wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 12:47 AM EDT

PDB ID	:	3TR9
Title	:	Structure of a dihydropteroate synthase (folP) in complex with pteroic acid from Coxiella burnetii
Authors	:	Cheung, J.; Franklin, M.C.; Rudolph, M.; Cassidy, M.; Gary, E.; Burshteyn, F.; Love, J.
Deposited on	:	2011-09-09
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

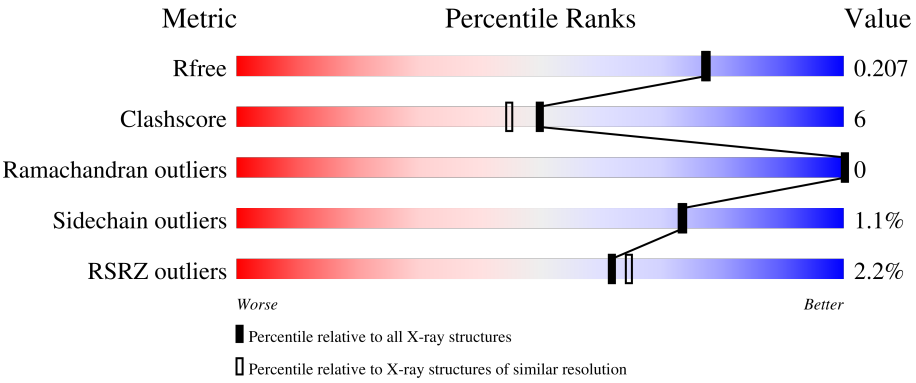
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	314	78% 10% 12%
1	B	314	% 72% 13% • 14%
1	C	314	3% 74% 12% 14%
1	D	314	4% 75% 12% • 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9301 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 Dihydropteroate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	Se	0	0	0
			2165	1367	382	407	2	7			
1	B	270	Total	C	N	O	S	Se	0	0	0
			2114	1334	374	397	2	7			
1	C	269	Total	C	N	O	S	Se	0	1	0
			2117	1335	376	397	2	7			
1	D	275	Total	C	N	O	S	Se	0	1	0
			2158	1362	381	406	2	7			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	-	expression tag	UNP Q83BY6
A	299	ASN	-	expression tag	UNP Q83BY6
A	300	LEU	-	expression tag	UNP Q83BY6
A	301	TYR	-	expression tag	UNP Q83BY6
A	302	PHE	-	expression tag	UNP Q83BY6
A	303	GLN	-	expression tag	UNP Q83BY6
A	304	GLY	-	expression tag	UNP Q83BY6
A	305	HIS	-	expression tag	UNP Q83BY6
A	306	HIS	-	expression tag	UNP Q83BY6
A	307	HIS	-	expression tag	UNP Q83BY6
A	308	HIS	-	expression tag	UNP Q83BY6
A	309	HIS	-	expression tag	UNP Q83BY6
A	310	HIS	-	expression tag	UNP Q83BY6
A	311	HIS	-	expression tag	UNP Q83BY6
A	312	HIS	-	expression tag	UNP Q83BY6
A	313	HIS	-	expression tag	UNP Q83BY6
A	314	HIS	-	expression tag	UNP Q83BY6
B	298	GLU	-	expression tag	UNP Q83BY6
B	299	ASN	-	expression tag	UNP Q83BY6
B	300	LEU	-	expression tag	UNP Q83BY6
B	301	TYR	-	expression tag	UNP Q83BY6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	PHE	-	expression tag	UNP Q83BY6
B	303	GLN	-	expression tag	UNP Q83BY6
B	304	GLY	-	expression tag	UNP Q83BY6
B	305	HIS	-	expression tag	UNP Q83BY6
B	306	HIS	-	expression tag	UNP Q83BY6
B	307	HIS	-	expression tag	UNP Q83BY6
B	308	HIS	-	expression tag	UNP Q83BY6
B	309	HIS	-	expression tag	UNP Q83BY6
B	310	HIS	-	expression tag	UNP Q83BY6
B	311	HIS	-	expression tag	UNP Q83BY6
B	312	HIS	-	expression tag	UNP Q83BY6
B	313	HIS	-	expression tag	UNP Q83BY6
B	314	HIS	-	expression tag	UNP Q83BY6
C	298	GLU	-	expression tag	UNP Q83BY6
C	299	ASN	-	expression tag	UNP Q83BY6
C	300	LEU	-	expression tag	UNP Q83BY6
C	301	TYR	-	expression tag	UNP Q83BY6
C	302	PHE	-	expression tag	UNP Q83BY6
C	303	GLN	-	expression tag	UNP Q83BY6
C	304	GLY	-	expression tag	UNP Q83BY6
C	305	HIS	-	expression tag	UNP Q83BY6
C	306	HIS	-	expression tag	UNP Q83BY6
C	307	HIS	-	expression tag	UNP Q83BY6
C	308	HIS	-	expression tag	UNP Q83BY6
C	309	HIS	-	expression tag	UNP Q83BY6
C	310	HIS	-	expression tag	UNP Q83BY6
C	311	HIS	-	expression tag	UNP Q83BY6
C	312	HIS	-	expression tag	UNP Q83BY6
C	313	HIS	-	expression tag	UNP Q83BY6
C	314	HIS	-	expression tag	UNP Q83BY6
D	298	GLU	-	expression tag	UNP Q83BY6
D	299	ASN	-	expression tag	UNP Q83BY6
D	300	LEU	-	expression tag	UNP Q83BY6
D	301	TYR	-	expression tag	UNP Q83BY6
D	302	PHE	-	expression tag	UNP Q83BY6
D	303	GLN	-	expression tag	UNP Q83BY6
D	304	GLY	-	expression tag	UNP Q83BY6
D	305	HIS	-	expression tag	UNP Q83BY6
D	306	HIS	-	expression tag	UNP Q83BY6
D	307	HIS	-	expression tag	UNP Q83BY6
D	308	HIS	-	expression tag	UNP Q83BY6
D	309	HIS	-	expression tag	UNP Q83BY6

