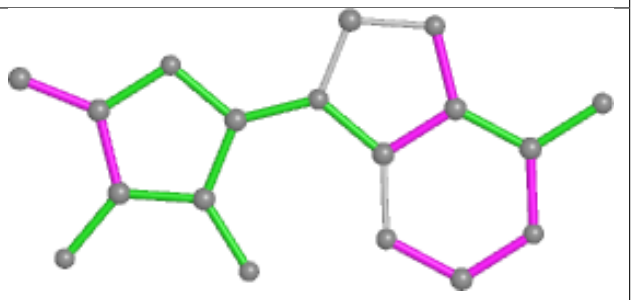

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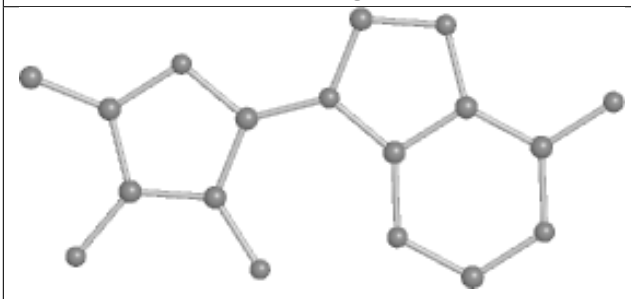

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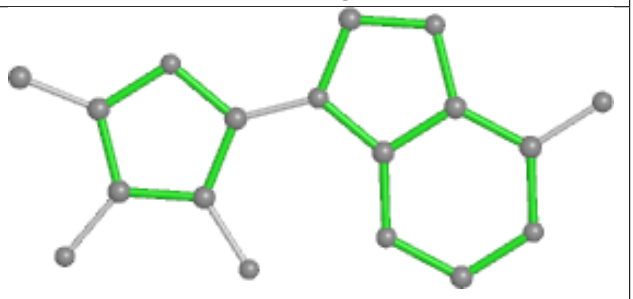
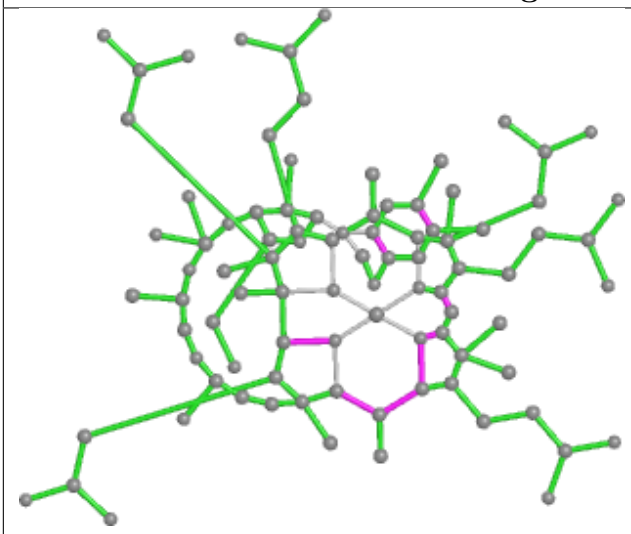


Rings

Ligand B12 K 1601



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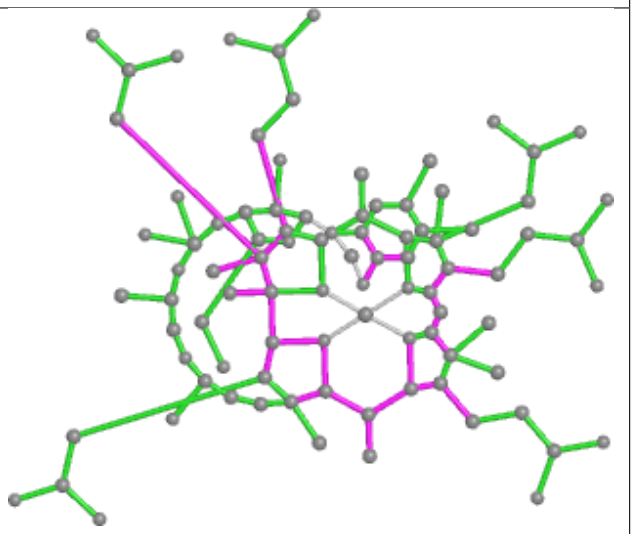
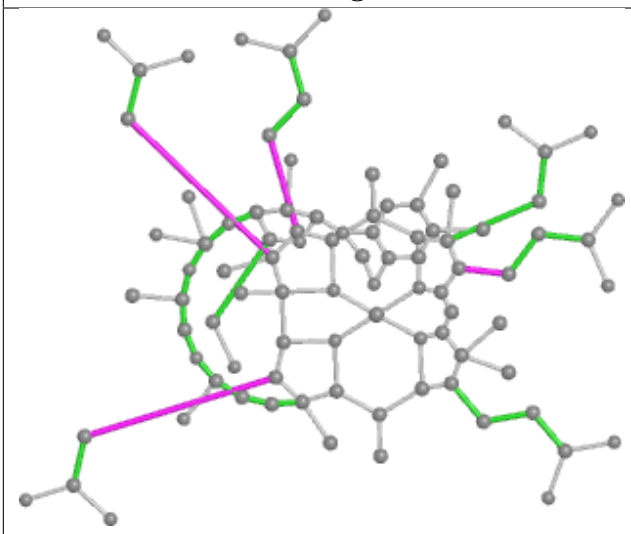


