Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2020 – 07:56 PM BST

PDB ID	:	6Y88
Title	:	IGPS (Indole-3-glycerol phosphate synthase) from Pseudomonas aeruginosa in complex with substrate inhibitor rCdRP
Authors	:	Soderholm, A.; Selmer, M.
Deposited on	:	2020-03-03
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

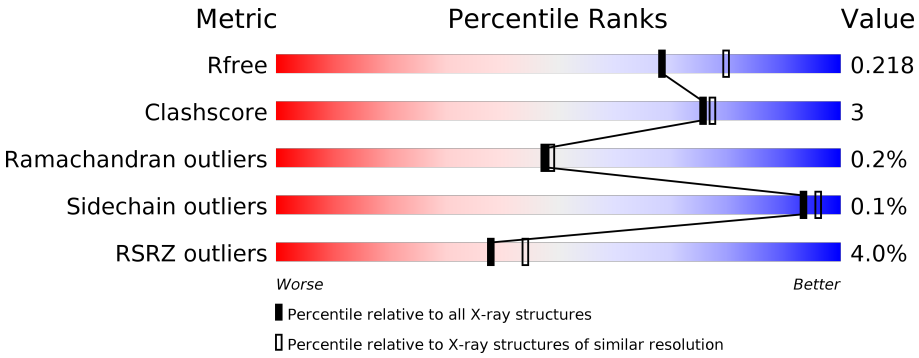
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.5
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.5

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	287	% 85% 7% 8%
1	B	287	86% 6% 8%
1	C	287	% 84% 8% 8%
1	D	287	6% 86% 7% 8%
1	E	287	% 86% 6% 8%
1	F	287	3% 86% 7% 8%

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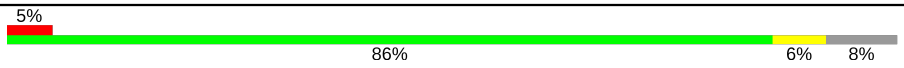
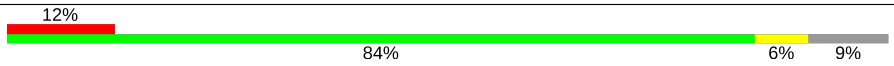
Mol	Chain	Length	Quality of chain
1	H	287	
2	G	277	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34437 atoms, of which 16871 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 Indole-3-glycerol phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	H	N	O	S	0	1	0
			4139	1292	2101	355	384	7			
1	B	265	Total	C	H	N	O	S	0	1	0
			4150	1295	2106	356	386	7			
1	C	264	Total	C	H	N	O	S	0	4	0
			4170	1299	2121	357	386	7			
1	D	265	Total	C	H	N	O	S	0	0	0
			4150	1294	2103	359	387	7			
1	E	265	Total	C	H	N	O	S	0	2	0
			4171	1300	2119	359	386	7			
1	F	265	Total	C	H	N	O	S	0	3	0
			4170	1301	2117	356	389	7			
1	H	264	Total	C	H	N	O	S	0	0	0
			4120	1286	2089	354	384	7			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	THR	-	expression tag	UNP A0A367MAM9
A	280	SER	-	expression tag	UNP A0A367MAM9
A	281	GLY	-	expression tag	UNP A0A367MAM9
A	282	HIS	-	expression tag	UNP A0A367MAM9
A	283	HIS	-	expression tag	UNP A0A367MAM9
A	284	HIS	-	expression tag	UNP A0A367MAM9
A	285	HIS	-	expression tag	UNP A0A367MAM9
A	286	HIS	-	expression tag	UNP A0A367MAM9
A	287	HIS	-	expression tag	UNP A0A367MAM9
B	279	THR	-	expression tag	UNP A0A367MAM9
B	280	SER	-	expression tag	UNP A0A367MAM9
B	281	GLY	-	expression tag	UNP A0A367MAM9
B	282	HIS	-	expression tag	UNP A0A367MAM9
B	283	HIS	-	expression tag	UNP A0A367MAM9
B	284	HIS	-	expression tag	UNP A0A367MAM9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	285	HIS	-	expression tag	UNP A0A367MAM9
B	286	HIS	-	expression tag	UNP A0A367MAM9
B	287	HIS	-	expression tag	UNP A0A367MAM9
C	279	THR	-	expression tag	UNP A0A367MAM9
C	280	SER	-	expression tag	UNP A0A367MAM9
C	281	GLY	-	expression tag	UNP A0A367MAM9
C	282	HIS	-	expression tag	UNP A0A367MAM9
C	283	HIS	-	expression tag	UNP A0A367MAM9
C	284	HIS	-	expression tag	UNP A0A367MAM9
C	285	HIS	-	expression tag	UNP A0A367MAM9
C	286	HIS	-	expression tag	UNP A0A367MAM9
C	287	HIS	-	expression tag	UNP A0A367MAM9
D	279	THR	-	expression tag	UNP A0A367MAM9
D	280	SER	-	expression tag	UNP A0A367MAM9
D	281	GLY	-	expression tag	UNP A0A367MAM9
D	282	HIS	-	expression tag	UNP A0A367MAM9
D	283	HIS	-	expression tag	UNP A0A367MAM9
D	284	HIS	-	expression tag	UNP A0A367MAM9
D	285	HIS	-	expression tag	UNP A0A367MAM9
D	286	HIS	-	expression tag	UNP A0A367MAM9
D	287	HIS	-	expression tag	UNP A0A367MAM9
E	279	THR	-	expression tag	UNP A0A367MAM9
E	280	SER	-	expression tag	UNP A0A367MAM9
E	281	GLY	-	expression tag	UNP A0A367MAM9
E	282	HIS	-	expression tag	UNP A0A367MAM9
E	283	HIS	-	expression tag	UNP A0A367MAM9
E	284	HIS	-	expression tag	UNP A0A367MAM9
E	285	HIS	-	expression tag	UNP A0A367MAM9
E	286	HIS	-	expression tag	UNP A0A367MAM9
E	287	HIS	-	expression tag	UNP A0A367MAM9
F	279	THR	-	expression tag	UNP A0A367MAM9
F	280	SER	-	expression tag	UNP A0A367MAM9
F	281	GLY	-	expression tag	UNP A0A367MAM9
F	282	HIS	-	expression tag	UNP A0A367MAM9
F	283	HIS	-	expression tag	UNP A0A367MAM9
F	284	HIS	-	expression tag	UNP A0A367MAM9
F	285	HIS	-	expression tag	UNP A0A367MAM9
F	286	HIS	-	expression tag	UNP A0A367MAM9
F	287	HIS	-	expression tag	UNP A0A367MAM9
H	279	THR	-	expression tag	UNP A0A367MAM9
H	280	SER	-	expression tag	UNP A0A367MAM9
H	281	GLY	-	expression tag	UNP A0A367MAM9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	282	HIS	-	expression tag	UNP A0A367MAM9
H	283	HIS	-	expression tag	UNP A0A367MAM9
H	284	HIS	-	expression tag	UNP A0A367MAM9
H	285	HIS	-	expression tag	UNP A0A367MAM9
H	286	HIS	-	expression tag	UNP A0A367MAM9
H	287	HIS	-	expression tag	UNP A0A367MAM9

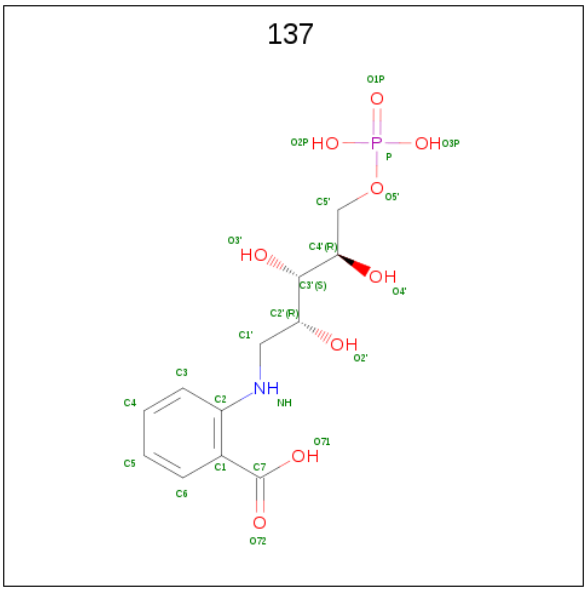
- Molecule 2 is a protein called Indole-3-glycerol phosphate synthase,Indole-3-glycerol phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	253	Total	C	H	N	O	S	0	1	0
			3830	1200	1928	329	366	7			

There are 9 discrepancies between the modelled and reference sequences:

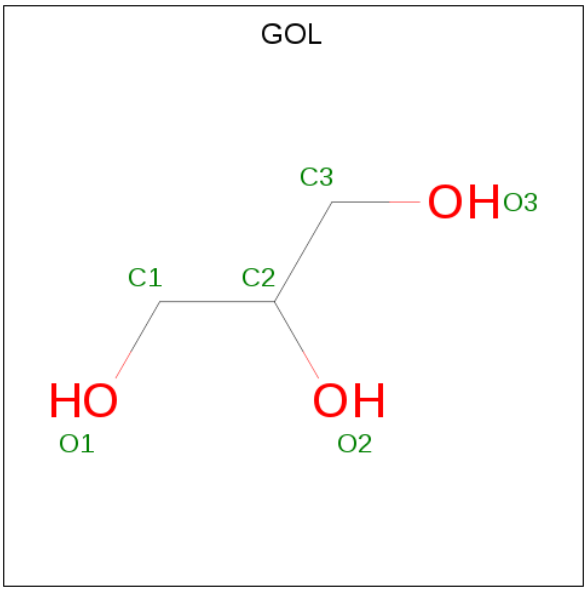
Chain	Residue	Modelled	Actual	Comment	Reference
G	279	THR	-	expression tag	UNP A0A367MAM9
G	280	SER	-	expression tag	UNP A0A367MAM9
G	281	GLY	-	expression tag	UNP A0A367MAM9
G	282	HIS	-	expression tag	UNP A0A367MAM9
G	283	HIS	-	expression tag	UNP A0A367MAM9
G	284	HIS	-	expression tag	UNP A0A367MAM9
G	285	HIS	-	expression tag	UNP A0A367MAM9
G	286	HIS	-	expression tag	UNP A0A367MAM9
G	287	HIS	-	expression tag	UNP A0A367MAM9

- Molecule 3 is 1-(O-CARBOXY-PHENYLAMINO)-1-DEOXY-D-RIBULOSE-5-PHOSPHATE (three-letter code: 137) (formula: $C_{12}H_{18}NO_9P$) (labeled as "Ligand of Interest" by author).