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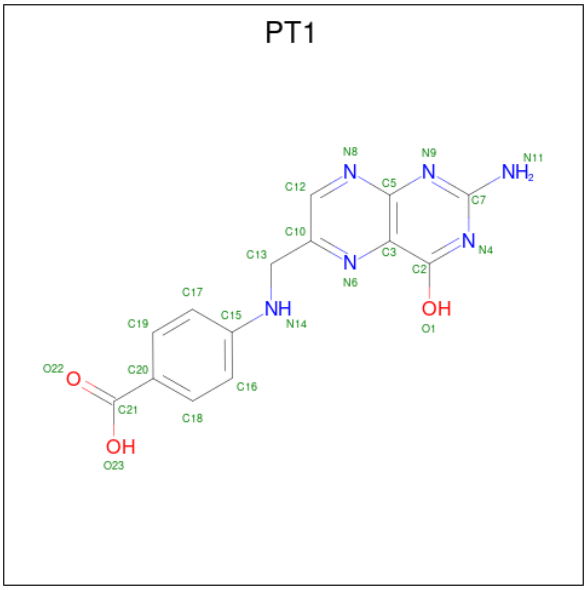
Chain	Residue	Modelled	Actual	Comment	Reference
D	310	HIS	-	expression tag	UNP Q83BY6
D	311	HIS	-	expression tag	UNP Q83BY6
D	312	HIS	-	expression tag	UNP Q83BY6
D	313	HIS	-	expression tag	UNP Q83BY6
D	314	HIS	-	expression tag	UNP Q83BY6

- Molecule 2 is PTEROIC ACID (three-letter code: PT1) (formula: $C_{14}H_{12}N_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 23 14 6 3	0	0
2	B	1	Total C N O 23 14 6 3	0	0
2	C	1	Total C N O 23 14 6 3	0	0
2	D	1	Total C N O 23 14 6 3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is water.

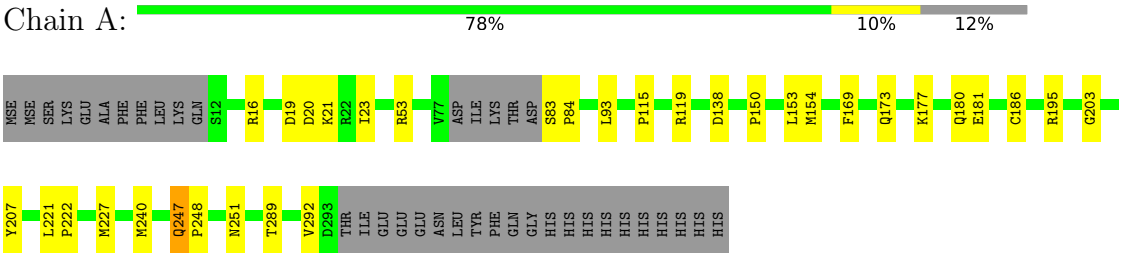
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	182	Total O 182 182	0	0
5	B	175	Total O 175 175	0	0
5	C	150	Total O 150 150	0	0
5	D	143	Total O 143 143	0	0

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.

