wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 10:01 am GMT

PDB ID	:	2CJF
Title	:	TYPE II DEHYDROQUINASE INHIBITOR COMPLEX
Authors	:	Payne, R.J.; Riboldi-Tunnicliffe, A.; Abell, A.D.; Lapthorn, A.J.; Abell, C.
Deposited on	:	2006-03-31
Resolution	:	1.95 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:

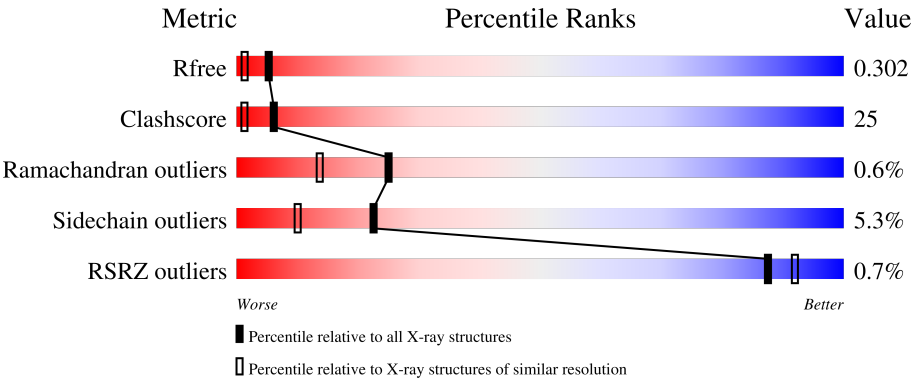
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	157	57% 34% · 5%
1	B	157	59% 31% 6% 5%
1	C	157	54% 38% · 5%
1	D	157	53% 36% 6% 5%
1	E	157	55% 35% · 5%

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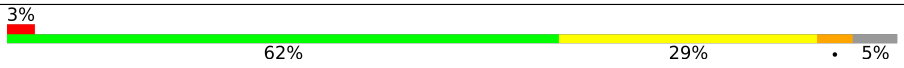
Mol	Chain	Length	Quality of chain
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RP4	A	1151	-	-	X	-
3	GOL	A	1152	-	-	X	-
3	GOL	D	1753	-	-	X	-
3	GOL	F	2153	-	-	X	-
3	GOL	G	2353	-	-	X	-
3	GOL	H	2552	-	-	X	-
3	GOL	J	2955	-	-	X	-
3	GOL	K	3153	-	-	X	-

2 Entry composition (i)

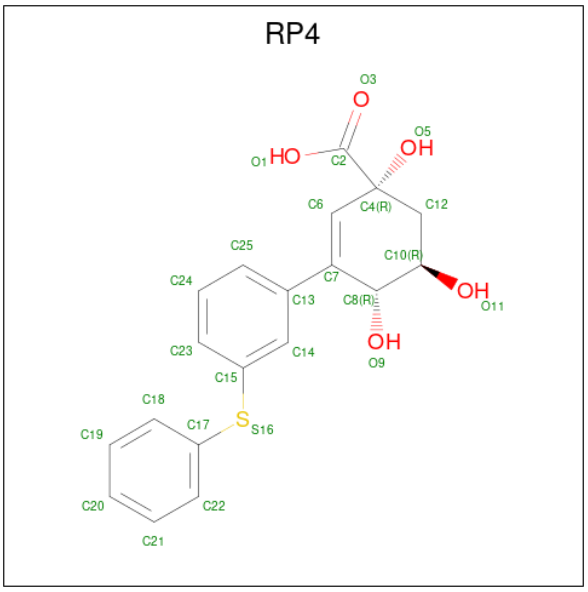
There are 6 unique types of molecules in this entry. The entry contains 15510 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-DEHYDROQUINATE DEHYDRATASE.

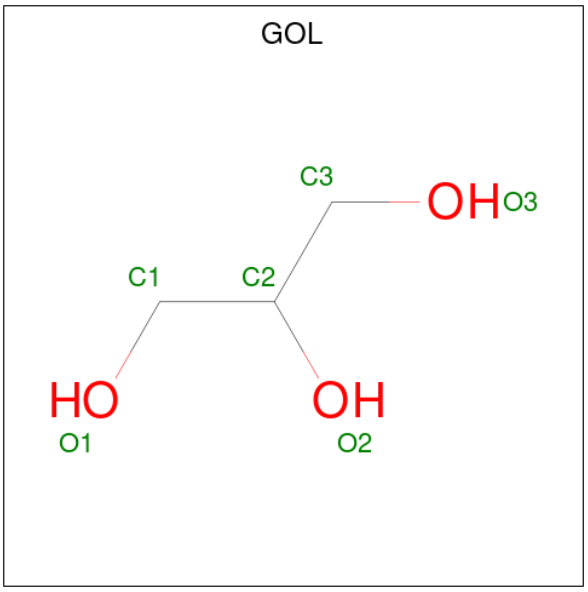
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	B	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	C	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	D	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	E	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	F	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	G	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	H	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	I	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	J	149	Total	C	N	O	S	0	2	0
			1132	704	213	210	5			
1	K	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	L	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			

- Molecule 2 is (1S,4S,5S)-1,4,5-TRIHYDROXY-3-[3-(PHENYLTHIO)PHENYL]CYCLOHEX-2-ENE-1-CARBOXYLIC ACID (three-letter code: RP4) (formula: $C_{19}H_{18}O_5S$).