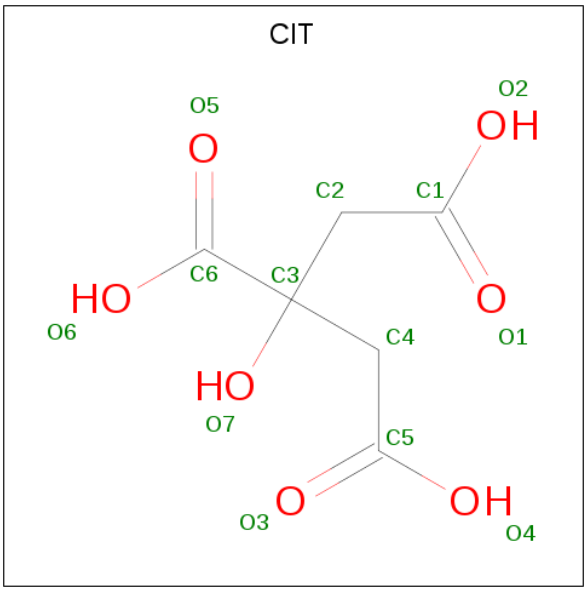
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			41	12	18	1	9	1		
3	B	1	Total	C	H	N	O	P	0	0
			41	12	18	1	9	1		
3	C	1	Total	C	H	N	O	P	0	0
			41	12	18	1	9	1		
3	D	1	Total	C	H	N	O	P	0	0
			41	12	18	1	9	1		
3	E	1	Total	C	H	N	O	P	0	0
			41	12	18	1	9	1		
3	F	1	Total	C	H	N	O	P	0	0
			41	12	18	1	9	1		
3	H	1	Total	C	H	N	O	P	0	0
			41	12	18	1	9	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



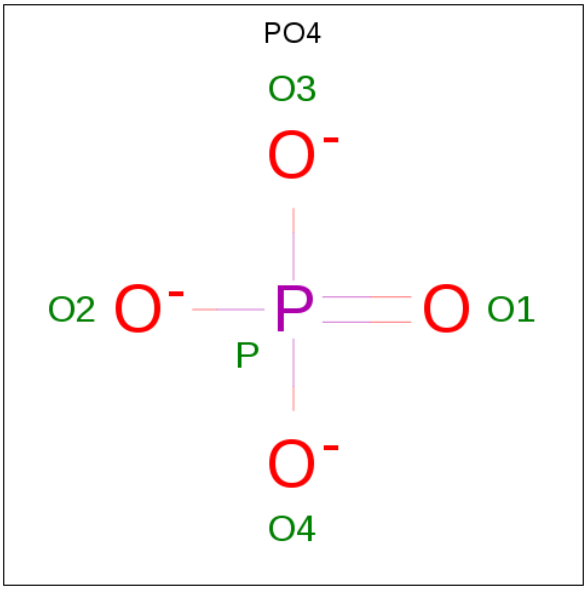
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C H O 18 6 5 7	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

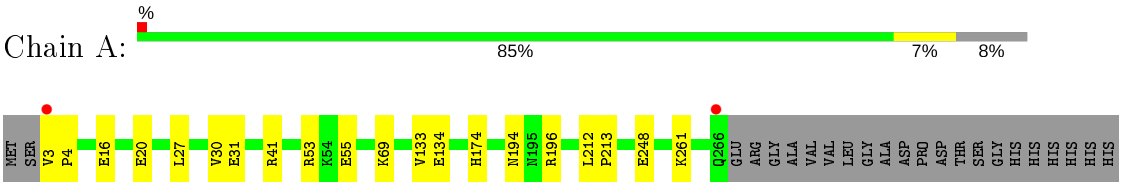
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	209	Total O 209 209	0	0
7	B	179	Total O 179 179	0	0
7	C	160	Total O 160 160	0	0
7	D	100	Total O 100 100	0	0
7	E	205	Total O 205 205	0	0
7	F	110	Total O 110 110	0	0
7	G	76	Total O 76 76	0	0
7	H	90	Total O 90 90	0	0

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.

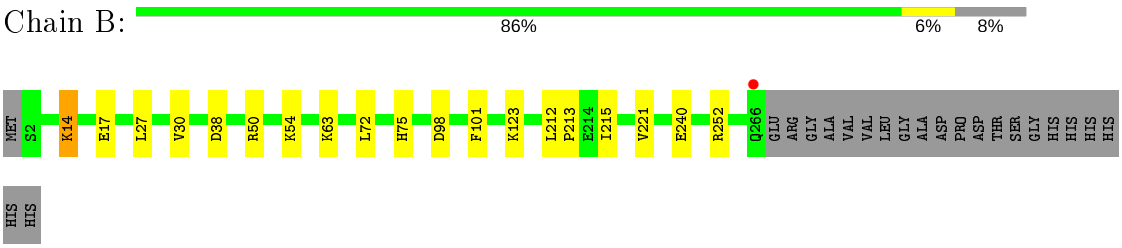
- Molecule 1: Indole-3-glycerol phosphate synthase

Chain A:



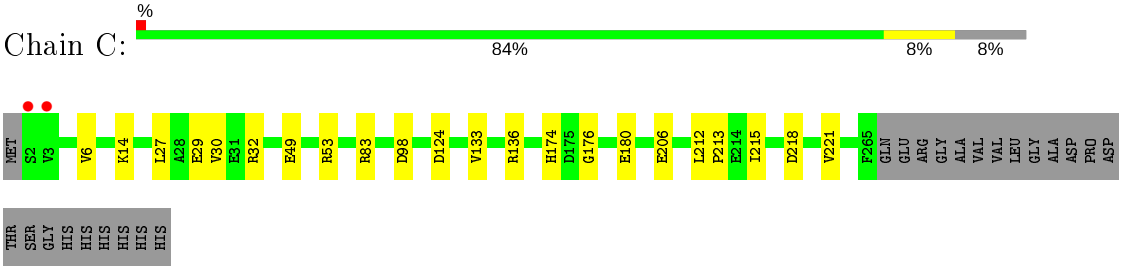
- Molecule 1: Indole-3-glycerol phosphate synthase

Chain B:



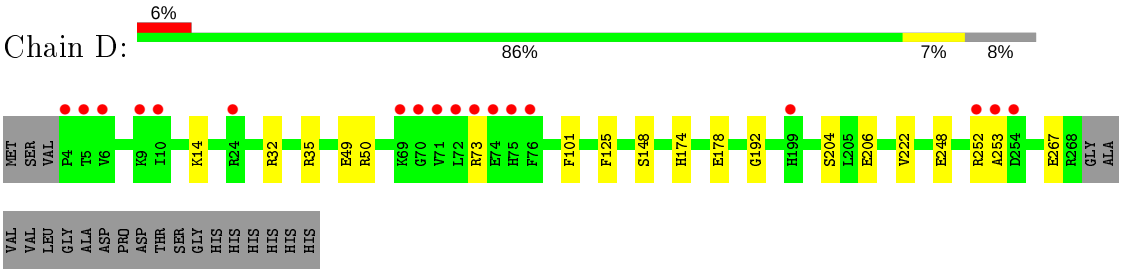
- Molecule 1: Indole-3-glycerol phosphate synthase

Chain C:



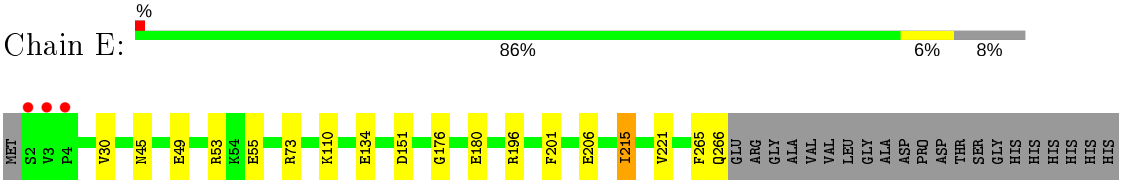
- Molecule 1: Indole-3-glycerol phosphate synthase

Chain D:



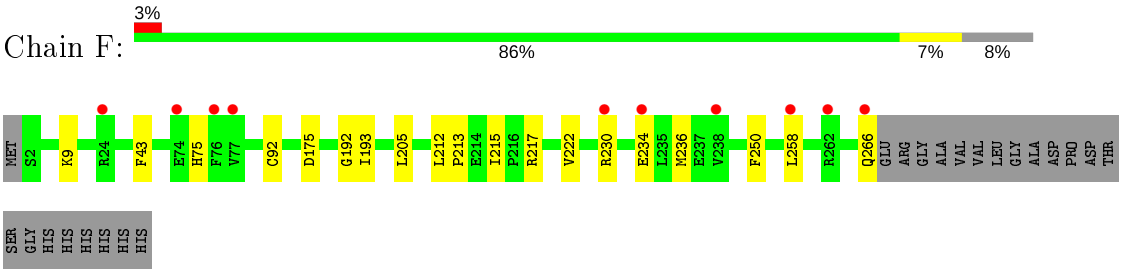
- Molecule 1: Indole-3-glycerol phosphate synthase

Chain E:



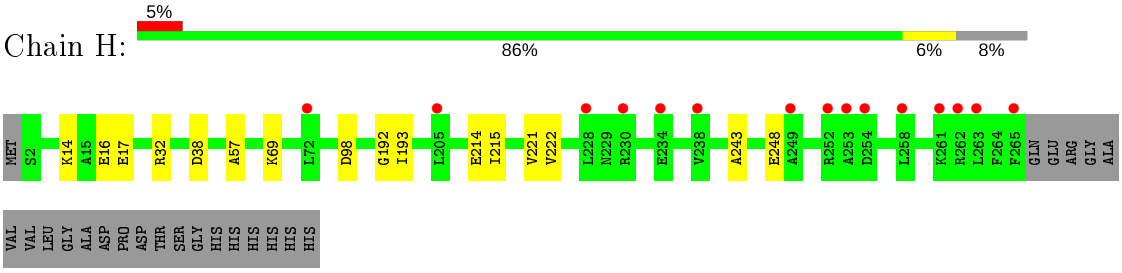
• Molecule 1: Indole-3-glycerol phosphate synthase

Chain F:



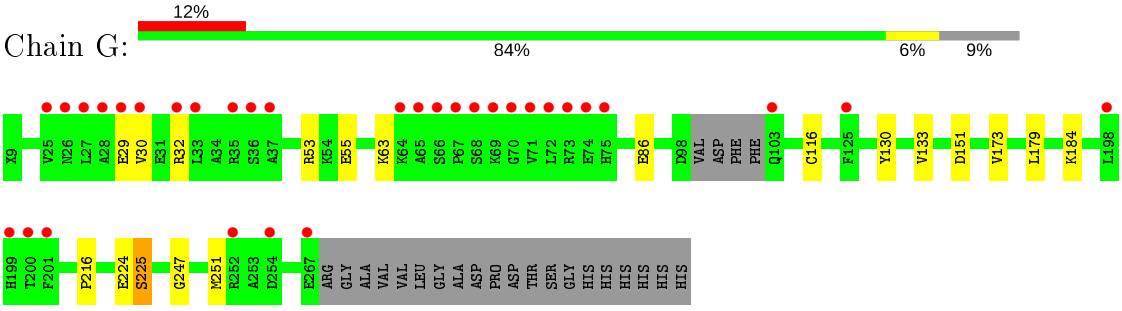
• Molecule 1: Indole-3-glycerol phosphate synthase

Chain H:



• Molecule 2: Indole-3-glycerol phosphate synthase,Indole-3-glycerol phosphate synthase