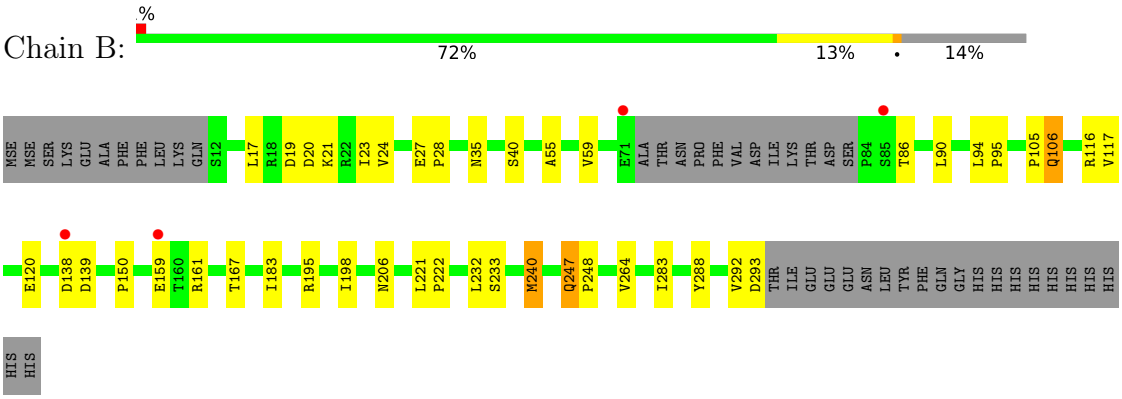
• Molecule 1: Dihydropteroate synthase

Chain A:



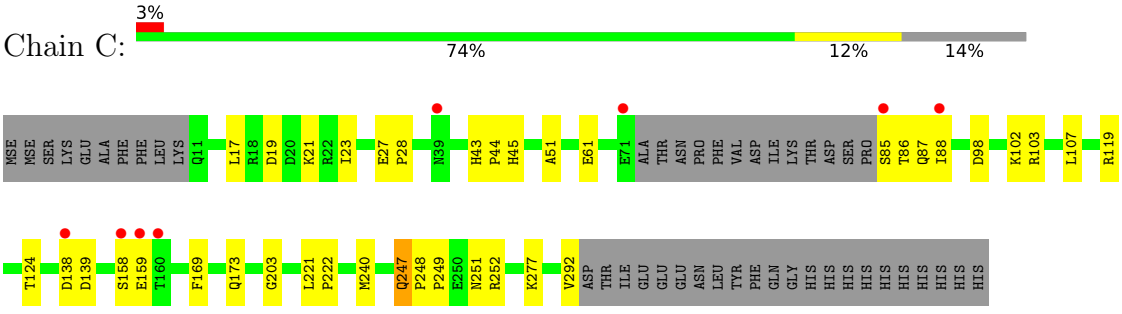
• Molecule 1: Dihydropteroate synthase

Chain B:



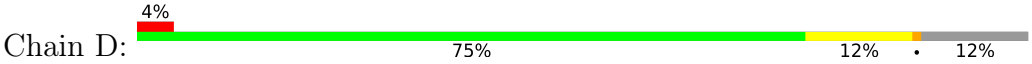
• Molecule 1: Dihydropteroate synthase

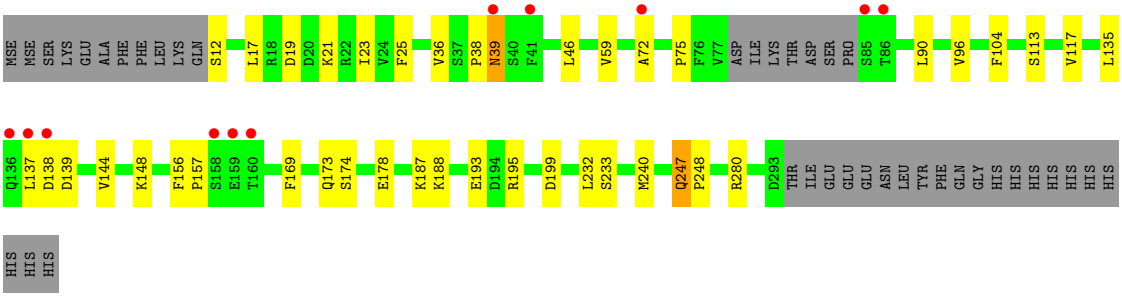
Chain C:



• Molecule 1: Dihydropteroate synthase

Chain D:




MSE MSE SER LYS GLU ALA PHE PHE LEU LYS GLN S12 L17 R18 D19 D20 K21 R22 I23 V24 F25 V36 S37 P38 N39 S40 F41 L46 V59 A72 P75 F76 V77 ASP ILE LYS THR ASP SER PRO S85 T86 L90 V96 F104 S113 V117 L135
Q136 L137 D138 D139 V144 K148 F156 P157 S158 E159 T160 F169 Q173 S174 E178 K187 K188 E193 D194 R195 D199 L232 S233 M240 Q247 P248 R280 D293 THR ILE GLU GLU GLU ASN LEU TYR PHE GLN GLY HIS HIS HIS HIS HIS HIS
HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.88Å 86.88Å 158.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 1.90 48.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.44-1.90) 99.5 (48.51-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.172 , 0.212 0.168 , 0.207	Depositor DCC
R_{free} test set	4782 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9301	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: CL, PT1, NA