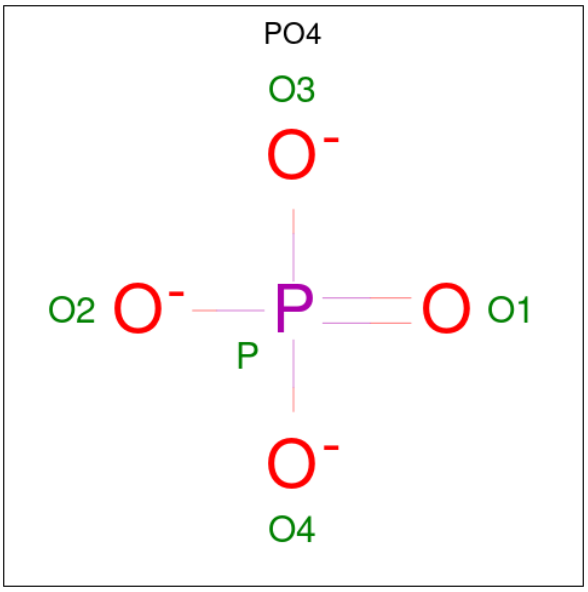
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			25	19	5	1		
2	B	1	Total	C	O	S	0	0
			25	19	5	1		
2	C	1	Total	C	O	S	0	0
			25	19	5	1		
2	D	1	Total	C	O	S	0	0
			25	19	5	1		
2	E	1	Total	C	O	S	0	0
			25	19	5	1		
2	F	1	Total	C	O	S	0	0
			25	19	5	1		
2	G	1	Total	C	O	S	0	0
			25	19	5	1		
2	H	1	Total	C	O	S	0	0
			25	19	5	1		
2	I	1	Total	C	O	S	0	0
			25	19	5	1		
2	J	1	Total	C	O	S	0	0
			25	19	5	1		
2	K	1	Total	C	O	S	0	0
			25	19	5	1		
2	L	1	Total	C	O	S	0	0
			25	19	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



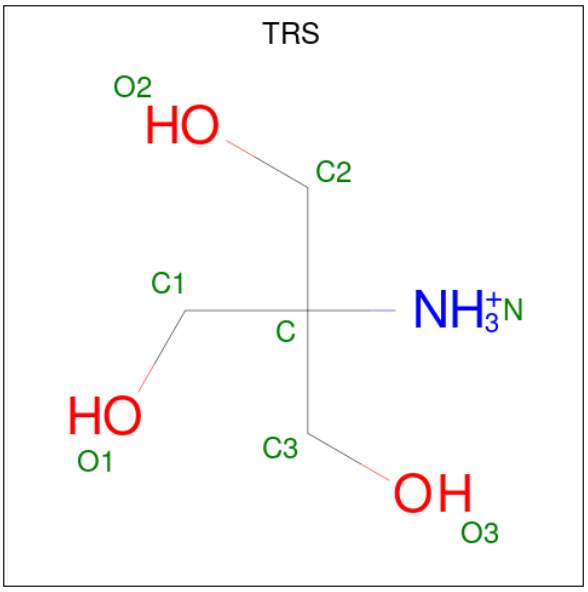
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	J	1	Total O P 5 4 1	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 8 4 1 3	0	0
5	D	1	Total C N O 8 4 1 3	0	0
5	I	1	Total C N O 8 4 1 3	0	0
5	J	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is water.

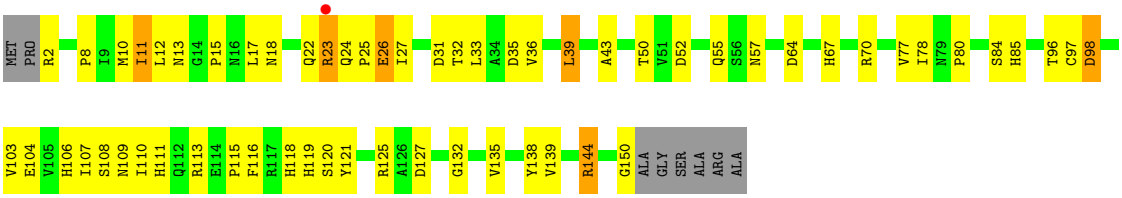
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	118	Total O 118 118	0	0
6	B	142	Total O 142 142	0	0
6	C	127	Total O 127 127	0	0
6	D	140	Total O 140 140	0	0
6	E	164	Total O 164 164	0	0
6	F	133	Total O 133 133	0	0
6	G	133	Total O 133 133	0	0
6	H	105	Total O 105 105	0	0
6	I	139	Total O 139 139	0	0
6	J	111	Total O 111 111	0	0
6	K	117	Total O 117 117	0	0
6	L	132	Total O 132 132	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.

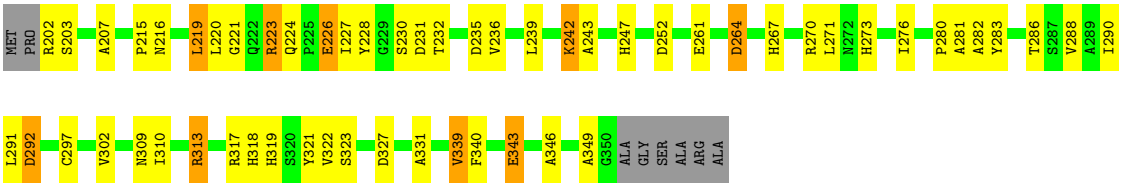
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain A:



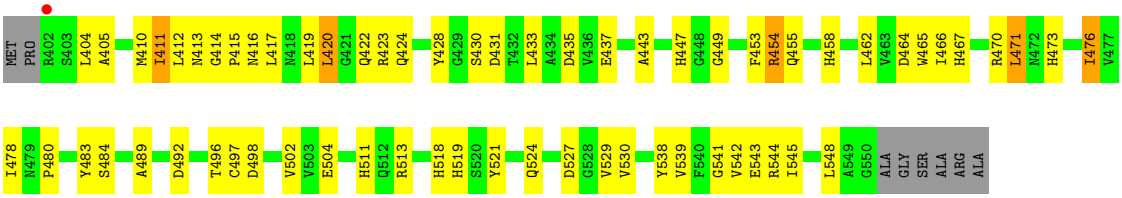
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain B:



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain C:

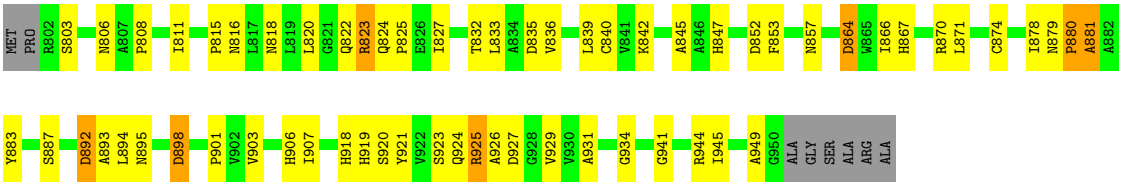


• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain D:

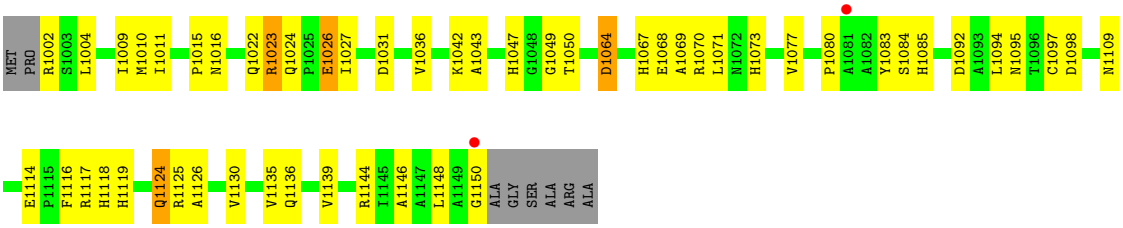
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain E:



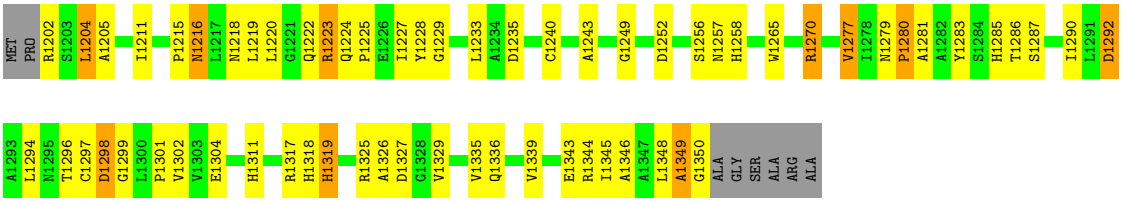
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain F:



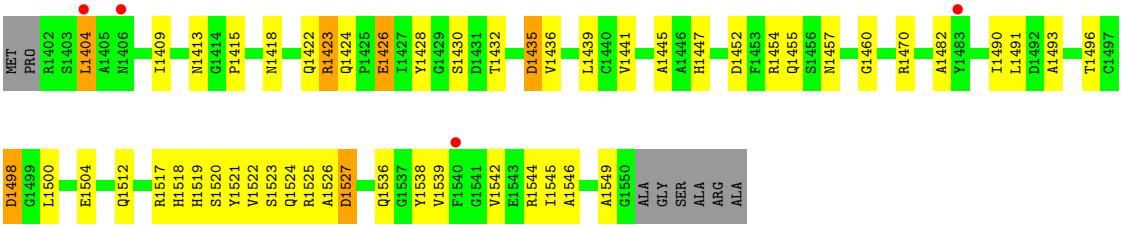
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:



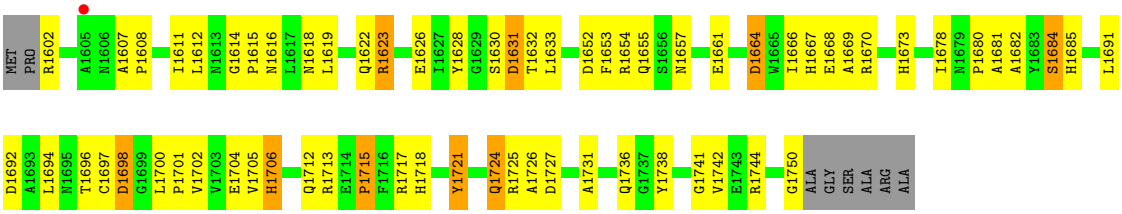
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:

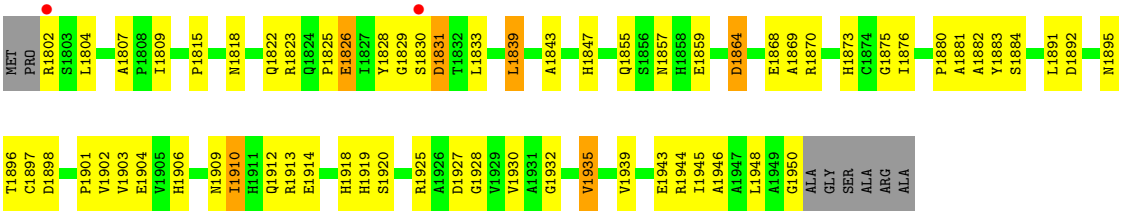


• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

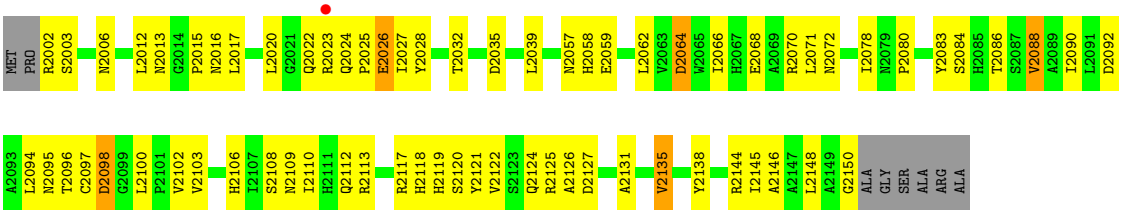
Chain I:



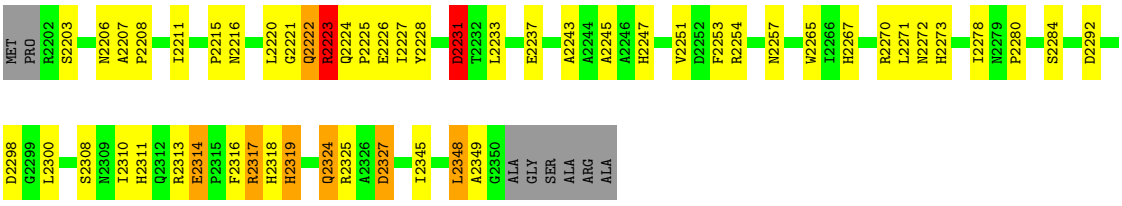
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	195.75Å 195.73Å 239.68Å 65.84° 65.89° 89.97°	Depositor
Resolution (Å)	25.00 – 1.95 25.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	76.2 (25.00-1.95) 76.0 (25.00-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.274 , 0.334 0.299 , 0.302	Depositor DCC
R_{free} test set	80795 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.406 for k,-h,-h+l 0.406 for -k,h,-k+l 0.417 for -h,k,-k-l 0.437 for h,-k,h-l 0.417 for -k,-h,-l 0.407 for k,h,h+k-l 0.416 for -h,-k,-h-k+l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	15510	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, TRS, RP4