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	164.71Å 150.68Å 114.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 2.10 49.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.04-2.10) 100.0 (49.50-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.173 , 0.218 0.173 , 0.218	Depositor DCC
R_{free} test set	8298 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	34437	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GOL, PO4, 137, CIT

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	0.62	0/2068	0.73	1/2802 (0.0%)
1	B	0.61	0/2074	0.72	1/2810 (0.0%)
1	C	0.62	1/2088 (0.0%)	0.70	1/2828 (0.0%)
1	D	0.50	0/2074	0.68	0/2807
1	E	0.61	1/2085 (0.0%)	0.75	1/2824 (0.0%)
1	F	0.48	0/2089	0.64	0/2830
1	H	0.48	0/2058	0.65	0/2788
2	G	0.55	0/1858	0.67	0/2517
All	All	0.56	2/16394 (0.0%)	0.69	4/22206 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	GLU	CB-CG	7.11	1.65	1.52
1	E	206	GLU	CB-CG	5.71	1.63	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	218	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	50	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	196	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	E	151	ASP	CB-CG-OD1	5.03	122.83	118.30

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	2038	2101	2101	15	0
1	B	2044	2106	2106	10	2
1	C	2049	2121	2121	18	0
1	D	2047	2103	2103	13	0
1	E	2052	2119	2119	12	0
1	F	2053	2117	2117	14	0
1	H	2031	2089	2089	11	0
2	G	1902	1928	1889	12	2
3	A	23	18	15	1	0
3	B	23	18	15	1	0
3	C	23	18	15	0	0
3	D	23	18	15	0	0
3	E	23	18	15	0	0
3	F	23	18	15	0	0
3	H	23	18	15	0	0
4	A	6	8	8	1	0
4	B	12	16	16	1	0
4	C	12	16	16	0	0
4	E	6	8	8	2	0
4	H	6	8	8	1	0
5	E	13	5	5	0	0
6	G	5	0	0	0	0
7	A	209	0	0	4	0
7	B	179	0	0	1	0
7	C	160	0	0	7	0
7	D	100	0	0	1	0
7	E	205	0	0	3	0
7	F	110	0	0	3	0
7	G	76	0	0	2	0
7	H	90	0	0	1	0
All	All	17566	16871	16811	103	2

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 (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LYS:NZ	3:B:301:137:O2'	2.12	0.80
1:E:53:ARG:NH1	1:E:55:GLU:OE1	2.21	0.73
1:C:53:ARG:NH1	7:C:401:HOH:O	2.22	0.71
2:G:151:ASP:OD2	7:G:401:HOH:O	2.12	0.67
1:B:252:ARG:NH2	7:B:404:HOH:O	2.29	0.65
1:C:29:GLU:OE1	1:C:32:ARG:NH2	2.30	0.65
1:F:217:ARG:NH2	7:F:404:HOH:O	2.32	0.62
2:G:86:GLU:OE1	2:G:116:CYS:HB2	2.01	0.60
1:H:14:LYS:NZ	1:H:98:ASP:OD1	2.36	0.59
1:C:49:GLU:OE2	1:C:53:ARG:NH2	2.36	0.58
1:H:32:ARG:NH2	7:H:402:HOH:O	2.36	0.58
1:A:53:ARG:NH1	1:A:55:GLU:OE2	2.37	0.58
1:D:204:SER:OG	1:D:206:GLU:OE1	2.22	0.57
1:E:215:ILE:HD12	1:E:221:VAL:HG22	1.86	0.57
1:F:175:ASP:OD2	7:F:401:HOH:O	2.17	0.56
1:B:14:LYS:NZ	1:B:98:ASP:OD1	2.39	0.56
1:D:248:GLU:OE2	1:D:252:ARG:NH2	2.39	0.55
1:E:49:GLU:OE2	1:E:53:ARG:NH2	2.31	0.55
1:E:73:ARG:HH21	4:E:303:GOL:H12	1.71	0.55
1:C:215:ILE:HD13	1:C:221:VAL:HG22	1.89	0.54
1:B:14:LYS:HE3	1:B:17:GLU:OE1	2.07	0.53
1:C:53:ARG:HD3	7:C:412:HOH:O	2.08	0.53
1:E:45:ASN:ND2	7:E:401:HOH:O	2.36	0.53
1:A:30[A]:VAL:HG12	1:A:133:VAL:HG12	1.89	0.52
2:G:29:GLU:OE2	2:G:32:ARG:NH2	2.43	0.52
1:D:148:SER:HB3	1:D:178:GLU:OE2	2.10	0.51
2:G:63:LYS:H	2:G:251:MET:HE2	1.75	0.51
2:G:30:VAL:HG21	2:G:130:TYR:CE1	2.45	0.51
1:F:75:HIS:O	7:F:402:HOH:O	2.19	0.50
3:A:301:137:H2'	7:A:411:HOH:O	2.12	0.50
2:G:53:ARG:NH1	2:G:55:GLU:OE2	2.45	0.50
2:G:63:LYS:H	2:G:251:MET:CE	2.25	0.49
1:F:193:ILE:HD11	1:F:215:ILE:HD11	1.93	0.49
1:C:136:ARG:NH1	7:C:404:HOH:O	2.44	0.49
1:D:32:ARG:HG2	1:D:35:ARG:NH2	2.27	0.49
1:H:193:ILE:HD11	1:H:215:ILE:HD11	1.93	0.49
1:B:215:ILE:HD13	1:B:221:VAL:HG22	1.94	0.49
1:E:110:LYS:NZ	7:E:408:HOH:O	2.46	0.49
1:H:14:LYS:HE3	1:H:17:GLU:OE1	2.12	0.48
1:A:31:GLU:HG2	7:A:529:HOH:O	2.13	0.48
1:H:57:ALA:O	1:H:243:ALA:HA	2.14	0.48
1:E:196[A]:ARG:NH1	1:E:201:PHE:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ARG:O	1:F:230:ARG:HG2	2.14	0.47
1:D:49:GLU:HG3	1:D:50:ARG:N	2.30	0.47
1:C:49:GLU:HG3	7:E:496:HOH:O	2.14	0.46
1:D:174:HIS:HE1	7:D:479:HOH:O	1.99	0.46
2:G:173:VAL:HG11	2:G:179:LEU:HA	1.96	0.46
1:C:83[B]:ARG:NH2	7:C:411:HOH:O	2.47	0.46
1:F:9:LYS:NZ	1:H:16:GLU:OE2	2.44	0.46
1:A:69:LYS:HE3	7:A:469:HOH:O	2.15	0.46
1:D:174:HIS:O	1:D:174:HIS:CG	2.68	0.46
1:A:27:LEU:HA	1:A:30[B]:VAL:HG22	1.97	0.46
1:B:101:PHE:O	4:B:302:GOL:H32	2.15	0.46
1:A:212:LEU:N	1:A:213:PRO:CD	2.78	0.45
1:F:258:LEU:C	1:F:258:LEU:HD13	2.36	0.45
2:G:30:VAL:HG12	2:G:133:VAL:HG12	1.97	0.45
1:C:49:GLU:OE2	1:C:53:ARG:CZ	2.64	0.45
1:A:174:HIS:O	1:A:174:HIS:CG	2.69	0.45
1:F:230:ARG:HD3	1:F:234:GLU:OE2	2.17	0.45
7:C:414:HOH:O	1:E:49:GLU:HG3	2.16	0.44
1:C:53:ARG:NH1	7:C:412:HOH:O	2.48	0.44
1:H:14:LYS:HE3	4:H:302:GOL:H12	1.99	0.44
1:B:212:LEU:HB2	1:B:213:PRO:HD3	1.99	0.44
1:A:134:GLU:OE1	7:A:401:HOH:O	2.21	0.44
1:D:174:HIS:O	1:D:174:HIS:CD2	2.71	0.44
1:A:3:VAL:HB	1:A:4:PRO:HD3	1.99	0.44
1:C:30[B]:VAL:HG12	1:C:133:VAL:HG12	1.99	0.44
1:F:250:PHE:N	1:F:250:PHE:CD1	2.84	0.44
1:A:16:GLU:O	1:A:20:GLU:HG3	2.18	0.44
1:B:54:LYS:HE3	1:B:240:GLU:OE1	2.17	0.44
1:E:73:ARG:HH21	4:E:303:GOL:C1	2.31	0.44
2:G:184:LYS:HE3	7:G:459:HOH:O	2.17	0.43
1:F:205:LEU:HB3	1:F:236:MET:HE2	2.00	0.43
1:A:41:ARG:HE	4:A:302:GOL:H2	1.82	0.43
1:B:27:LEU:O	1:B:30[B]:VAL:HG12	2.19	0.43
1:C:14:LYS:NZ	1:C:98:ASP:OD1	2.51	0.43
1:H:69:LYS:HE3	1:H:248:GLU:OE1	2.18	0.43
1:D:73:ARG:NH2	1:D:253:ALA:O	2.41	0.43
1:B:63:LYS:HE3	1:B:72:LEU:CD1	2.48	0.43
2:G:216:PRO:HB3	1:H:214:GLU:HA	2.01	0.42
1:A:69:LYS:HE2	1:A:248:GLU:OE1	2.19	0.42
1:F:43:PHE:CE2	1:F:92:CYS:HB3	2.54	0.42
1:C:14:LYS:HE2	1:C:124:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:HG2	1:A:133:VAL:HG11	2.02	0.42
1:H:215:ILE:HD13	1:H:221:VAL:HG22	2.02	0.42
1:E:176:GLY:O	1:E:180:GLU:HG2	2.20	0.41
1:F:266:GLN:HG3	1:F:266:GLN:O	2.20	0.41
1:E:265:PHE:O	1:E:266:GLN:HG2	2.20	0.41
1:F:212:LEU:N	1:F:213:PRO:HD2	2.35	0.41
1:C:174:HIS:O	1:C:174:HIS:CG	2.73	0.41
1:D:101:PHE:N	1:D:101:PHE:CD1	2.88	0.41
1:F:192:GLY:HA2	1:F:222:VAL:O	2.20	0.41
1:A:174:HIS:HD2	1:A:194:ASN:O	2.03	0.41
1:C:27:LEU:HA	1:C:30[A]:VAL:HG22	2.03	0.41
1:D:192:GLY:HA2	1:D:222:VAL:O	2.21	0.41
1:A:261:LYS:HD2	1:D:267:GLU:O	2.20	0.41
1:H:192:GLY:HA2	1:H:222:VAL:O	2.21	0.41
1:D:14:LYS:HG3	1:D:125:PHE:HB2	2.03	0.40
1:E:30[B]:VAL:CG1	1:E:134:GLU:HA	2.52	0.40
2:G:224:GLU:O	2:G:225:SER:CB	2.69	0.40
1:C:176:GLY:O	1:C:180:GLU:HG2	2.21	0.40
1:C:212:LEU:N	1:C:213:PRO:CD	2.85	0.40
1:C:6:VAL:HG12	7:C:449:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:HIS:HD1	2:G:86:GLU:OE2[4_557]	1.30	0.30
1:B:75:HIS:ND1	2:G:86:GLU:OE2[4_557]	2.10	0.10

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	263/287 (92%)	259 (98%)	4 (2%)	0	100 100
1	B	264/287 (92%)	260 (98%)	3 (1%)	1 (0%)	34 32
1	C	266/287 (93%)	262 (98%)	4 (2%)	0	100 100
1	D	263/287 (92%)	256 (97%)	7 (3%)	0	100 100
1	E	265/287 (92%)	262 (99%)	3 (1%)	0	100 100
1	F	266/287 (93%)	260 (98%)	6 (2%)	0	100 100
1	H	262/287 (91%)	252 (96%)	9 (3%)	1 (0%)	34 32
2	G	236/277 (85%)	227 (96%)	7 (3%)	2 (1%)	19 15
All	All	2085/2286 (91%)	2038 (98%)	43 (2%)	4 (0%)	47 49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	38	ASP
1	B	38	ASP
2	G	225	SER
2	G	247	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	215/232 (93%)	215 (100%)	0	100 100
1	B	216/232 (93%)	215 (100%)	1 (0%)	88 92
1	C	218/232 (94%)	218 (100%)	0	100 100
1	D	215/232 (93%)	215 (100%)	0	100 100
1	E	217/232 (94%)	216 (100%)	1 (0%)	88 92
1	F	218/232 (94%)	218 (100%)	0	100 100
1	H	214/232 (92%)	214 (100%)	0	100 100
2	G	194/212 (92%)	194 (100%)	0	100 100
All	All	1707/1836 (93%)	1705 (100%)	2 (0%)	93 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	LYS
1	E	215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

16 ligands are modelled in this entry.