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	0.28	0/2199	0.46	0/2965
1	B	0.28	0/2146	0.46	0/2890
1	C	0.29	0/2148	0.47	0/2892
1	D	0.26	0/2191	0.44	0/2953
All	All	0.28	0/8684	0.46	0/11700

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2165	0	2186	22	0
1	B	2114	0	2139	27	0
1	C	2117	0	2142	26	0
1	D	2158	0	2178	28	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	0	0
2	D	23	0	11	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	182	0	0	3	0
5	B	175	0	0	2	0
5	C	150	0	0	7	0
5	D	143	0	0	2	0
All	All	9301	0	8689	101	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 6.

The worst 5 of 101 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:21:LYS:HE3	1:B:23:ILE:HD11	1.40	1.03
1:A:21:LYS:HE3	1:A:23:ILE:HD11	1.46	0.95
1:D:21:LYS:HE3	1:D:23:ILE:HD11	1.49	0.92
1:C:85:SER:C	5:C:608:HOH:O	2.16	0.84
1:A:16:ARG:HD2	1:A:195:ARG:NH2	1.99	0.76

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	273/314 (87%)	267 (98%)	6 (2%)	0	100	100
1	B	266/314 (85%)	258 (97%)	8 (3%)	0	100	100
1	C	266/314 (85%)	260 (98%)	6 (2%)	0	100	100
1	D	272/314 (87%)	266 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1077/1256 (86%)	1051 (98%)	26 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	241/267 (90%)	240 (100%)	1 (0%)	91 91
1	B	235/267 (88%)	230 (98%)	5 (2%)	53 48
1	C	235/267 (88%)	233 (99%)	2 (1%)	78 79
1	D	240/267 (90%)	238 (99%)	2 (1%)	81 82
All	All	951/1068 (89%)	941 (99%)	10 (1%)	73 73

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	292	VAL
1	D	39	ASN
1	D	247	GLN
1	B	240	MSE
1	B	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	247	GLN
1	C	247	GLN
1	D	247	GLN
1	A	184	GLN
1	A	180	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PT1	A	1001	-	24,25,25	1.85	3 (12%)	31,35,35	2.06	6 (19%)
2	PT1	B	1001	-	24,25,25	1.86	3 (12%)	31,35,35	2.17	6 (19%)
2	PT1	C	1001	-	24,25,25	1.85	3 (12%)	31,35,35	2.06	6 (19%)
2	PT1	D	1001	-	24,25,25	1.91	3 (12%)	31,35,35	2.00	6 (19%)

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
2	PT1	A	1001	-	-	2/9/9/9	0/3/3/3
2	PT1	B	1001	-	-	1/9/9/9	0/3/3/3
2	PT1	C	1001	-	-	1/9/9/9	0/3/3/3
2	PT1	D	1001	-	-	1/9/9/9	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	PT1	C15-N14	6.02	1.56	1.38
2	B	1001	PT1	C15-N14	5.88	1.55	1.38
2	C	1001	PT1	C15-N14	5.88	1.55	1.38
2	A	1001	PT1	C15-N14	5.73	1.55	1.38
2	D	1001	PT1	C7-N11	5.60	1.45	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	PT1	C7-N9-C5	5.59	121.74	115.36
2	C	1001	PT1	C7-N9-C5	5.31	121.42	115.36
2	D	1001	PT1	C7-N9-C5	5.24	121.35	115.36
2	B	1001	PT1	C7-N9-C5	4.95	121.02	115.36
2	A	1001	PT1	N8-C5-N9	4.91	121.43	115.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PT1	C10-C13-N14-C15
2	B	1001	PT1	C10-C13-N14-C15
2	C	1001	PT1	C10-C13-N14-C15
2	D	1001	PT1	C10-C13-N14-C15
2	A	1001	PT1	C17-C15-N14-C13

There are no ring outliers.