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	1.00	1/1161 (0.1%)	1.09	5/1582 (0.3%)
1	B	1.04	1/1155 (0.1%)	1.12	4/1574 (0.3%)
1	C	0.96	1/1161 (0.1%)	1.06	4/1582 (0.3%)
1	D	1.06	1/1161 (0.1%)	1.06	5/1582 (0.3%)
1	E	1.06	1/1155 (0.1%)	1.12	8/1574 (0.5%)
1	F	0.96	1/1155 (0.1%)	0.99	2/1574 (0.1%)
1	G	1.11	0/1161	1.12	6/1582 (0.4%)
1	H	0.96	0/1161	1.05	3/1582 (0.2%)
1	I	1.06	1/1161 (0.1%)	1.09	4/1582 (0.3%)
1	J	0.96	1/1166 (0.1%)	1.04	4/1588 (0.3%)
1	K	1.01	2/1155 (0.2%)	1.04	3/1574 (0.2%)
1	L	1.03	0/1161	1.12	5/1582 (0.3%)
All	All	1.02	10/13913 (0.1%)	1.08	53/18958 (0.3%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	2121	TYR	CD1-CE1	6.82	1.49	1.39
1	F	1130	VAL	CB-CG2	-6.78	1.38	1.52
1	A	121	TYR	CD1-CE1	6.45	1.49	1.39
1	C	521	TYR	CD2-CE2	6.12	1.48	1.39
1	D	683	TYR	CG-CD2	5.99	1.47	1.39

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	864	ASP	CB-CG-OD2	9.20	126.58	118.30
1	I	1652	ASP	CB-CG-OD2	8.76	126.18	118.30
1	E	927	ASP	CB-CG-OD2	8.48	125.93	118.30
1	L	2317	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	L	2317	ARG	NE-CZ-NH2	-8.06	116.27	120.30

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	1127	0	1093	51	0
1	B	1126	0	1092	54	0
1	C	1127	0	1093	58	0
1	D	1127	0	1093	61	0
1	E	1126	0	1092	59	0
1	F	1126	0	1092	59	0
1	G	1127	0	1093	56	0
1	H	1127	0	1093	50	0
1	I	1127	0	1093	54	0
1	J	1132	0	1102	68	0
1	K	1126	0	1092	69	0
1	L	1127	0	1093	55	0
2	A	25	0	17	9	0
2	B	25	0	17	2	0
2	C	25	0	17	2	0
2	D	25	0	17	0	0
2	E	25	0	17	2	0
2	F	25	0	17	2	0
2	G	25	0	17	1	0
2	H	25	0	17	2	0
2	I	25	0	17	1	0
2	J	25	0	18	0	0
2	K	25	0	17	4	0
2	L	25	0	17	5	0
3	A	6	0	8	4	0
3	B	6	0	8	1	0
3	D	6	0	8	8	0
3	E	6	0	8	2	0
3	F	6	0	8	5	0
3	G	6	0	8	4	0
3	H	6	0	8	4	0
3	J	12	0	16	7	0
3	K	12	0	16	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	6	0	8	2	0
4	B	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	J	5	0	0	0	0
5	B	8	0	12	0	0
5	D	8	0	12	0	0
5	I	8	0	12	1	0
5	J	8	0	12	1	0
6	A	118	0	0	18	0
6	B	142	0	0	15	0
6	C	127	0	0	14	0
6	D	140	0	0	23	0
6	E	164	0	0	16	0
6	F	133	0	0	16	0
6	G	133	0	0	19	0
6	H	105	0	0	13	0
6	I	139	0	0	17	0
6	J	111	0	0	10	0
6	K	117	0	0	19	0
6	L	132	0	0	17	0
All	All	15510	0	13470	674	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 25.

The worst 5 of 674 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:D:710:ILE:CD1	1:D:710:ILE:CG1	1.74	1.59
1:C:447:HIS:CD2	6:C:2051:HOH:O	1.84	1.28
3:K:3153:GOL:H32	6:K:7116:HOH:O	1.34	1.26
1:C:447:HIS:HD2	6:C:2051:HOH:O	1.16	1.19
1:G:1228:TYR:CE1	6:G:2032:HOH:O	1.96	1.17

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	149/157 (95%)	138 (93%)	11 (7%)	0	100 100
1	B	148/157 (94%)	140 (95%)	8 (5%)	0	100 100
1	C	149/157 (95%)	133 (89%)	15 (10%)	1 (1%)	22 11
1	D	149/157 (95%)	138 (93%)	9 (6%)	2 (1%)	12 3
1	E	148/157 (94%)	137 (93%)	10 (7%)	1 (1%)	22 11
1	F	148/157 (94%)	138 (93%)	8 (5%)	2 (1%)	11 3
1	G	149/157 (95%)	138 (93%)	9 (6%)	2 (1%)	12 3
1	H	149/157 (95%)	140 (94%)	9 (6%)	0	100 100
1	I	149/157 (95%)	133 (89%)	16 (11%)	0	100 100
1	J	148/157 (94%)	135 (91%)	13 (9%)	0	100 100
1	K	148/157 (94%)	134 (90%)	14 (10%)	0	100 100
1	L	149/157 (95%)	140 (94%)	6 (4%)	3 (2%)	7 1
All	All	1783/1884 (95%)	1644 (92%)	128 (7%)	11 (1%)	25 14

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1023	ARG
1	E	949	ALA
1	G	1349	ALA
1	L	2223	ARG
1	C	420	LEU