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	GOL	H	302	-	5,5,5	0.14	0	5,5,5	0.85	0
6	PO4	G	301	-	4,4,4	0.94	0	6,6,6	0.37	0
4	GOL	B	302	-	5,5,5	0.30	0	5,5,5	0.73	0
3	137	H	301	-	21,23,23	0.86	1 (4%)	27,32,32	0.77	0
4	GOL	A	302	-	5,5,5	0.43	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CIT	E	302	-	3,12,12	1.23	1 (33%)	3,17,17	3.59	1 (33%)
3	137	A	301	-	21,23,23	0.44	0	27,32,32	1.11	3 (11%)
3	137	C	301	-	21,23,23	0.63	0	27,32,32	1.01	1 (3%)
4	GOL	B	303	-	5,5,5	0.43	0	5,5,5	0.37	0
4	GOL	C	302	-	5,5,5	0.33	0	5,5,5	0.59	0
3	137	E	301	-	21,23,23	0.74	1 (4%)	27,32,32	1.05	2 (7%)
4	GOL	C	303	-	5,5,5	0.43	0	5,5,5	0.35	0
4	GOL	E	303	-	5,5,5	0.39	0	5,5,5	0.85	0
3	137	F	301	-	21,23,23	0.96	2 (9%)	27,32,32	0.86	0
3	137	D	301	-	21,23,23	0.82	1 (4%)	27,32,32	0.80	0
3	137	B	301	-	21,23,23	0.80	1 (4%)	27,32,32	1.29	2 (7%)

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	GOL	H	302	-	-	2/4/4/4	-
4	GOL	B	302	-	-	2/4/4/4	-
3	137	H	301	-	-	8/19/23/23	0/1/1/1
3	137	A	301	-	-	7/19/23/23	0/1/1/1
5	CIT	E	302	-	-	0/6/16/16	-
3	137	C	301	-	-	6/19/23/23	0/1/1/1
4	GOL	B	303	-	-	4/4/4/4	-
4	GOL	C	302	-	-	2/4/4/4	-
3	137	E	301	-	-	10/19/23/23	0/1/1/1
4	GOL	C	303	-	-	2/4/4/4	-
4	GOL	E	303	-	-	2/4/4/4	-
3	137	F	301	-	-	5/19/23/23	0/1/1/1
3	137	D	301	-	-	8/19/23/23	0/1/1/1
3	137	B	301	-	-	2/19/23/23	0/1/1/1
4	GOL	A	302	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	137	C1-C7	3.57	1.50	1.47
3	H	301	137	C1-C7	3.35	1.50	1.47
3	F	301	137	C1-C7	3.19	1.50	1.47
3	B	301	137	C1-C7	2.90	1.50	1.47
3	E	301	137	C1-C7	2.81	1.50	1.47
3	F	301	137	P-O1P	-2.51	1.42	1.50
5	E	302	CIT	O7-C3	2.04	1.46	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	302	CIT	C3-C4-C5	-5.88	105.57	114.98
3	B	301	137	C2'-C1'-NH	3.90	122.72	111.52
3	E	301	137	O3P-P-O2P	2.54	117.35	107.64
3	A	301	137	O3P-P-O5'	-2.50	100.07	106.73
3	E	301	137	C2'-C3'-C4'	-2.26	108.66	113.36
3	C	301	137	O3'-C3'-C2'	2.14	113.99	108.81
3	A	301	137	O3'-C3'-C2'	2.14	113.98	108.81
3	A	301	137	C2'-C3'-C4'	-2.12	108.96	113.36
3	B	301	137	O5'-P-O1P	2.08	112.31	106.47

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	GOL	C1-C2-C3-O3
3	H	301	137	C1'-C2'-C3'-C4'
3	C	301	137	C1'-C2'-C3'-C4'
4	B	303	GOL	O1-C1-C2-C3
4	C	302	GOL	O1-C1-C2-C3
3	E	301	137	C1'-C2'-C3'-C4'
4	E	303	GOL	C1-C2-C3-O3
3	D	301	137	C1'-C2'-C3'-C4'
3	D	301	137	C1'-C2'-C3'-O3'
3	B	301	137	NH-C1'-C2'-C3'
3	B	301	137	NH-C1'-C2'-O2'
3	D	301	137	O2'-C2'-C3'-C4'
4	B	303	GOL	O2-C2-C3-O3
4	C	302	GOL	O1-C1-C2-O2
3	D	301	137	NH-C1'-C2'-C3'
3	H	301	137	O2'-C2'-C3'-O3'
3	C	301	137	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
3	E	301	137	O2'-C2'-C3'-O3'
3	D	301	137	O2'-C2'-C3'-O3'
3	H	301	137	O2'-C2'-C3'-C4'
3	C	301	137	O2'-C2'-C3'-C4'
3	E	301	137	C2'-C3'-C4'-O4'
3	E	301	137	O2'-C2'-C3'-C4'
4	H	302	GOL	O1-C1-C2-C3
4	A	302	GOL	O1-C1-C2-C3
4	B	303	GOL	C1-C2-C3-O3
4	C	303	GOL	O1-C1-C2-C3
4	B	302	GOL	O2-C2-C3-O3
4	A	302	GOL	O1-C1-C2-O2
4	C	303	GOL	O1-C1-C2-O2
4	E	303	GOL	O2-C2-C3-O3
3	A	301	137	O2'-C2'-C3'-O3'
3	F	301	137	O2'-C2'-C3'-O3'
3	F	301	137	O2'-C2'-C3'-C4'
3	C	301	137	NH-C1'-C2'-C3'
3	E	301	137	NH-C1'-C2'-C3'
3	F	301	137	NH-C1'-C2'-C3'
4	B	303	GOL	O1-C1-C2-O2
3	E	301	137	O3'-C3'-C4'-O4'
3	H	301	137	NH-C1'-C2'-C3'
3	A	301	137	C2'-C1'-NH-C2
3	C	301	137	C2'-C1'-NH-C2
3	A	301	137	O2'-C2'-C3'-C4'
3	A	301	137	NH-C1'-C2'-C3'
3	H	301	137	C1'-C2'-C3'-O3'
3	C	301	137	C1'-C2'-C3'-O3'
3	E	301	137	C1'-C2'-C3'-O3'
3	D	301	137	C2'-C3'-C4'-O4'
3	E	301	137	C2'-C3'-C4'-C5'
3	H	301	137	C2'-C1'-NH-C2
3	E	301	137	C2'-C1'-NH-C2
3	F	301	137	C2'-C1'-NH-C2
3	D	301	137	C2'-C1'-NH-C2
3	H	301	137	C2'-C3'-C4'-O4'
3	A	301	137	C2'-C3'-C4'-O4'
4	H	302	GOL	O1-C1-C2-O2
3	E	301	137	O3'-C3'-C4'-C5'
3	H	301	137	NH-C1'-C2'-O2'
3	A	301	137	C1'-C2'-C3'-O3'

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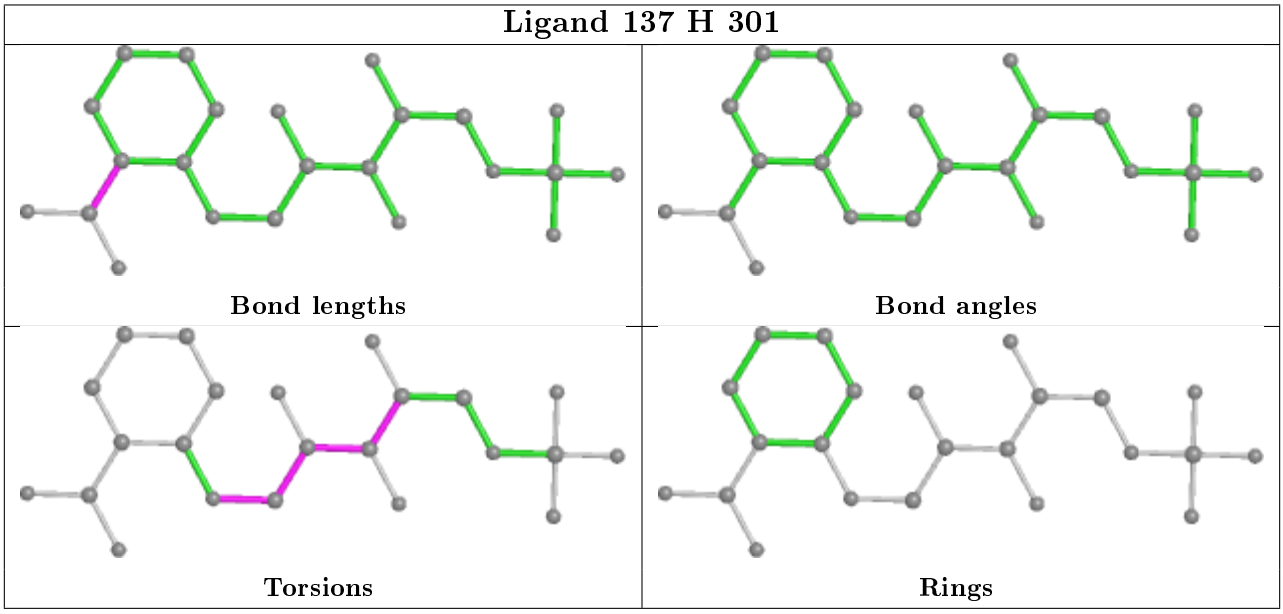
Mol	Chain	Res	Type	Atoms
3	A	301	137	NH-C1'-C2'-O2'
3	F	301	137	C1'-C2'-C3'-O3'
3	D	301	137	NH-C1'-C2'-O2'

There are no ring outliers.