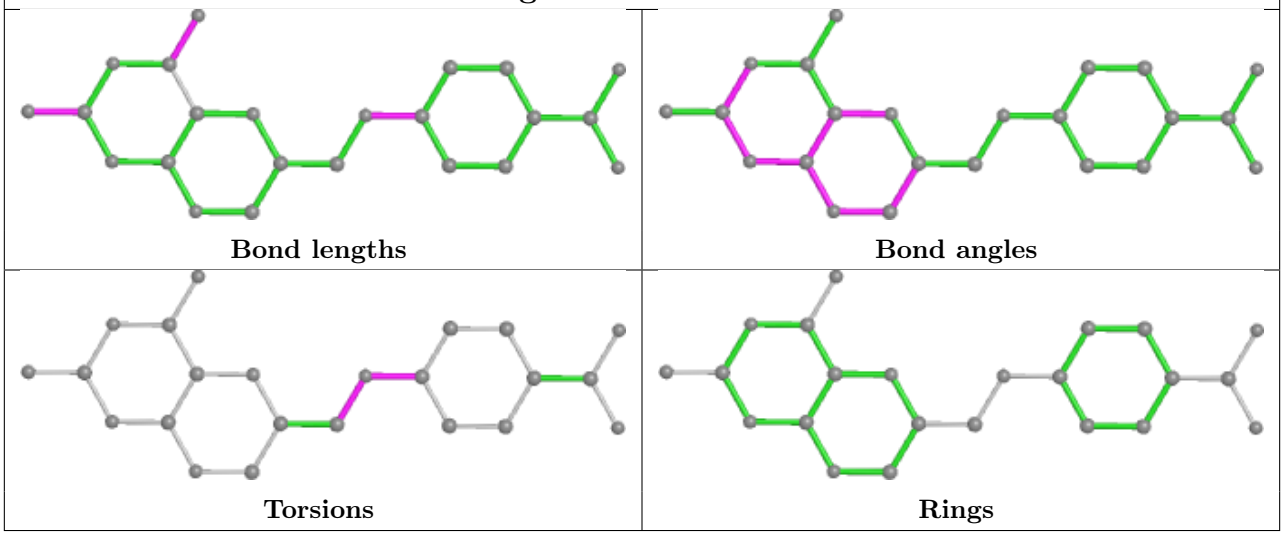
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	PT1	2	0

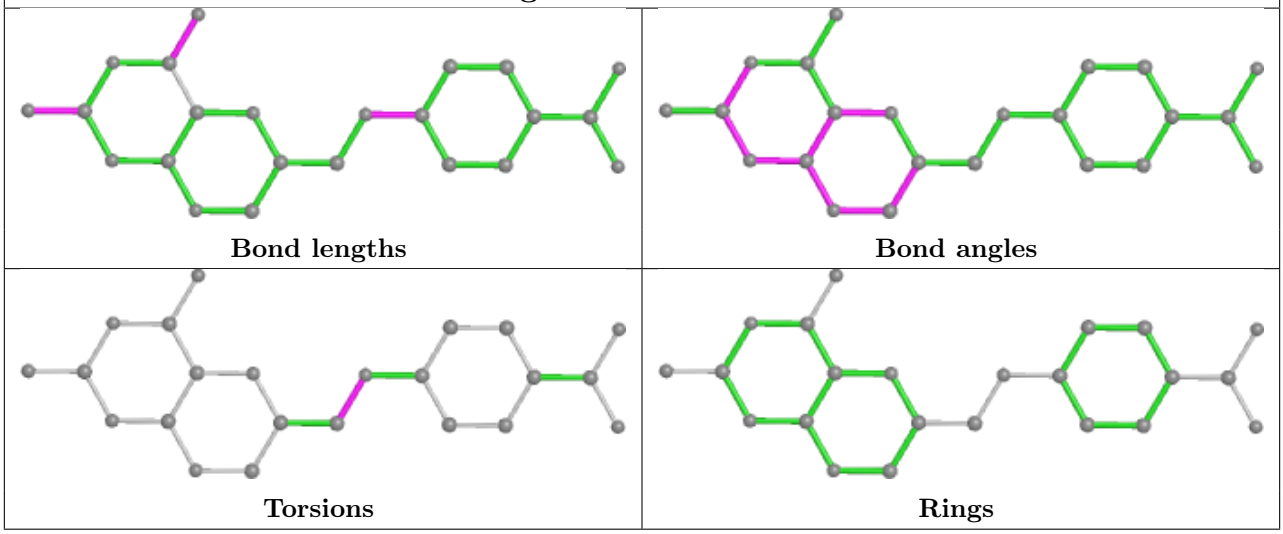
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