Bond angles



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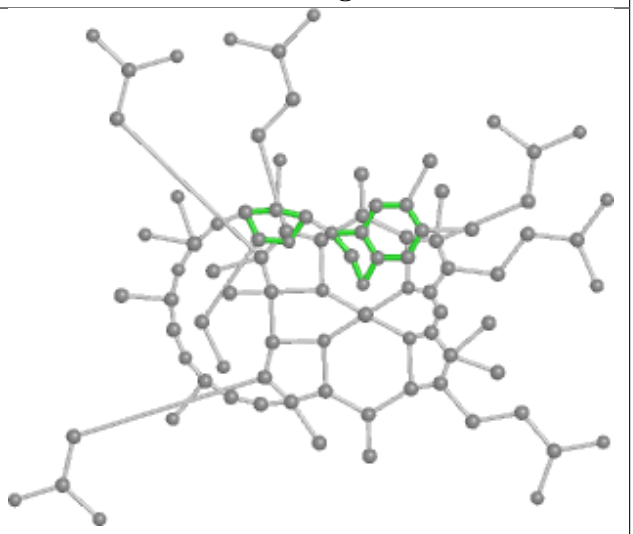

Rings

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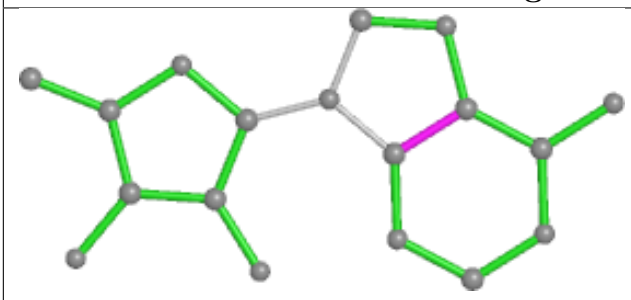

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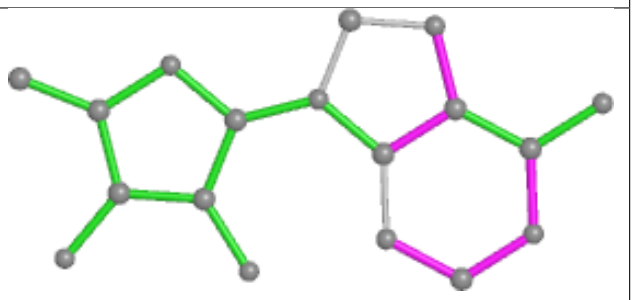

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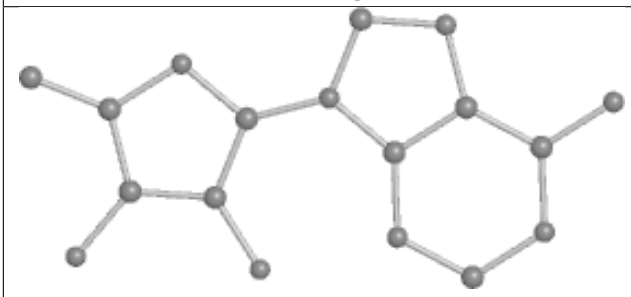

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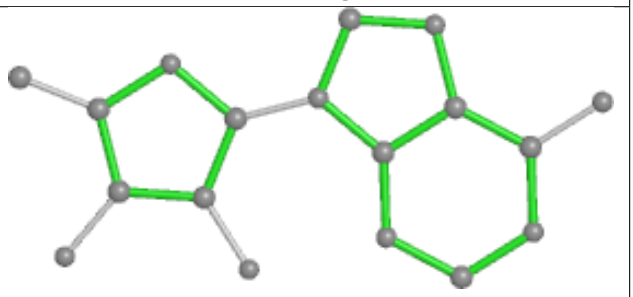

Rings

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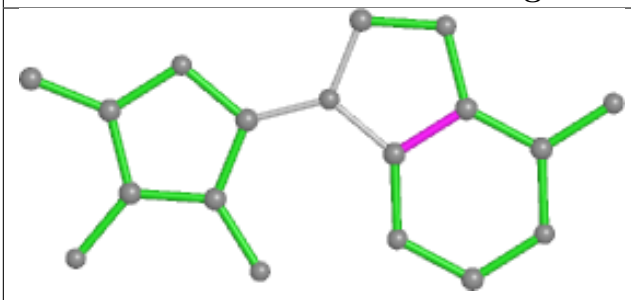

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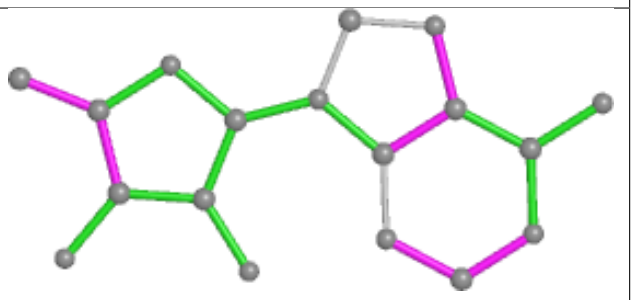