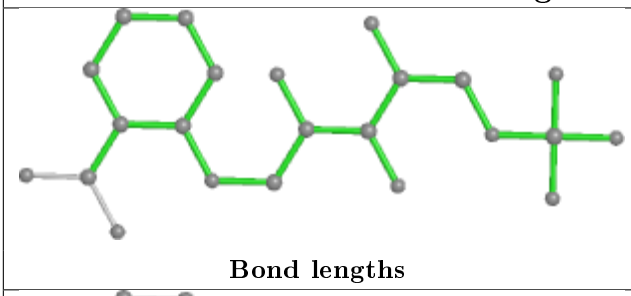
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	302	GOL	1	0
4	B	302	GOL	1	0
4	A	302	GOL	1	0
3	A	301	137	1	0
4	E	303	GOL	2	0
3	B	301	137	1	0

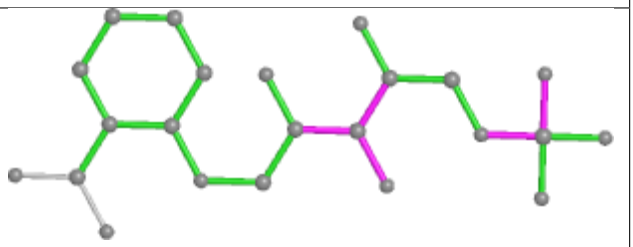
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