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	119/121 (98%)	114 (96%)	5 (4%)	30	17
1	B	118/121 (98%)	112 (95%)	6 (5%)	24	11
1	C	119/121 (98%)	113 (95%)	6 (5%)	24	11
1	D	119/121 (98%)	108 (91%)	11 (9%)	9	2
1	E	118/121 (98%)	116 (98%)	2 (2%)	60	55
1	F	118/121 (98%)	113 (96%)	5 (4%)	30	17
1	G	119/121 (98%)	111 (93%)	8 (7%)	16	5
1	H	119/121 (98%)	115 (97%)	4 (3%)	37	25
1	I	119/121 (98%)	110 (92%)	9 (8%)	13	4
1	J	119/121 (98%)	112 (94%)	7 (6%)	19	8
1	K	118/121 (98%)	113 (96%)	5 (4%)	30	17
1	L	119/121 (98%)	109 (92%)	10 (8%)	11	3
All	All	1424/1452 (98%)	1346 (94%)	78 (6%)	22	9

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	1830	SER
1	L	2271	LEU
1	J	1839	LEU
1	K	2027	ILE
1	L	2319[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	1906	HIS
1	K	2112	GLN
1	J	1912	GLN
1	K	2022	GLN
1	L	2247	HIS

5.3.3 RNA

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)

32 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	$\#\|Z\| > 2$
5	TRS	I	2752	-	7,7,7	1.00	1 (14%)	9,9,9	1.48	1 (11%)
2	RP4	E	1951	-	25,27,27	1.51	4 (16%)	27,39,39	0.90	1 (3%)
3	GOL	F	2153	-	5,5,5	0.59	0	5,5,5	0.99	0
4	PO4	B	1352	-	4,4,4	0.74	0	6,6,6	0.85	0
2	RP4	H	2551	-	25,27,27	1.57	2 (8%)	27,39,39	1.59	6 (22%)
3	GOL	K	3152	-	5,5,5	0.58	0	5,5,5	0.42	0
4	PO4	J	2952	-	4,4,4	0.46	0	6,6,6	1.07	0
3	GOL	K	3153	-	5,5,5	0.49	0	5,5,5	1.57	1 (20%)
5	TRS	B	1353	-	7,7,7	0.72	0	9,9,9	1.49	1 (11%)
3	GOL	J	2954	-	5,5,5	0.50	0	5,5,5	0.62	0
3	GOL	G	2353	-	5,5,5	0.62	0	5,5,5	0.56	0
2	RP4	D	1751	-	25,27,27	1.70	3 (12%)	27,39,39	1.96	7 (25%)
3	GOL	A	1152	-	5,5,5	0.58	0	5,5,5	0.45	0
3	GOL	J	2955	-	5,5,5	0.53	0	5,5,5	0.72	0
5	TRS	D	1752	-	7,7,7	0.54	0	9,9,9	0.80	0
2	RP4	B	1351	-	25,27,27	1.73	4 (16%)	27,39,39	1.61	5 (18%)
2	RP4	F	2151	-	25,27,27	1.43	3 (12%)	27,39,39	1.48	3 (11%)
3	GOL	H	2552	-	5,5,5	0.49	0	5,5,5	1.13	0
4	PO4	F	2152	-	4,4,4	0.70	0	6,6,6	1.31	0
2	RP4	A	1151	-	25,27,27	1.55	3 (12%)	27,39,39	1.49	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	TRS	J	2953	-	7,7,7	0.56	0	9,9,9	0.94	0
4	PO4	G	2352	-	4,4,4	1.01	0	6,6,6	1.58	1 (16%)
2	RP4	G	2351	-	25,27,27	1.49	4 (16%)	27,39,39	1.45	3 (11%)
2	RP4	L	3351	-	25,27,27	2.17	6 (24%)	27,39,39	1.33	5 (18%)
2	RP4	I	2751	-	25,27,27	1.43	3 (12%)	27,39,39	1.55	5 (18%)
3	GOL	D	1753	-	5,5,5	0.61	0	5,5,5	1.23	0
2	RP4	C	1551	-	25,27,27	1.55	4 (16%)	27,39,39	1.46	5 (18%)
2	RP4	J	2951	-	25,27,27	1.68	3 (12%)	27,39,39	2.27	4 (14%)
3	GOL	L	3352	-	5,5,5	0.57	0	5,5,5	1.00	0
3	GOL	B	1354	-	5,5,5	0.64	0	5,5,5	0.72	0
3	GOL	E	1952	-	5,5,5	1.05	0	5,5,5	1.67	0
2	RP4	K	3151	-	25,27,27	1.76	3 (12%)	27,39,39	1.91	9 (33%)

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
5	TRS	I	2752	-	-	3/9/9/9	-
2	RP4	E	1951	-	-	1/14/32/32	0/3/3/3
3	GOL	F	2153	-	-	4/4/4/4	-
2	RP4	H	2551	-	-	2/14/32/32	0/3/3/3
3	GOL	K	3152	-	-	4/4/4/4	-
3	GOL	K	3153	-	-	3/4/4/4	-
5	TRS	B	1353	-	-	1/9/9/9	-
3	GOL	J	2954	-	-	2/4/4/4	-
3	GOL	G	2353	-	-	1/4/4/4	-
2	RP4	D	1751	-	-	0/14/32/32	0/3/3/3
3	GOL	A	1152	-	-	0/4/4/4	-
3	GOL	J	2955	-	-	3/4/4/4	-
5	TRS	D	1752	-	-	0/9/9/9	-
2	RP4	B	1351	-	-	2/14/32/32	0/3/3/3
2	RP4	F	2151	-	-	0/14/32/32	0/3/3/3
3	GOL	H	2552	-	-	3/4/4/4	-
2	RP4	A	1151	-	-	2/14/32/32	0/3/3/3
5	TRS	J	2953	-	-	1/9/9/9	-
2	RP4	G	2351	-	-	0/14/32/32	0/3/3/3
2	RP4	L	3351	-	-	2/14/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RP4	I	2751	-	-	2/14/32/32	0/3/3/3
3	GOL	D	1753	-	-	2/4/4/4	-
2	RP4	C	1551	-	-	2/14/32/32	0/3/3/3
2	RP4	J	2951	-	-	0/14/32/32	0/3/3/3
3	GOL	L	3352	-	-	4/4/4/4	-
3	GOL	B	1354	-	-	2/4/4/4	-
3	GOL	E	1952	-	-	4/4/4/4	-
2	RP4	K	3151	-	-	1/14/32/32	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1751	RP4	C15-S16	-5.77	1.66	1.77
2	B	1351	RP4	C15-S16	-5.14	1.67	1.77
2	H	2551	RP4	C17-S16	-5.12	1.67	1.77
2	K	3151	RP4	C17-S16	-5.05	1.67	1.77
2	L	3351	RP4	C17-S16	-4.95	1.67	1.77