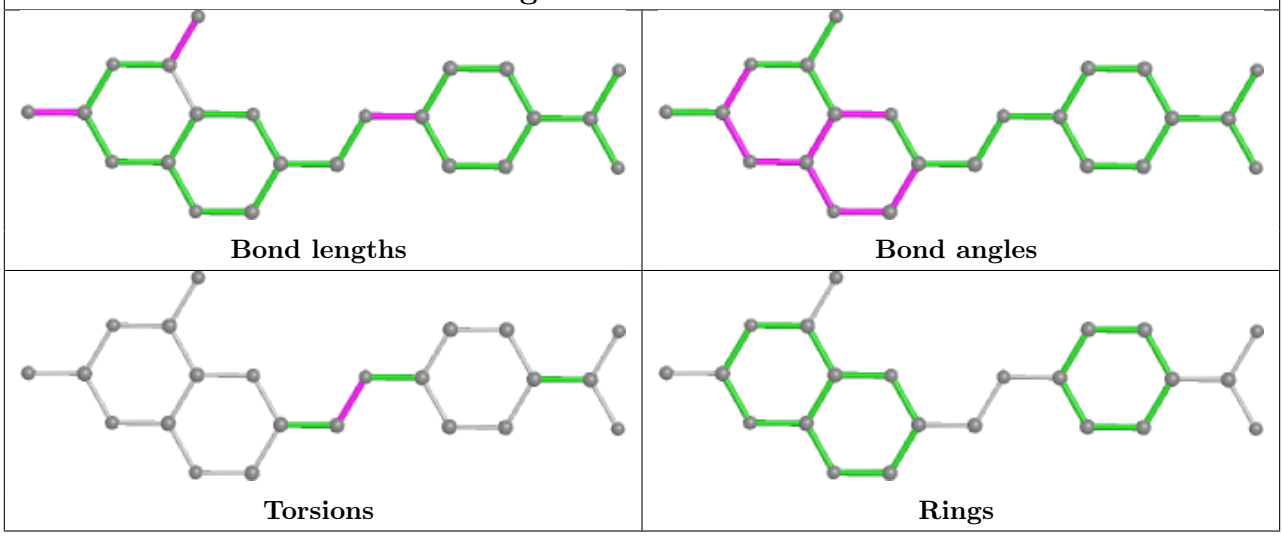
Ligand PT1 A 1001



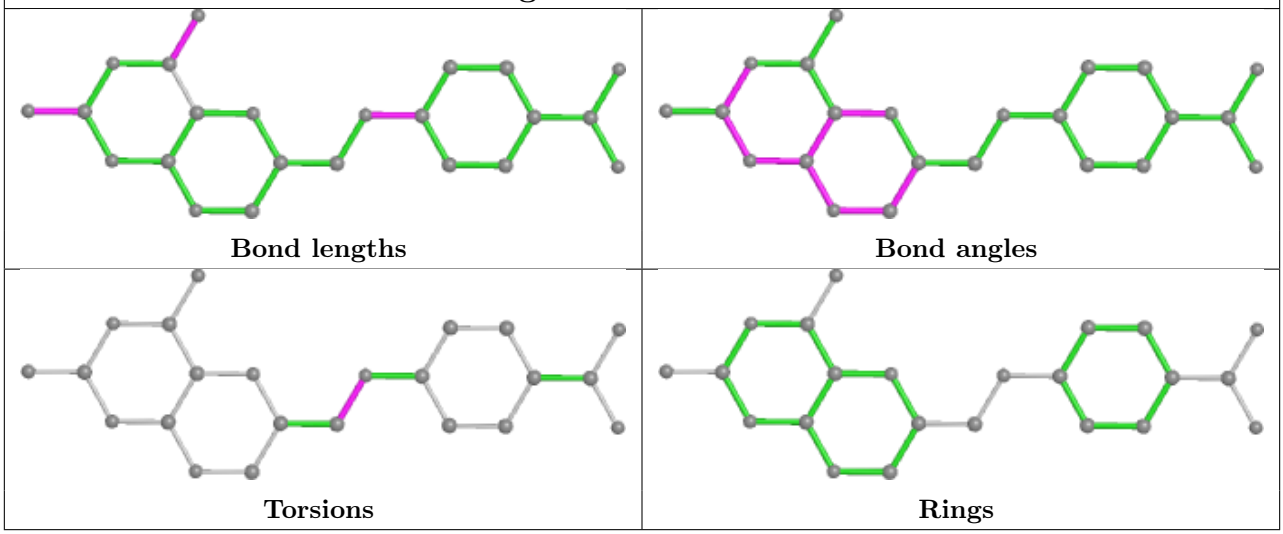
Ligand PT1 B 1001



Ligand PT1 C 1001



Ligand PT1 D 1001



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	270/314 (85%)	-0.39	0 100 100	12, 24, 43, 67	0
1	B	263/314 (83%)	-0.23	4 (1%) 73 76	13, 26, 51, 90	0
1	C	262/314 (83%)	-0.23	8 (3%) 49 51	12, 23, 55, 99	0
1	D	268/314 (85%)	-0.04	11 (4%) 37 40	15, 31, 65, 87	0
All	All	1063/1256 (84%)	-0.22	23 (2%) 62 64	12, 25, 56, 99	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	ASP	4.4
1	D	137	LEU	4.4
1	C	159	GLU	4.1
1	C	71	GLU	4.0
1	D	41	PHE	3.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