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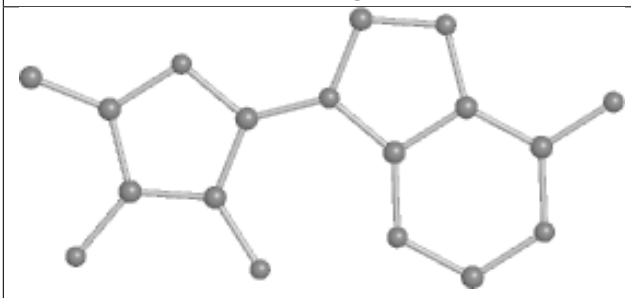
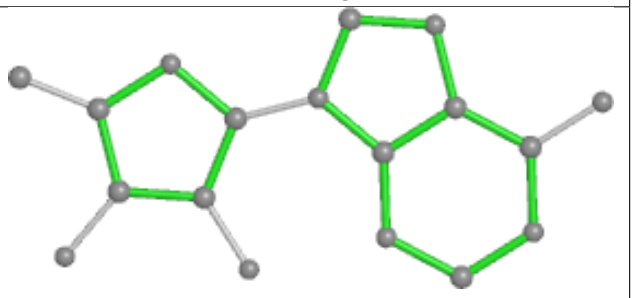
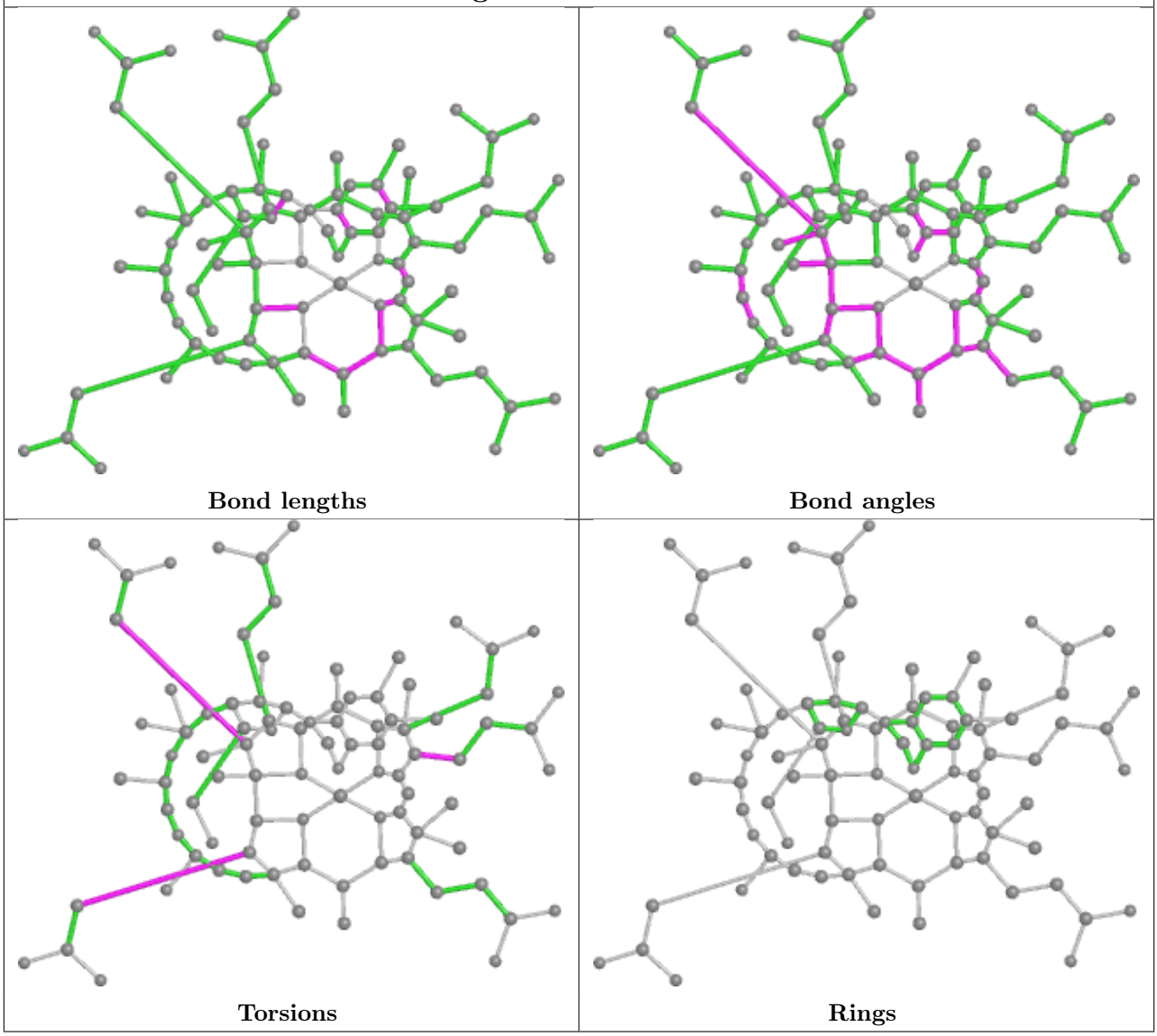


Torsions



Rings

Ligand B12 E 1601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	551/554 (99%)	-0.61	1 (0%) 95 95	9, 14, 26, 64	0
1	D	551/554 (99%)	-0.54	2 (0%) 92 93	9, 16, 30, 66	0
1	G	554/554 (100%)	-0.63	1 (0%) 95 95	9, 14, 25, 49	0
1	J	554/554 (100%)	-0.60	3 (0%) 91 92	8, 14, 27, 66	1 (0%)
2	B	182/200 (91%)	-0.43	4 (2%) 62 66	12, 22, 39, 57	0
2	E	178/200 (89%)	-0.48	1 (0%) 89 91	12, 21, 35, 57	0
2	H	178/200 (89%)	-0.60	0 100 100	12, 17, 29, 44	0
2	K	182/200 (91%)	-0.66	1 (0%) 91 92	10, 16, 35, 61	0
3	C	136/137 (99%)	-0.55	0 100 100	11, 20, 37, 48	1 (0%)
3	F	136/137 (99%)	-0.16	2 (1%) 73 77	17, 28, 44, 53	0
3	I	136/137 (99%)	-0.60	0 100 100	12, 19, 32, 42	1 (0%)
3	L	136/137 (99%)	-0.57	0 100 100	12, 20, 37, 44	0
All	All	3474/3564 (97%)	-0.56	15 (0%) 92 93	8, 16, 33, 66	3 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	ASN	3.7
2	K	58	THR	3.6
1	D	551	ASN	3.4
1	J	554	ASP	3.1
2	E	59	GLN	2.8
2	B	43	GLY	2.8
3	F	52	TRP	2.6
1	J	1	MET	2.6
2	B	74	ALA	2.5
2	B	60	GLN	2.4
1	J	553	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	548	LEU	2.3
1	G	45	ASN	2.1
2	B	59	GLN	2.1
3	F	56	ALA	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
7	CL	C	201	1/1	0.94	0.07	33,33,33,33	0
7	CL	G	606	1/1	0.94	0.05	28,28,28,28	0
7	CL	L	201	1/1	0.95	0.07	32,32,32,32	0
6	5AD	D	604	18/18	0.96	0.08	11,15,18,19	0
7	CL	J	606	1/1	0.97	0.05	30,30,30,30	0
6	5AD	G	604	18/18	0.97	0.07	10,13,17,19	0
7	CL	F	201	1/1	0.98	0.05	24,24,24,24	0
6	5AD	J	604	18/18	0.98	0.09	9,13,15,17	0
7	CL	A	606	1/1	0.98	0.06	25,25,25,25	0
6	5AD	A	604	18/18	0.98	0.08	9,14,16,17	0
8	B12	B	1601	91/91	0.98	0.08	8,12,16,20	0
8	B12	E	1601	91/91	0.98	0.08	8,13,17,21	0
8	B12	H	1601	91/91	0.98	0.07	8,11,15,18	0
7	CL	J	605	1/1	0.99	0.07	26,26,26,26	0
7	CL	D	605	1/1	0.99	0.08	28,28,28,28	0
7	CL	D	606	1/1	0.99	0.06	30,30,30,30	0
5	K	D	602	1/1	0.99	0.05	13,13,13,13	0
7	CL	G	605	1/1	0.99	0.04	25,25,25,25	0
7	CL	A	605	1/1	0.99	0.04	28,28,28,28	0