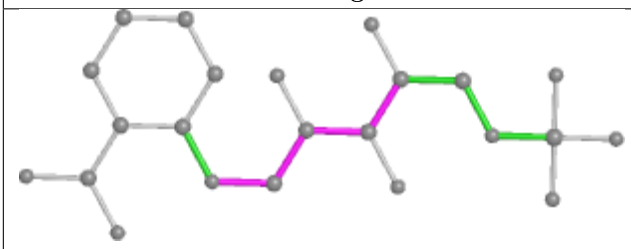
Ligand 137 A 301



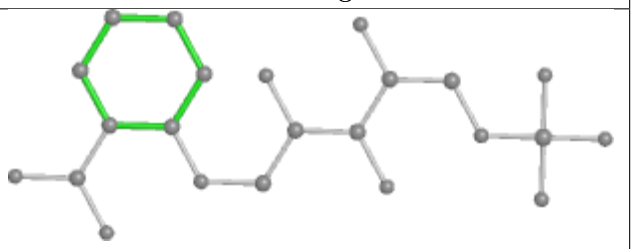
Bond lengths



Bond angles

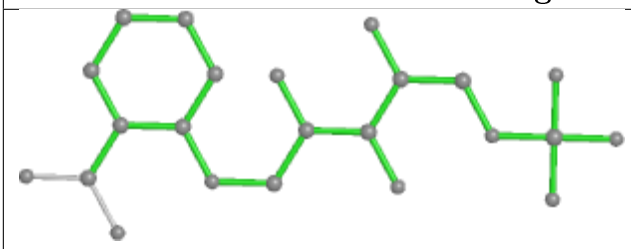


Torsions

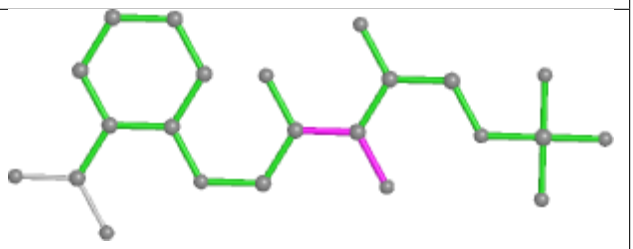


Rings

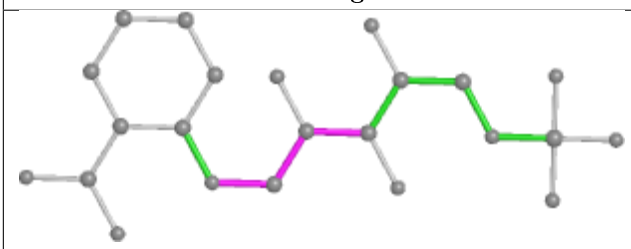
Ligand 137 C 301



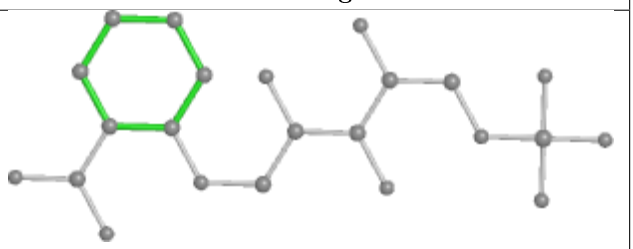
Bond lengths



Bond angles

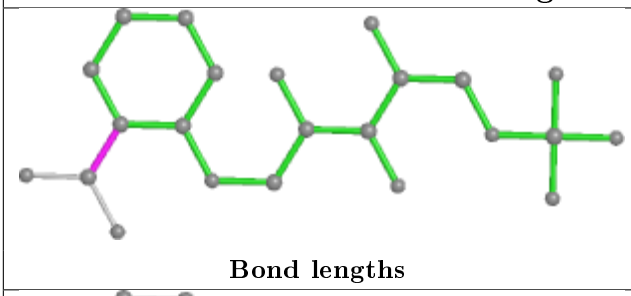


Torsions

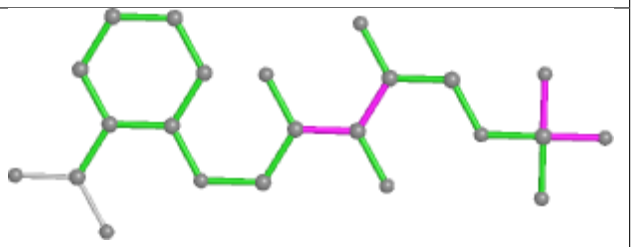


Rings

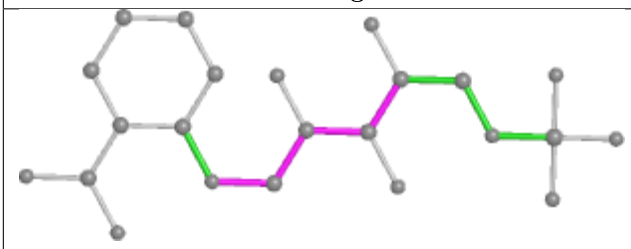
Ligand 137 E 301



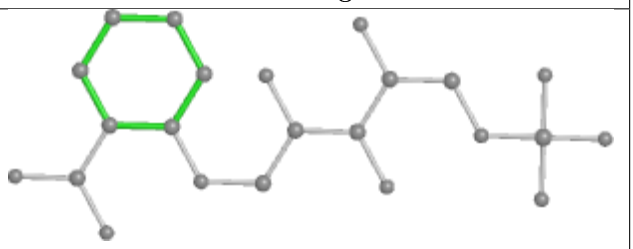
Bond lengths



Bond angles

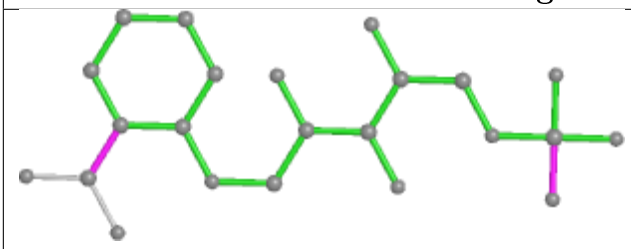


Torsions

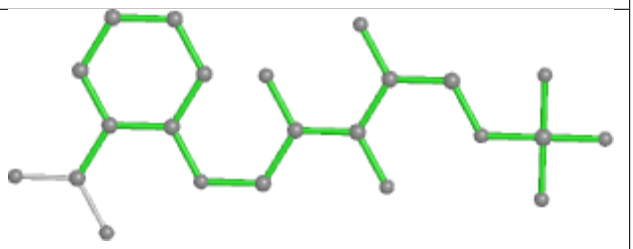


Rings

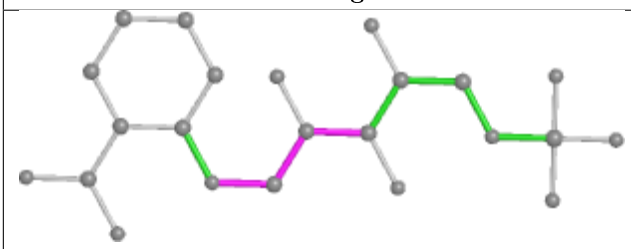
Ligand 137 F 301



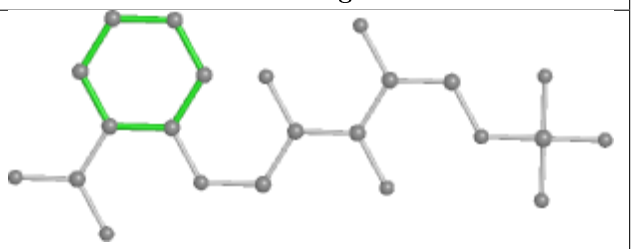
Bond lengths



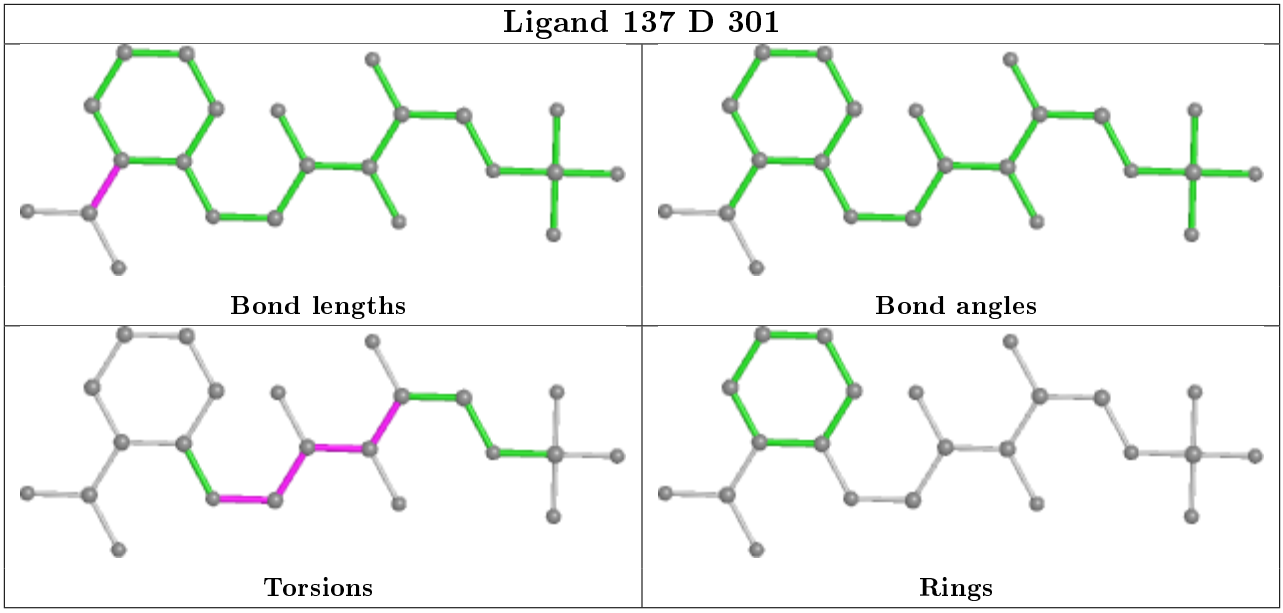
Bond angles

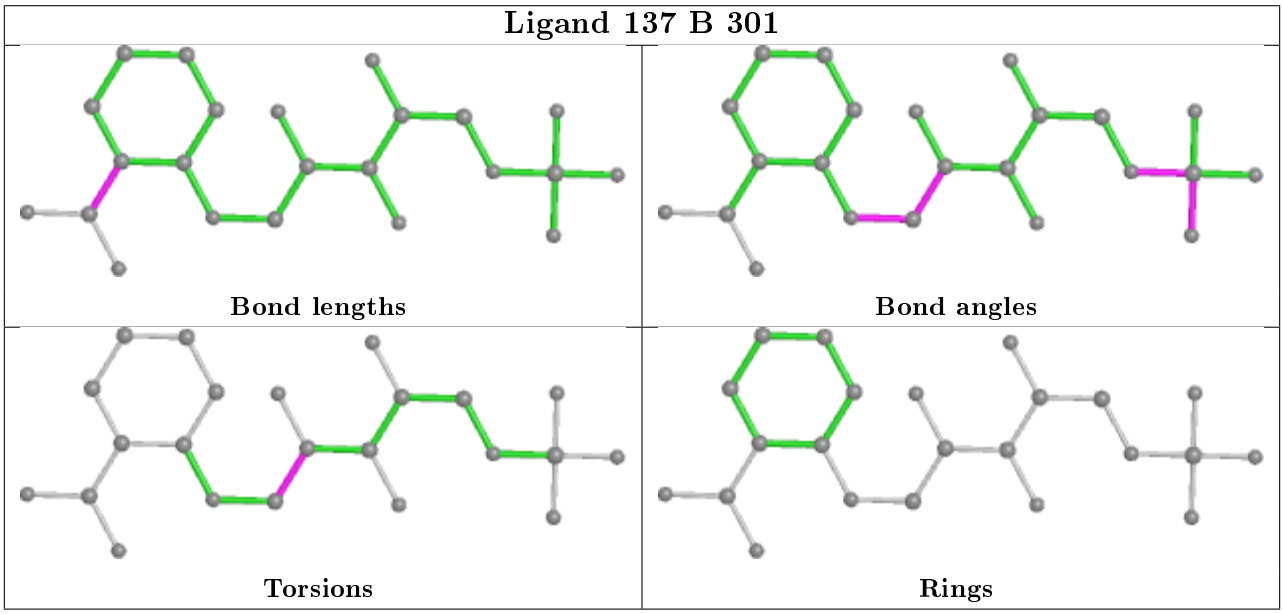


Torsions



Rings





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	22:UNK	C	25:VAL	N	7.20

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	264/287 (91%)	-0.51	2 (0%) 86 88	20, 27, 46, 70	0
1	B	265/287 (92%)	-0.45	1 (0%) 92 93	18, 27, 47, 72	0
1	C	264/287 (91%)	-0.46	2 (0%) 86 88	20, 29, 49, 85	0
1	D	265/287 (92%)	0.16	18 (6%) 17 21	24, 38, 76, 91	0
1	E	265/287 (92%)	-0.55	3 (1%) 80 84	22, 28, 48, 91	0
1	F	265/287 (92%)	-0.06	10 (3%) 40 46	25, 41, 64, 90	0
1	H	264/287 (91%)	0.04	15 (5%) 23 29	24, 42, 67, 97	0
2	G	239/277 (86%)	0.23	32 (13%) 3 4	24, 36, 94, 108	0
All	All	2091/2286 (91%)	-0.20	83 (3%) 38 44	18, 33, 65, 108	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	67	PRO	7.2
2	G	70	GLY	6.4
2	G	66	SER	6.3
2	G	71	VAL	6.3
2	G	68	SER	6.0
2	G	72	LEU	5.2
1	D	6	VAL	5.1
2	G	201	PHE	4.9
1	H	258	LEU	4.9
2	G	32	ARG	4.9
2	G	65	ALA	4.7
1	D	75	HIS	4.7
1	E	2	SER	4.2
1	F	74	GLU	4.2
1	D	253	ALA	4.1
2	G	252	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	262	ARG	4.0
2	G	267	GLU	4.0
1	H	263	LEU	3.8
2	G	35	ARG	3.8
1	H	265	PHE	3.8
1	D	5	THR	3.7
1	F	234	GLU	3.7
1	F	258	LEU	3.6
2	G	199	HIS	3.6
1	D	74	GLU	3.6
2	G	198	LEU	3.4
1	E	3	VAL	3.4
1	H	238	VAL	3.4
1	D	199	HIS	3.3
1	F	238	VAL	3.3
1	E	4	PRO	3.2
1	D	72	LEU	3.2
1	H	252	ARG	3.2
2	G	103	GLN	3.1
2	G	27	LEU	3.1
2	G	69	LYS	3.1
2	G	25	VAL	3.1
1	H	72	LEU	3.0
2	G	29	GLU	3.0
2	G	33	LEU	3.0
1	H	230	ARG	3.0
1	H	262	ARG	3.0
1	F	266	GLN	2.9
1	H	228	LEU	2.9
1	D	4	PRO	2.9
2	G	74	GLU	2.9
1	D	252	ARG	2.9
2	G	30	VAL	2.8
2	G	75	HIS	2.8
2	G	26	ASN	2.8
1	D	254	ASP	2.8
1	F	230	ARG	2.8
2	G	36	SER	2.7
1	D	76	PHE	2.7
1	F	77	VAL	2.7
1	H	205	LEU	2.7
1	H	261	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	125	PHE	2.6
1	H	234	GLU	2.5
2	G	37	ALA	2.5
1	B	266	GLN	2.5
2	G	64	LYS	2.5
2	G	28	ALA	2.5
1	D	10	ILE	2.4
2	G	254	ASP	2.4
1	D	71	VAL	2.4
1	A	266	GLN	2.4
1	F	76	PHE	2.4
1	F	24	ARG	2.3
1	D	73	ARG	2.2
1	C	2	SER	2.2
1	D	69	LYS	2.2
2	G	200	THR	2.1
1	H	253	ALA	2.1
1	H	254	ASP	2.1
1	D	24	ARG	2.1
1	A	3	VAL	2.1
1	D	70	GLY	2.1
1	C	3	VAL	2.0
1	H	249	ALA	2.0
2	G	73	ARG	2.0
1	D	9	LYS	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)

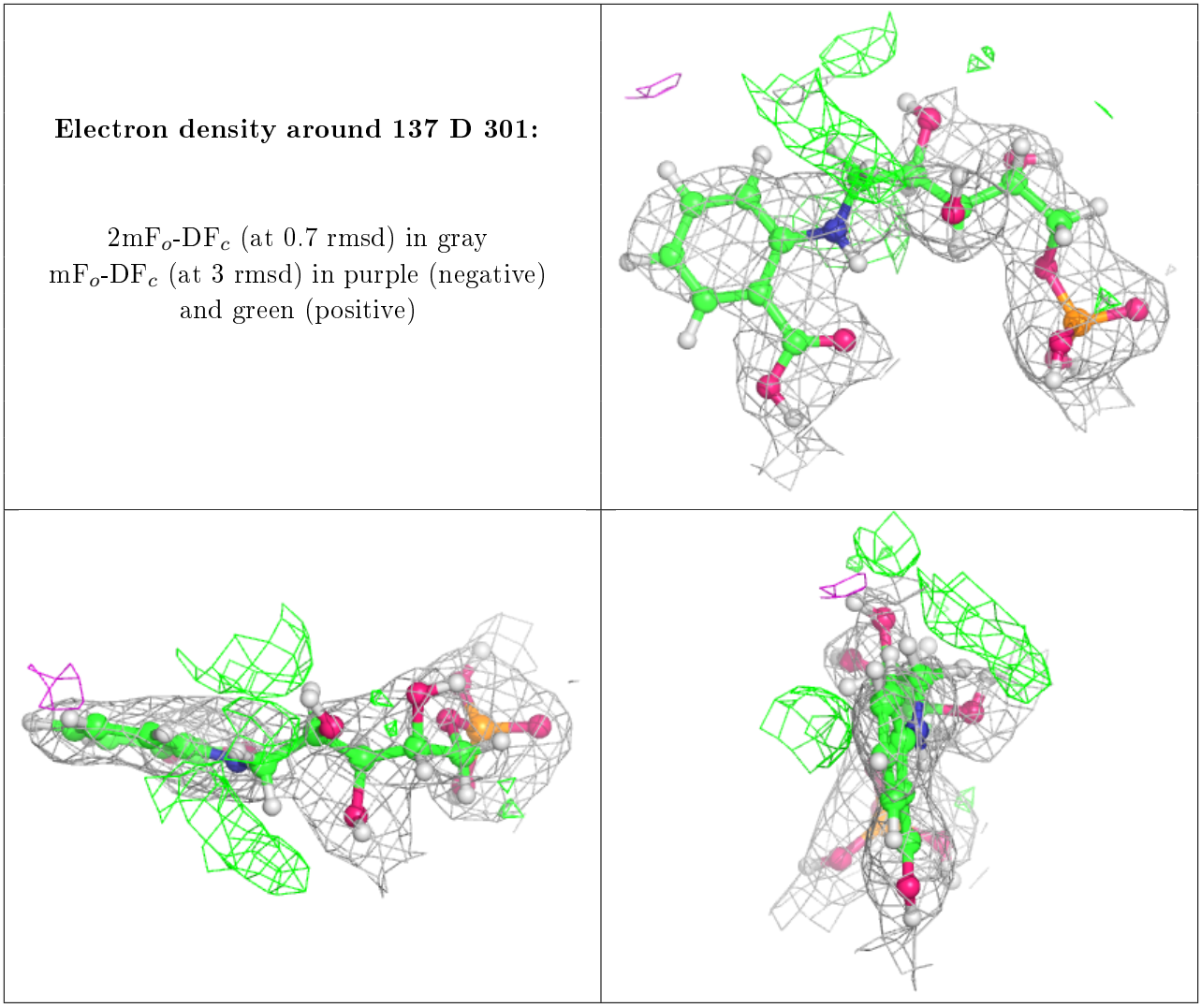
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GOL	C	303	6/6	0.75	0.24	51,62,74,74	0
4	GOL	A	302	6/6	0.82	0.22	46,57,68,72	0
4	GOL	B	303	6/6	0.86	0.22	43,59,71,82	0
4	GOL	E	303	6/6	0.88	0.32	32,53,82,86	0
4	GOL	C	302	6/6	0.91	0.19	39,56,65,67	0
4	GOL	B	302	6/6	0.92	0.10	24,44,62,67	0
4	GOL	H	302	6/6	0.94	0.12	40,51,59,61	0
5	CIT	E	302	13/13	0.94	0.10	35,45,62,62	0
3	137	D	301	23/23	0.95	0.14	38,62,77,83	0
3	137	F	301	23/23	0.96	0.10	39,48,59,65	0
3	137	H	301	23/23	0.97	0.14	42,53,67,73	0
6	PO4	G	301	5/5	0.97	0.10	41,55,61,64	0
3	137	C	301	23/23	0.98	0.09	25,35,48,58	0
3	137	E	301	23/23	0.98	0.09	19,29,41,61	0
3	137	B	301	23/23	0.98	0.11	22,27,43,48	0
3	137	A	301	23/23	0.99	0.08	22,31,43,56	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.