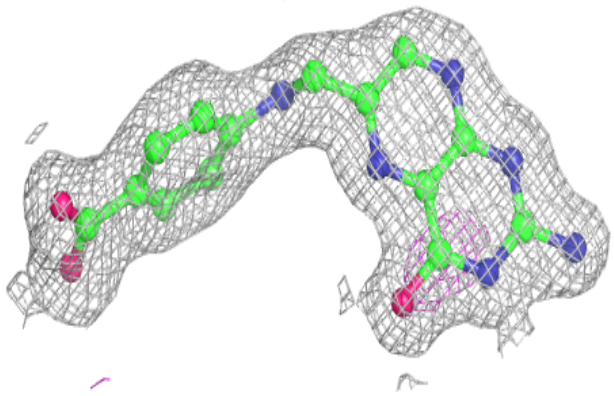
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

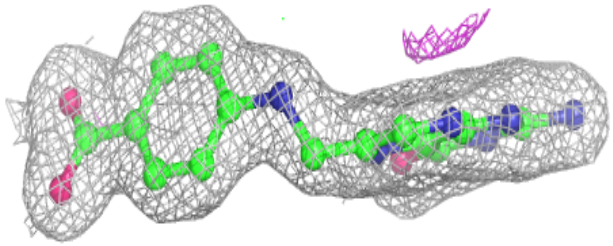
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	A	316	1/1	0.94	0.09	31,31,31,31	0
4	NA	A	317	1/1	0.95	0.15	34,34,34,34	0
2	PT1	D	1001	23/23	0.96	0.09	17,20,23,25	0
2	PT1	C	1001	23/23	0.97	0.08	15,17,21,22	0
2	PT1	B	1001	23/23	0.97	0.08	13,17,20,21	0
3	CL	B	315	1/1	0.98	0.06	25,25,25,25	0
2	PT1	A	1001	23/23	0.98	0.08	13,16,18,18	0
3	CL	A	315	1/1	0.98	0.07	27,27,27,27	0
4	NA	C	315	1/1	0.99	0.07	26,26,26,26	0

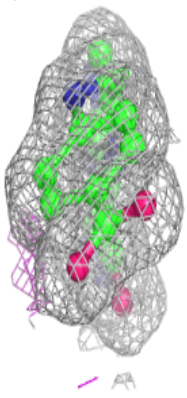
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PT1 D 1001:

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

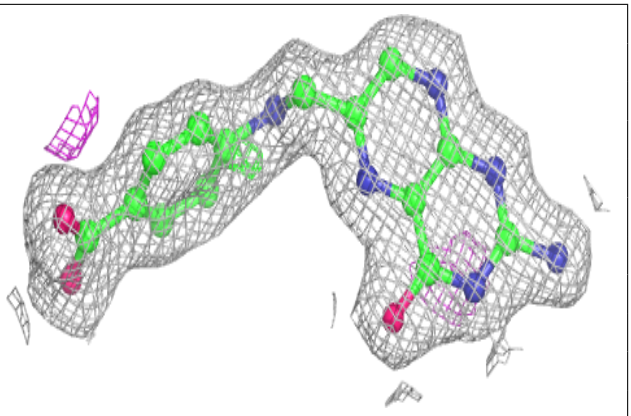


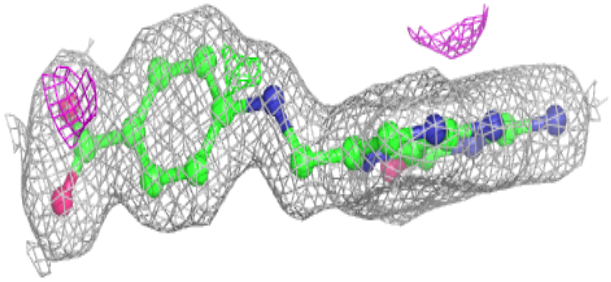


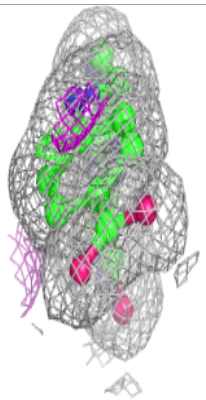


Electron density around PT1 C 1001:

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

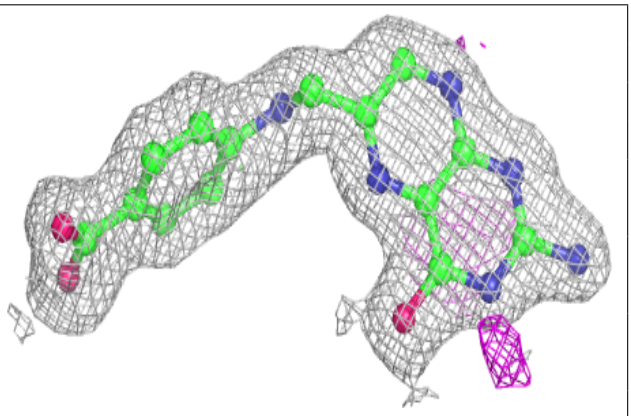


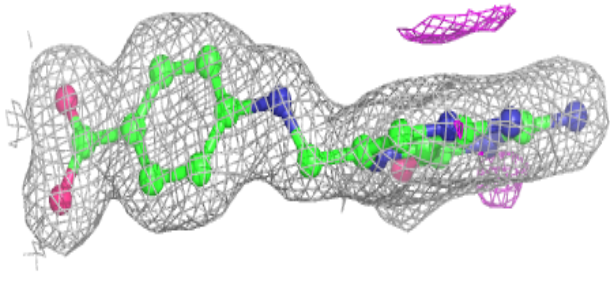


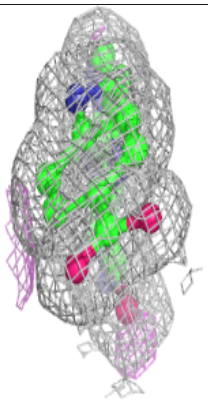


Electron density around PT1 B 1001:

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

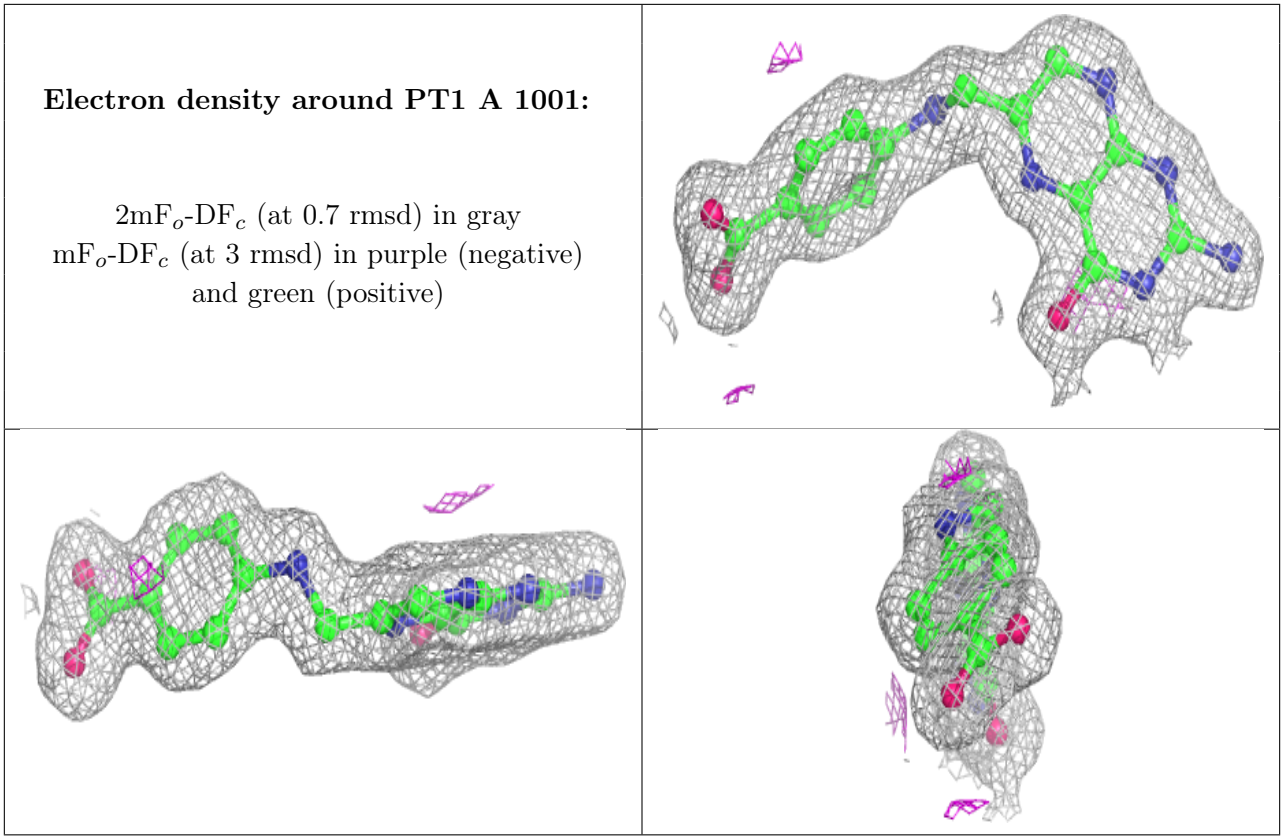






Electron density around PT1 A 1001:

$2mF_o$-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.