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2951	RP4	O11-C10-C8	-9.91	93.07	109.73
2	A	1151	RP4	C17-S16-C15	5.86	115.75	103.18
2	I	2751	RP4	O11-C10-C8	-4.80	101.67	109.73
2	D	1751	RP4	O11-C10-C8	-4.65	101.92	109.73
2	D	1751	RP4	O5-C4-C2	-4.60	99.25	108.54

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1151	RP4	O1-C2-C4-O5
2	B	1351	RP4	O1-C2-C4-O5
2	C	1551	RP4	O1-C2-C4-O5
2	E	1951	RP4	O1-C2-C4-O5
2	H	2551	RP4	O1-C2-C4-O5

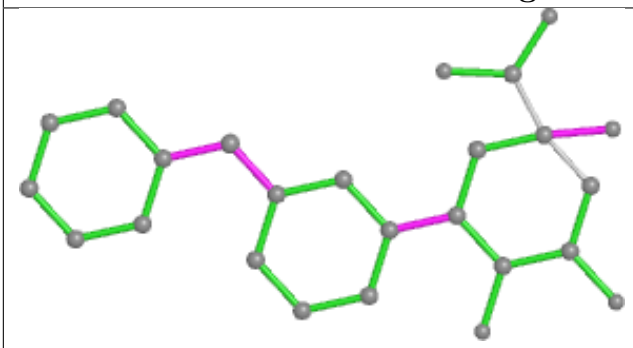
There are no ring outliers.

24 monomers are involved in 79 short contacts:

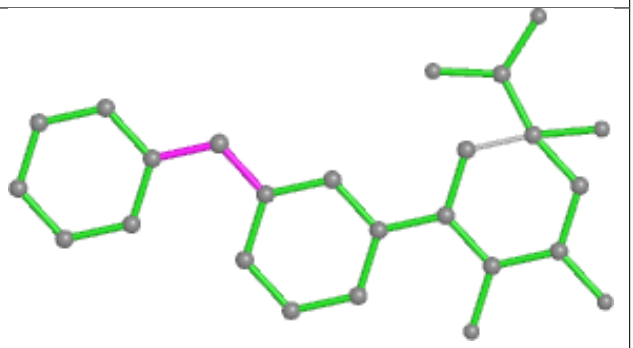
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2752	TRS	1	0
2	E	1951	RP4	2	0
3	F	2153	GOL	5	0
2	H	2551	RP4	2	0
3	K	3152	GOL	3	0
3	K	3153	GOL	7	0
3	J	2954	GOL	3	0
3	G	2353	GOL	4	0
3	A	1152	GOL	4	0
3	J	2955	GOL	4	0
2	B	1351	RP4	2	0
2	F	2151	RP4	2	0
3	H	2552	GOL	4	0
2	A	1151	RP4	9	0
5	J	2953	TRS	1	0
2	G	2351	RP4	1	0
2	L	3351	RP4	5	0
2	I	2751	RP4	1	0
3	D	1753	GOL	8	0
2	C	1551	RP4	2	0
3	L	3352	GOL	2	0
3	B	1354	GOL	1	0
3	E	1952	GOL	2	0
2	K	3151	RP4	4	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.

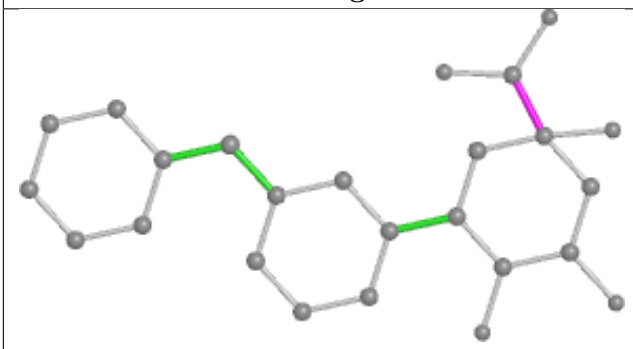
Ligand RP4 E 1951



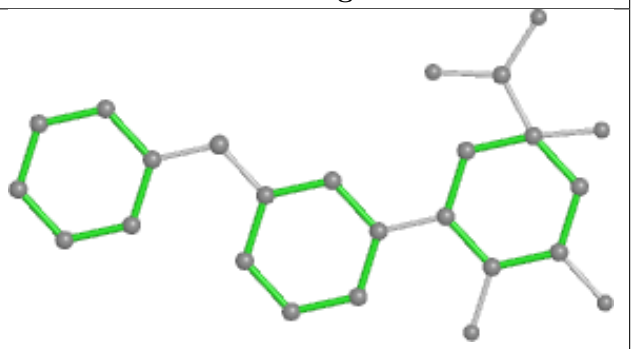
Bond lengths



Bond angles

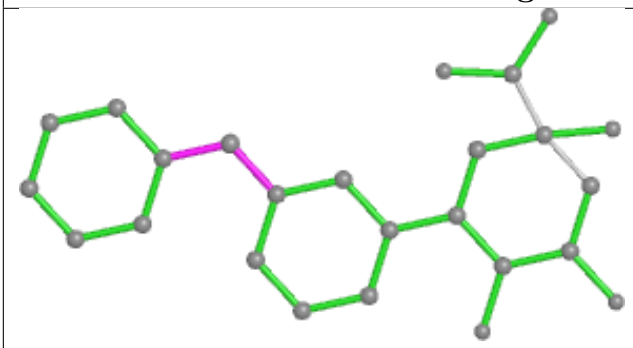


Torsions



Rings

Ligand RP4 H 2551



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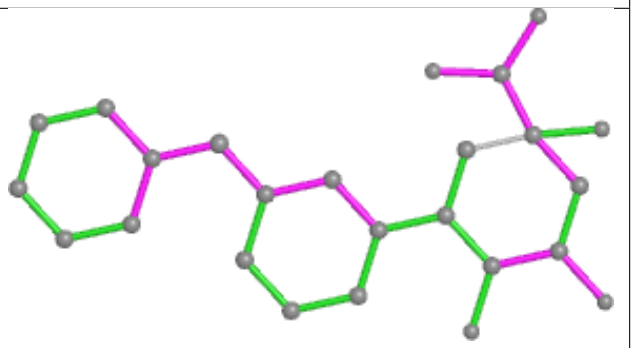