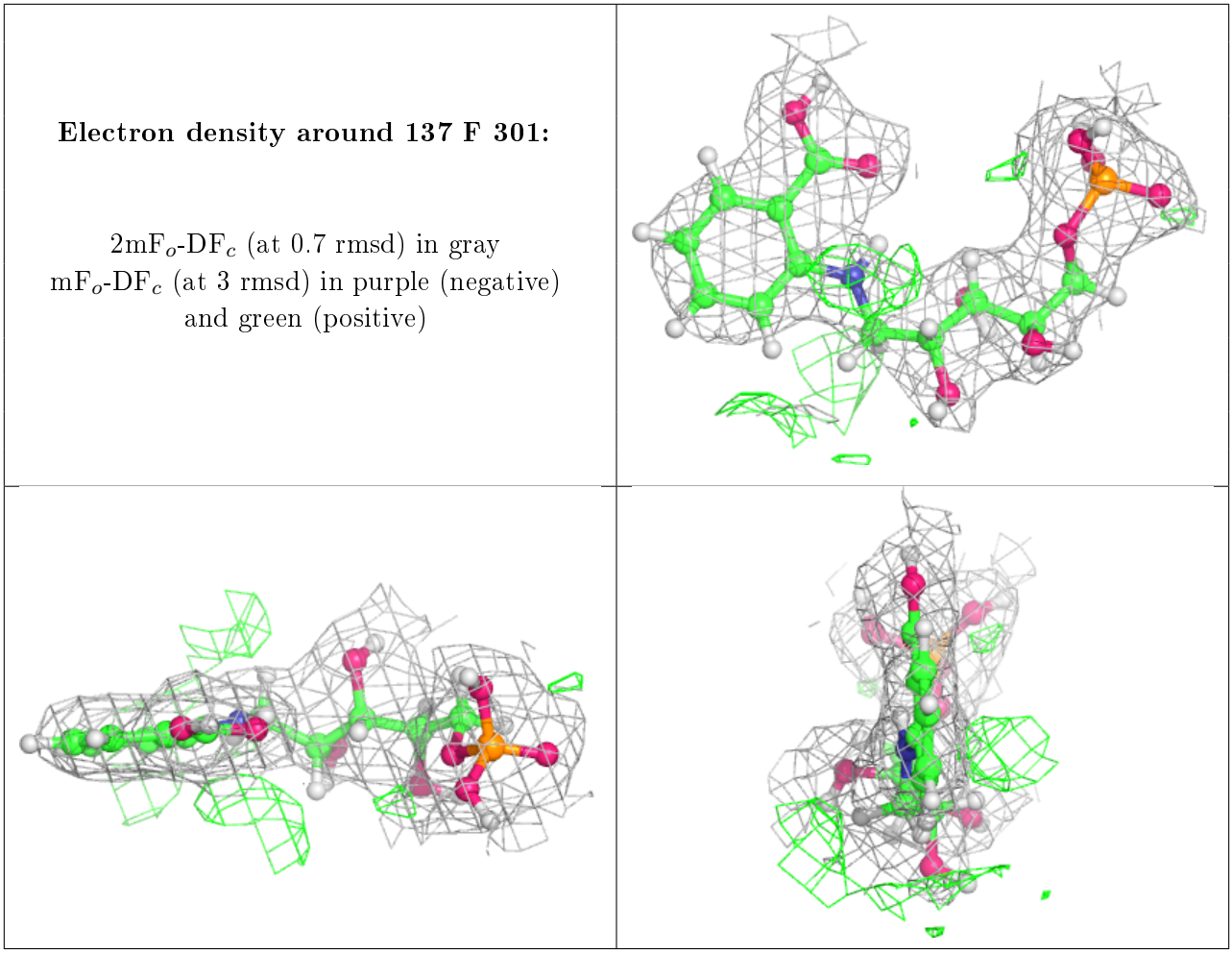
Electron density around 137 D 301:

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



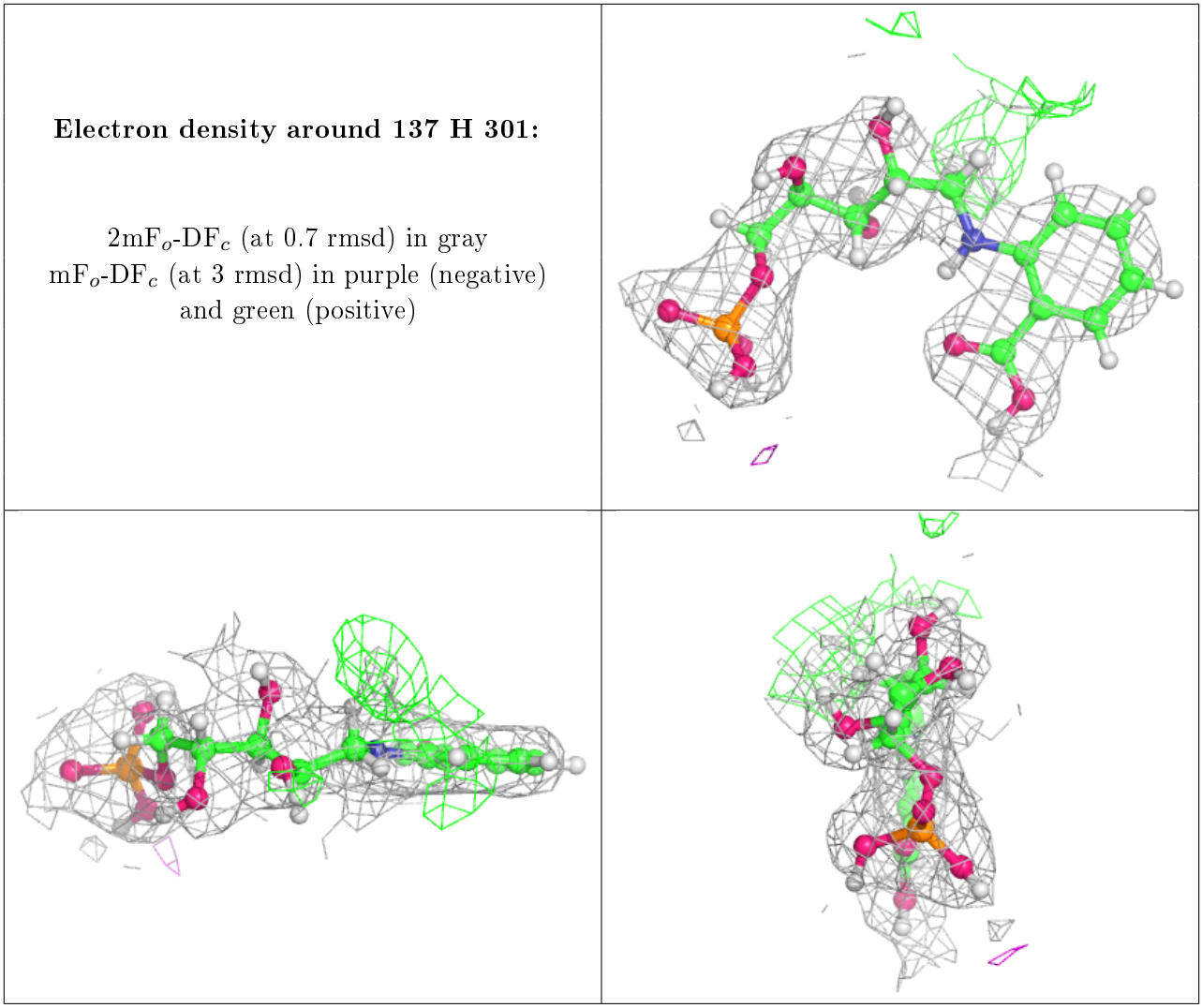
Electron density around 137 F 301:

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



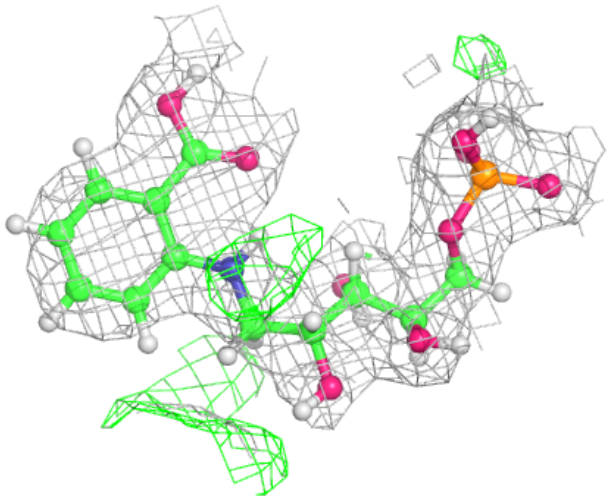
Electron density around 137 H 301:

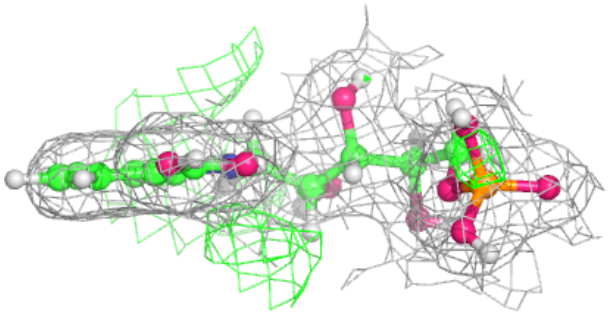
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

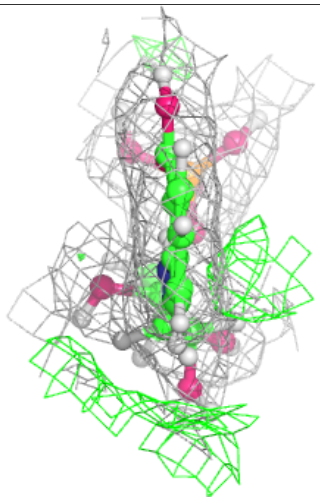


Electron density around 137 C 301:

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

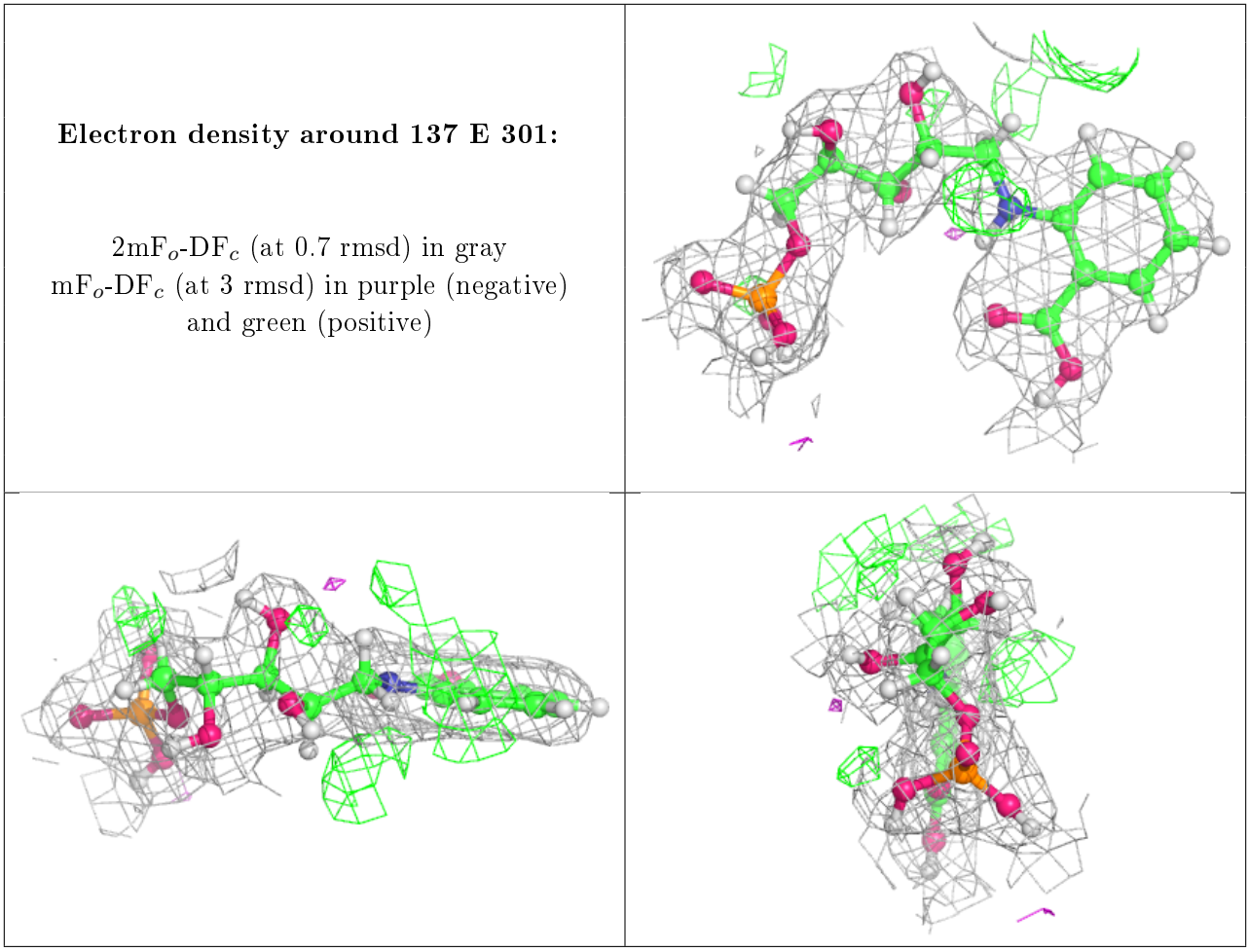






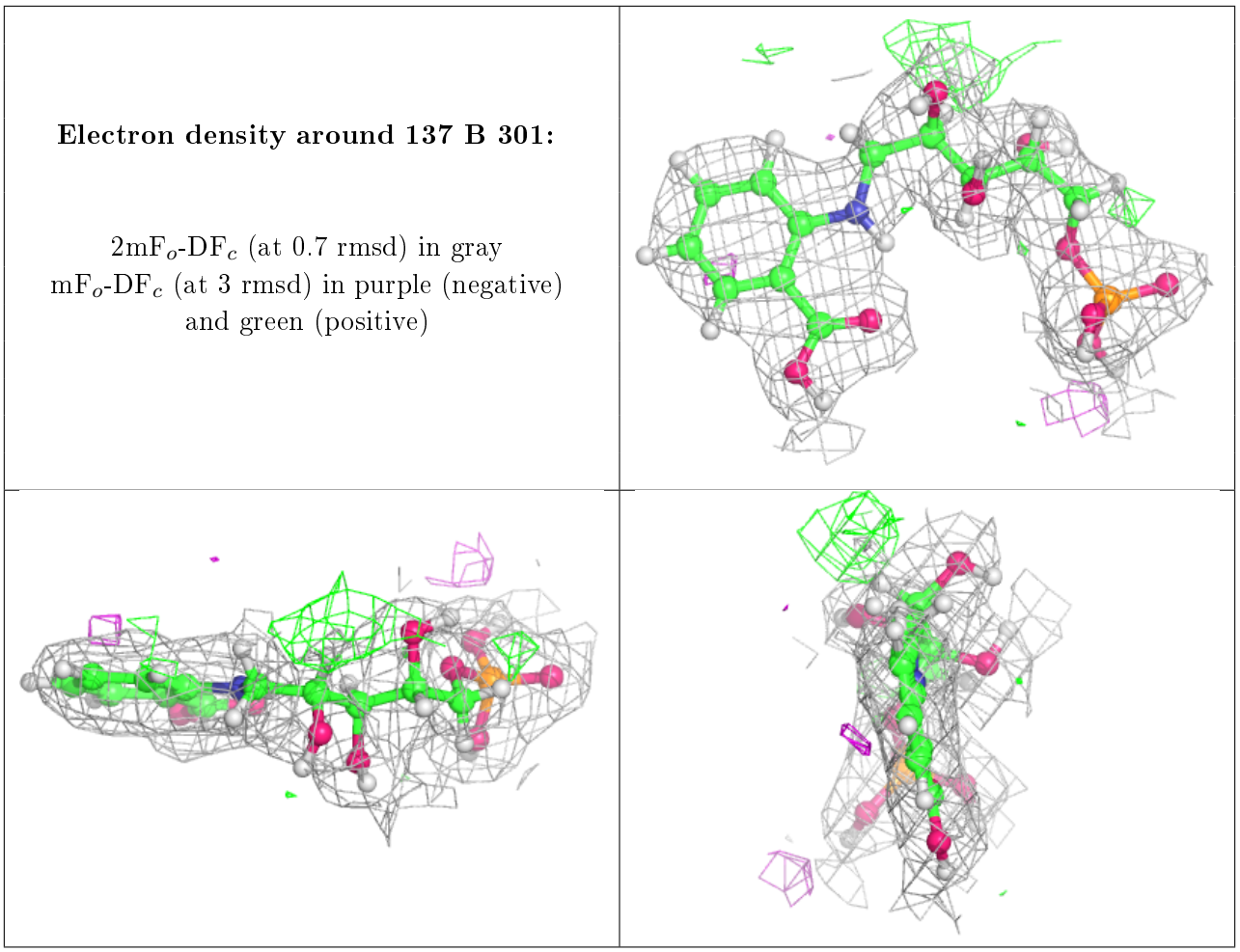
Electron density around 137 E 301:

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



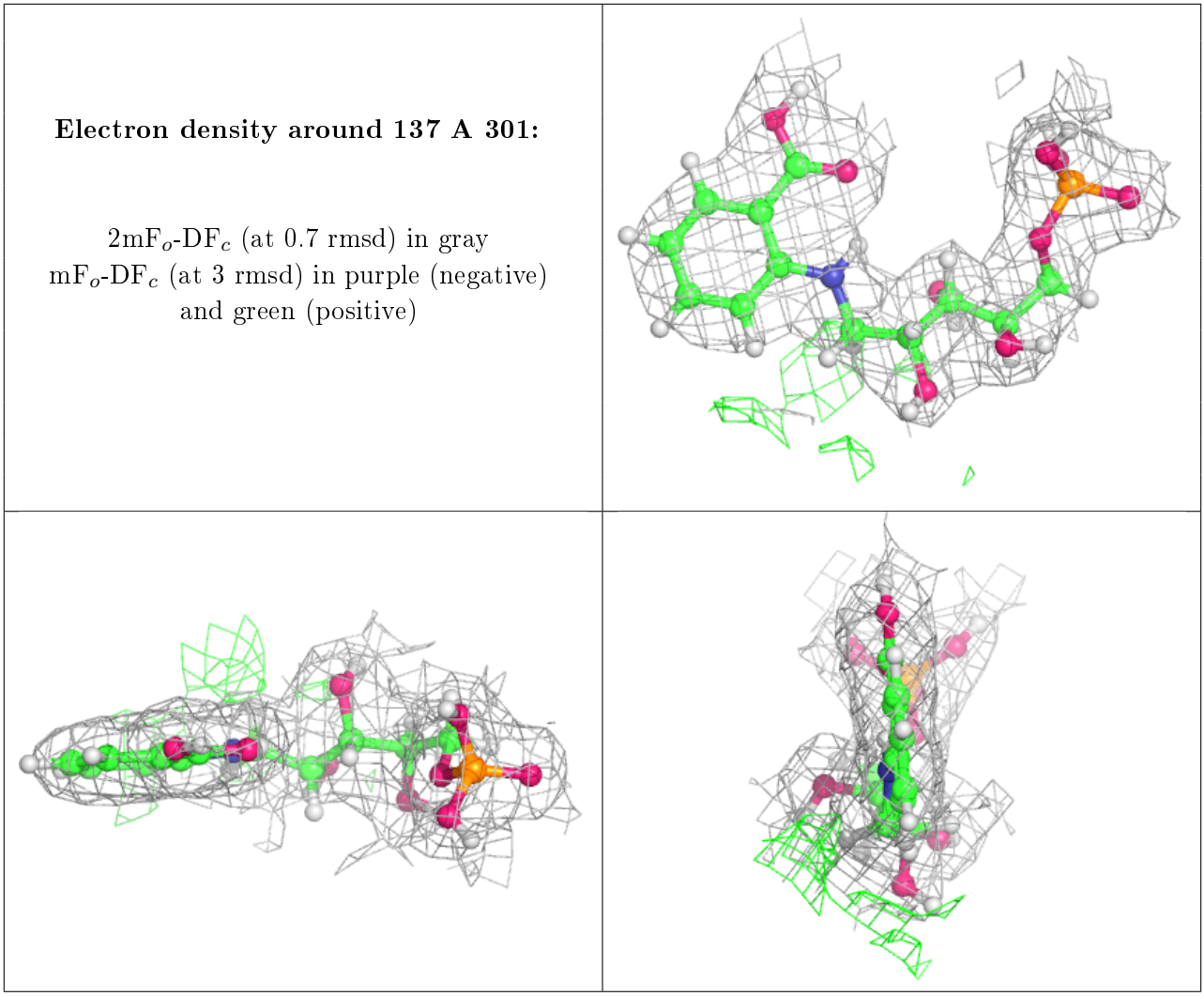
Electron density around 137 B 301:

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



Electron density around 137 A 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.