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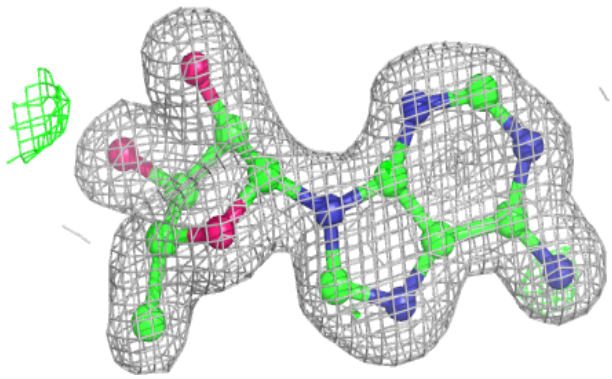
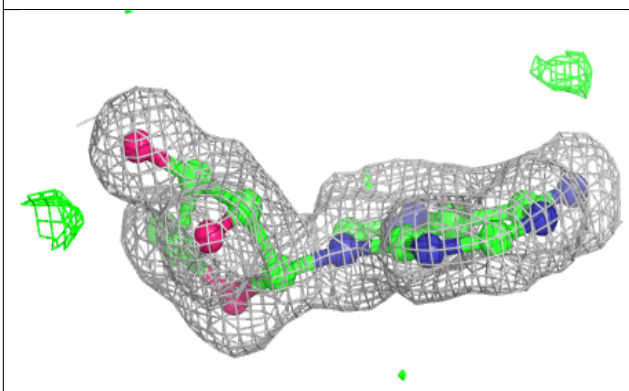
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	B12	K	1601	91/91	0.99	0.07	7,11,13,15	0
5	K	G	603	1/1	1.00	0.08	13,13,13,13	0
5	K	J	602	1/1	1.00	0.07	12,12,12,12	0
5	K	J	603	1/1	1.00	0.04	12,12,12,12	0
4	CA	D	601	1/1	1.00	0.04	13,13,13,13	0
7	CL	I	201	1/1	1.00	0.02	15,15,15,15	0
4	CA	G	601	1/1	1.00	0.05	11,11,11,11	0
4	CA	J	601	1/1	1.00	0.03	10,10,10,10	0
5	K	A	602	1/1	1.00	0.06	11,11,11,11	0
5	K	A	603	1/1	1.00	0.05	14,14,14,14	0
4	CA	A	601	1/1	1.00	0.06	12,12,12,12	0
5	K	D	603	1/1	1.00	0.03	15,15,15,15	0
5	K	G	602	1/1	1.00	0.04	11,11,11,11	0

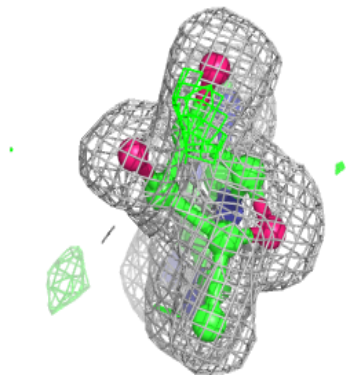
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD D 604:

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

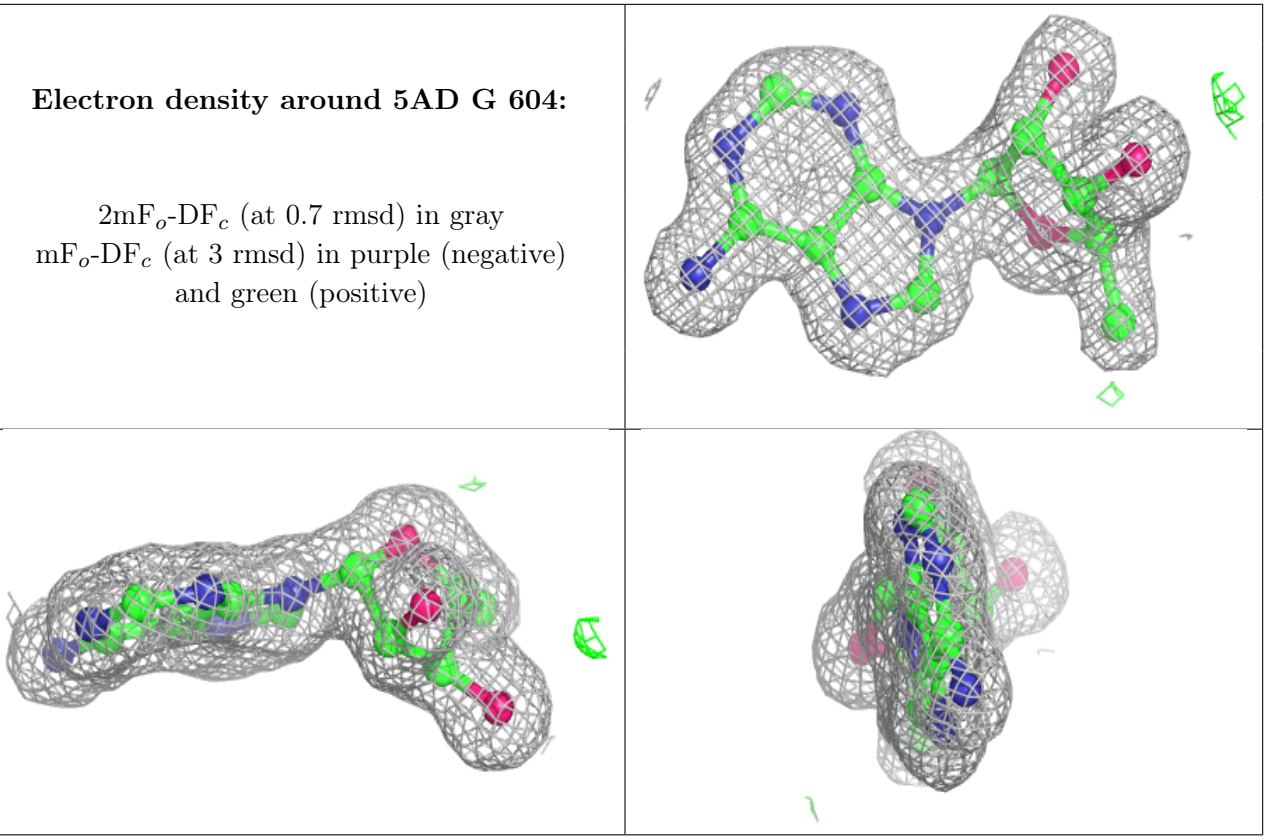






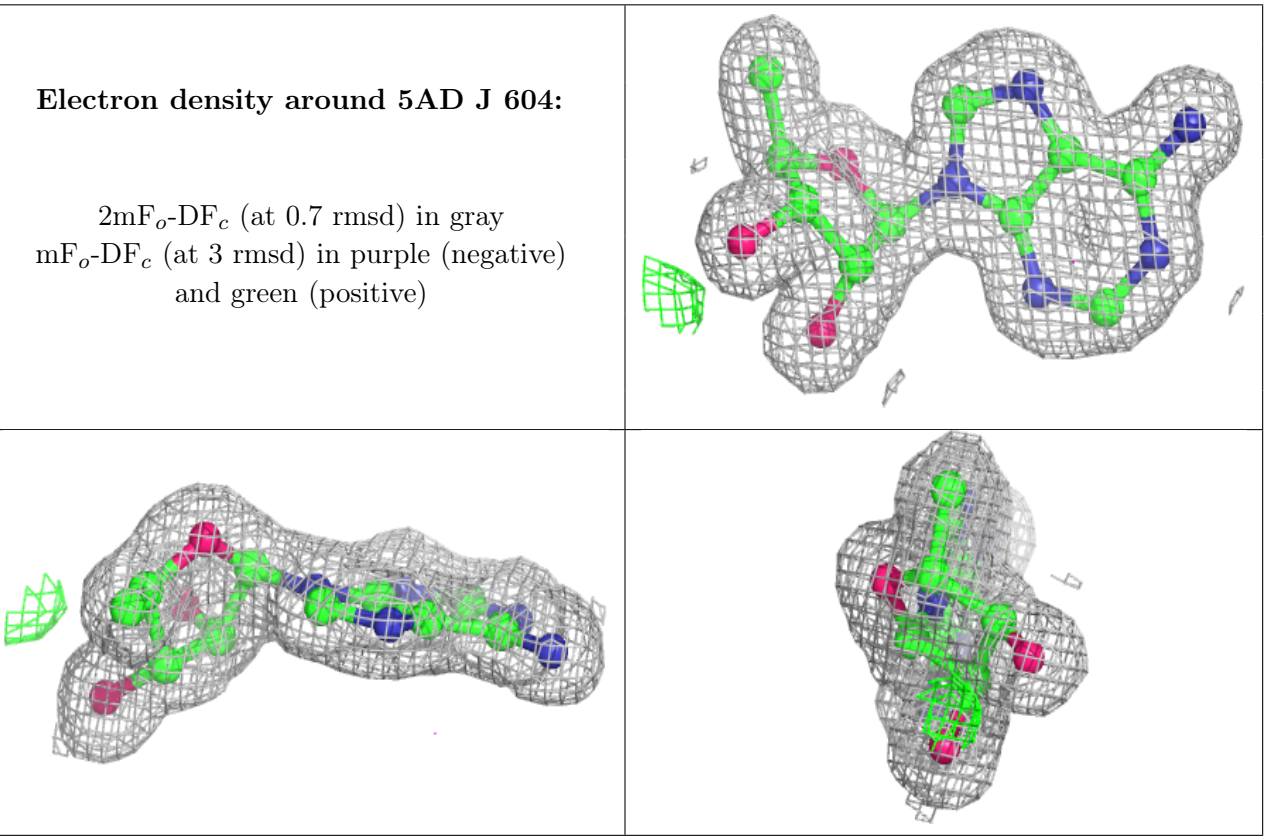
Electron density around 5AD G 604:

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



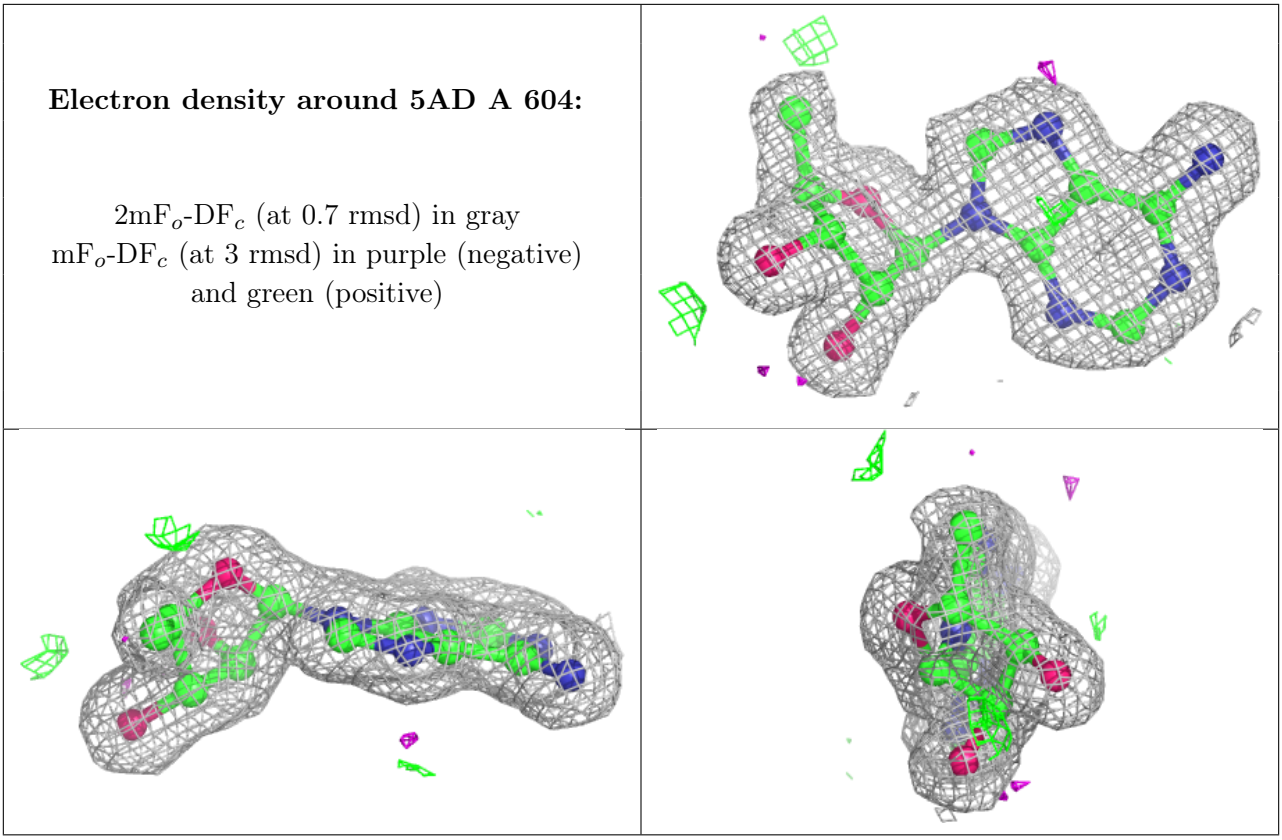
Electron density around 5AD J 604:

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



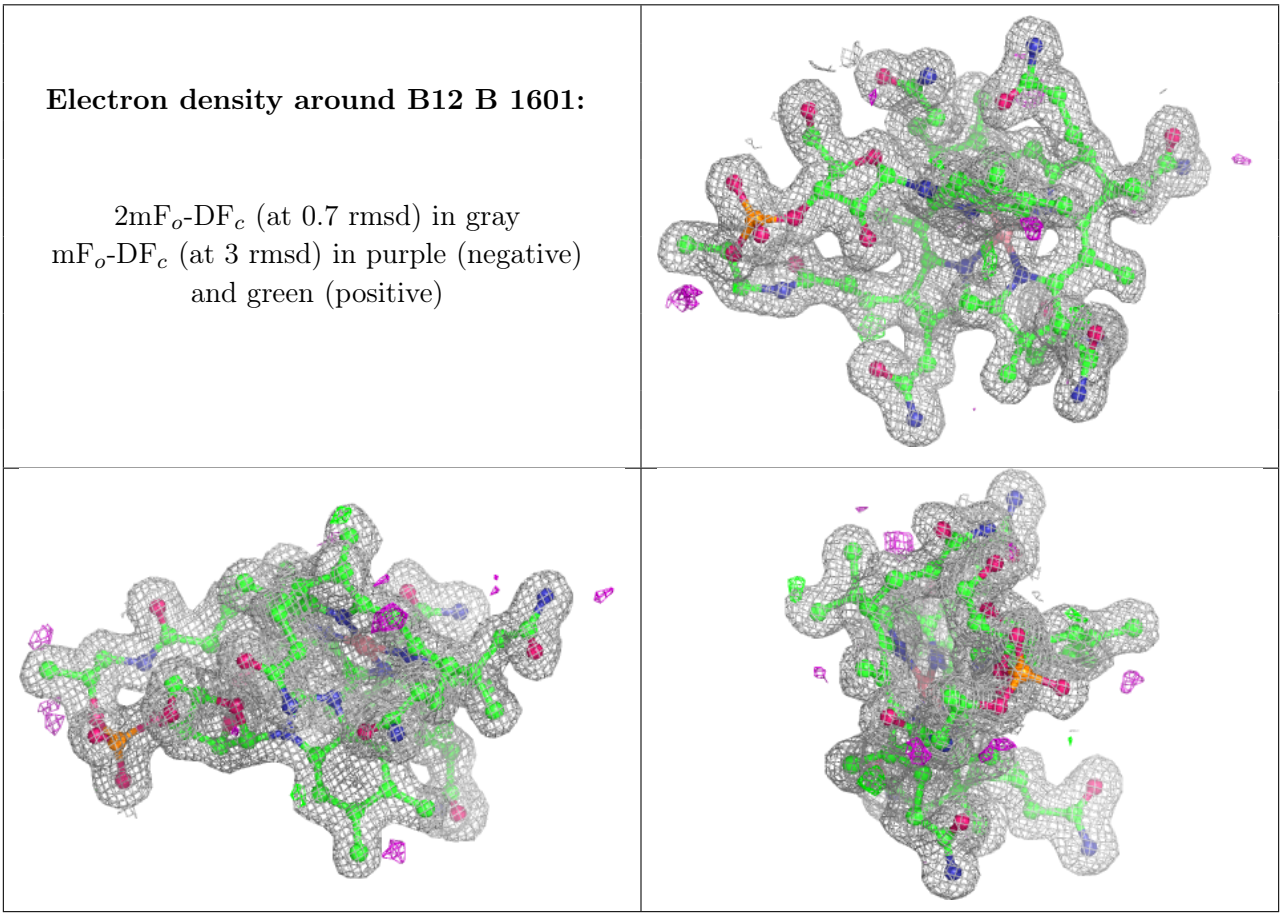
Electron density around 5AD A 604:

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



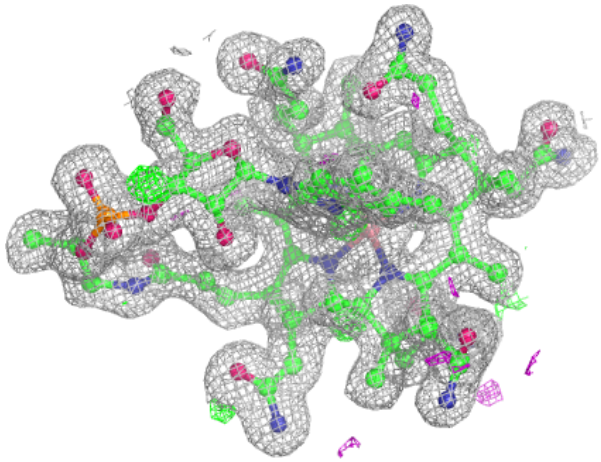
Electron density around B12 B 1601:

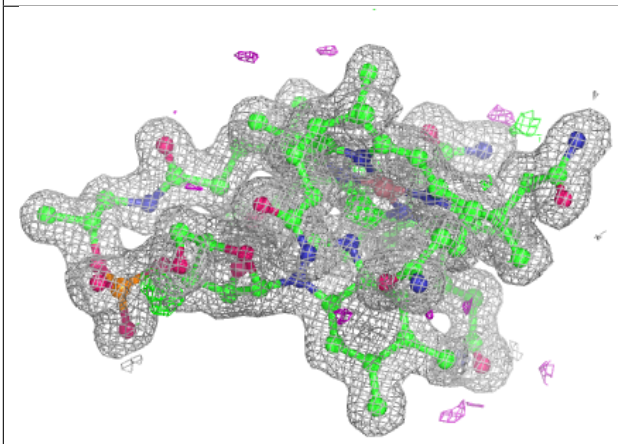
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

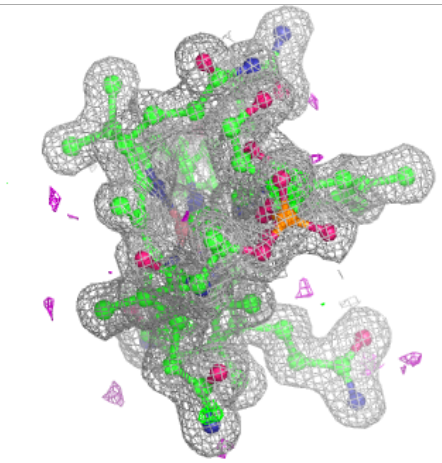


Electron density around B12 E 1601:

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

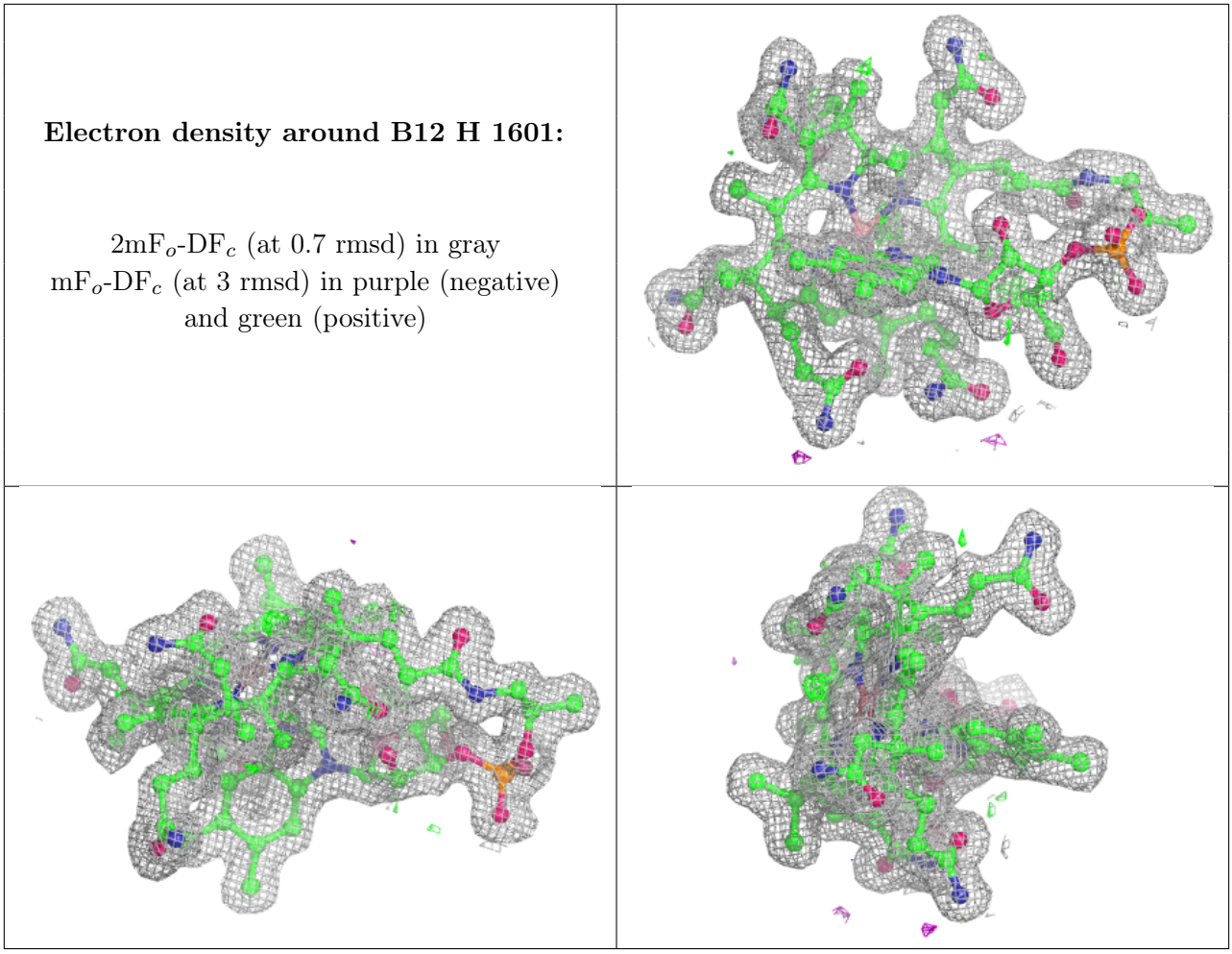






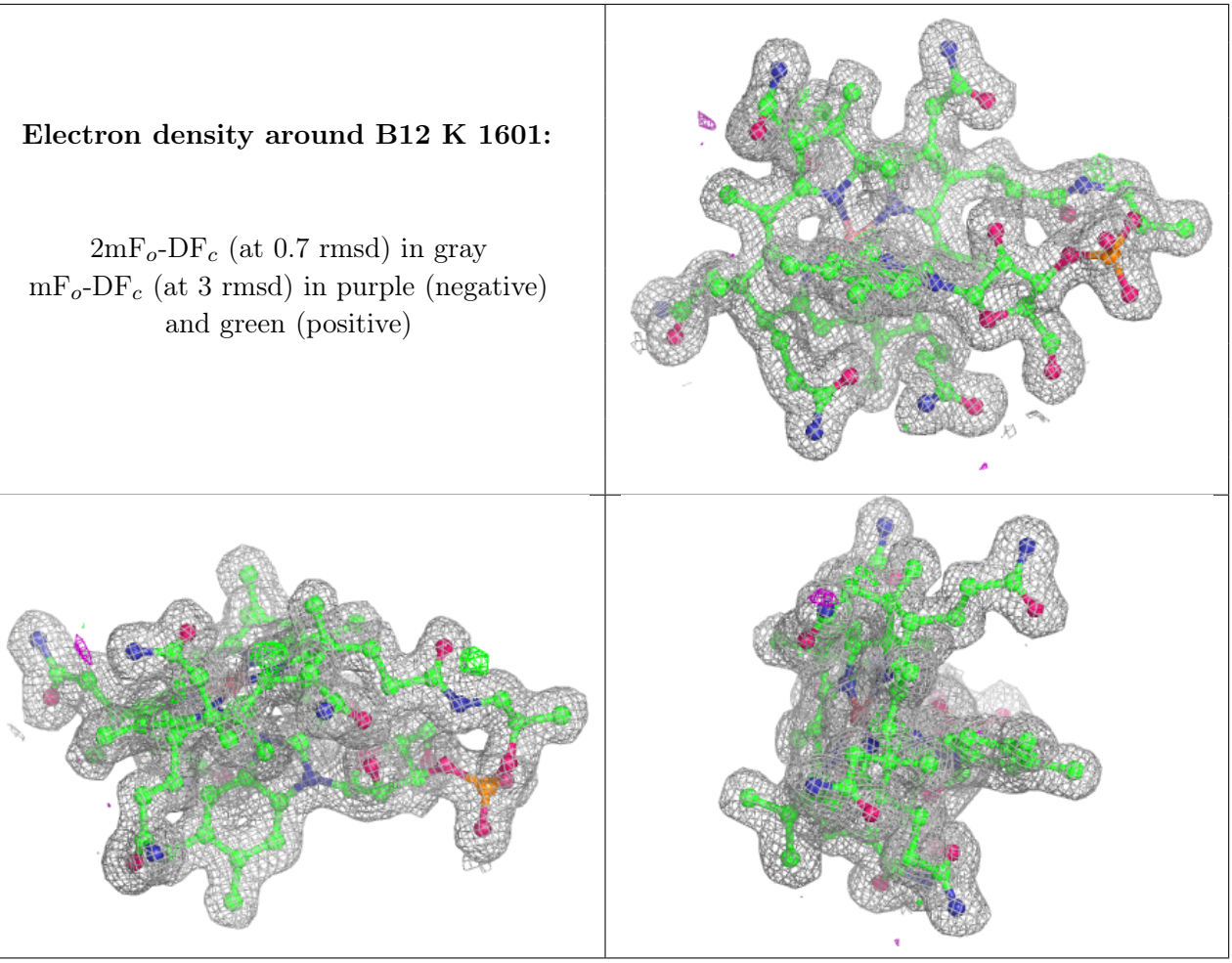
Electron density around B12 H 1601:

$2mF_o$-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 K 1601:

$2mF_o$-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.