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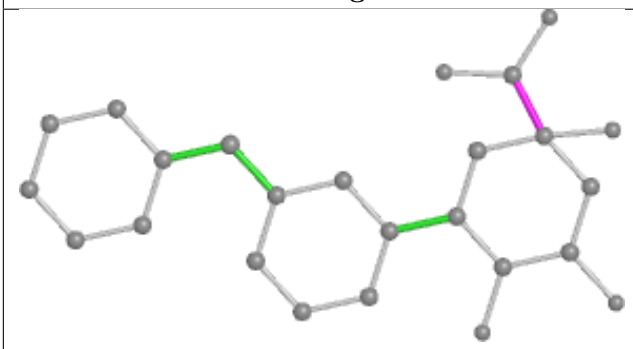

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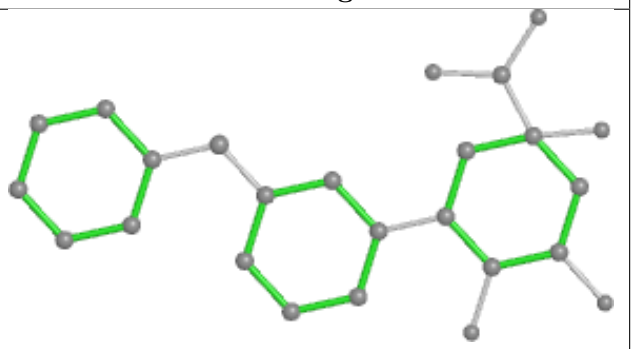
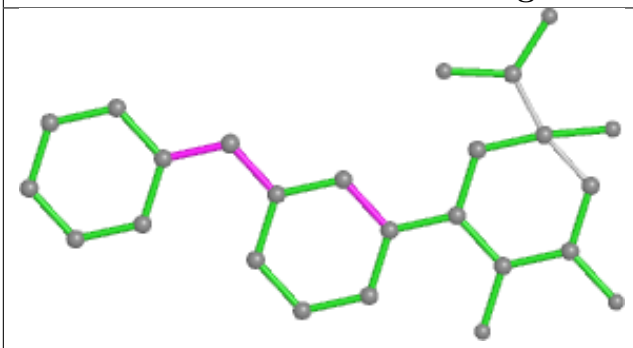


Rings

Ligand RP4 D 1751



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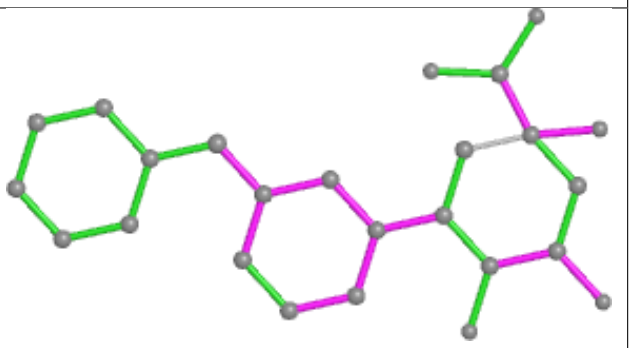

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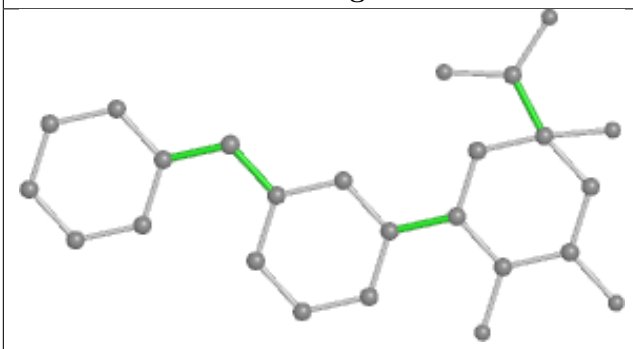

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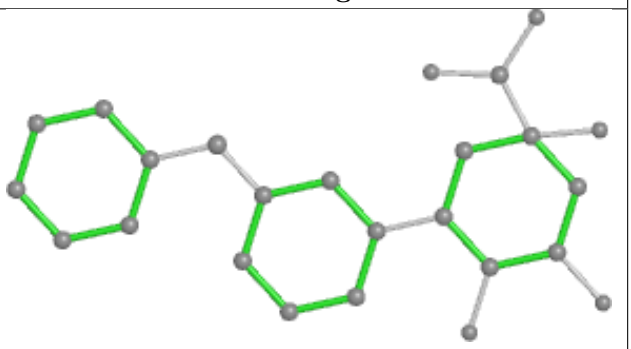
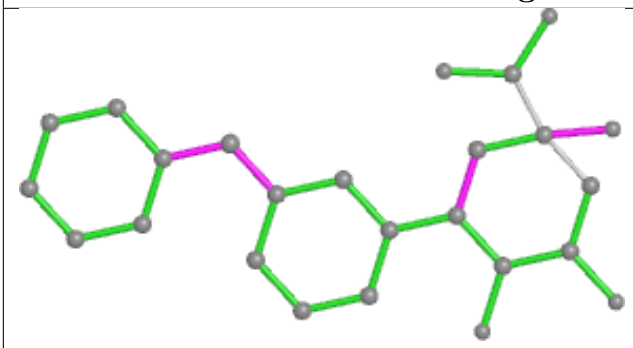
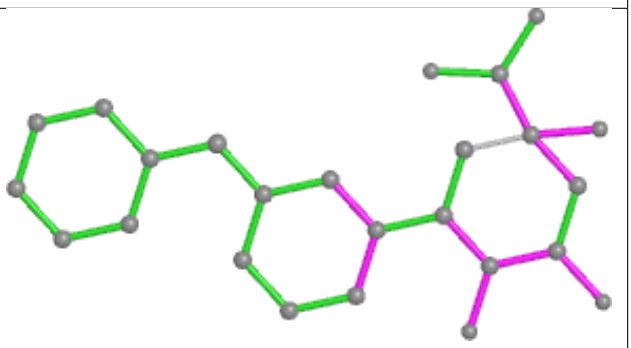


Rings

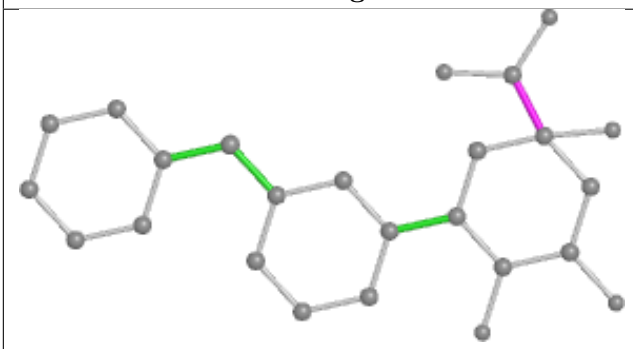
Ligand RP4 B 1351



Bond lengths



Bond angles



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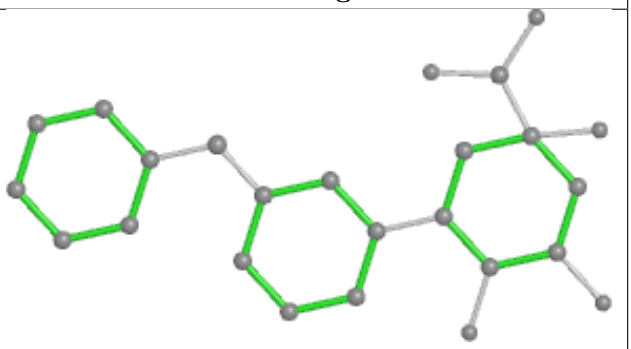
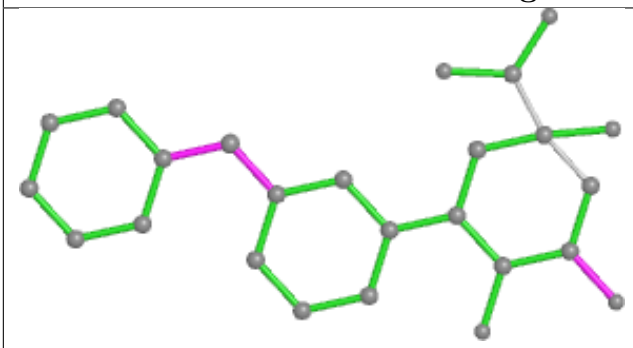
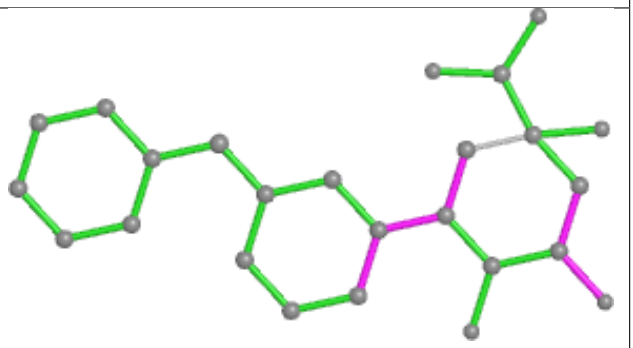


Rings

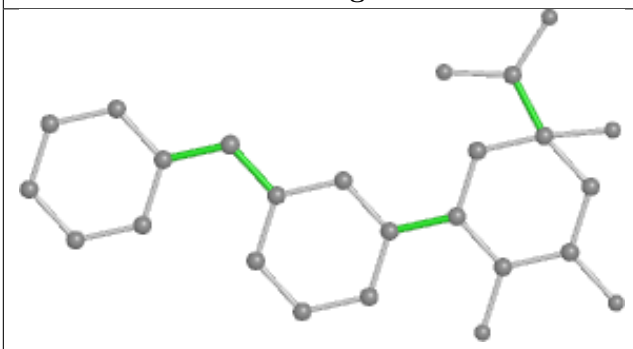
Ligand RP4 F 2151



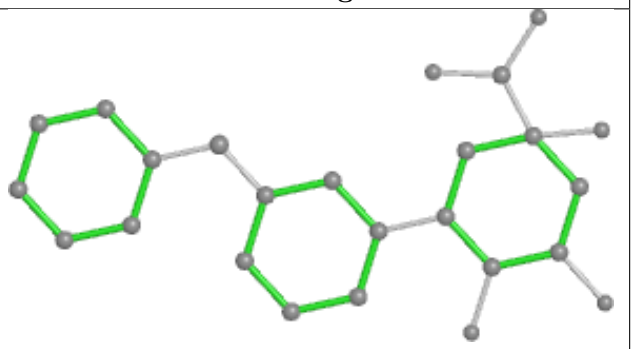
Bond lengths



Bond angles

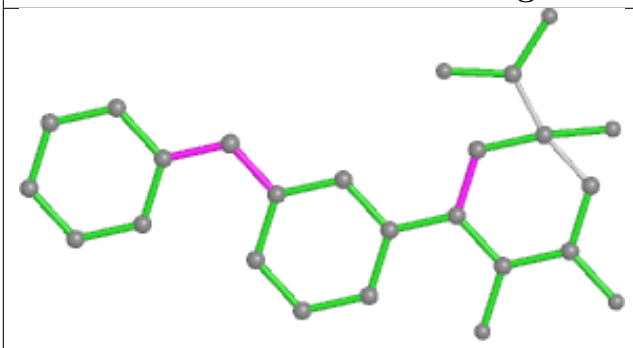


Torsions

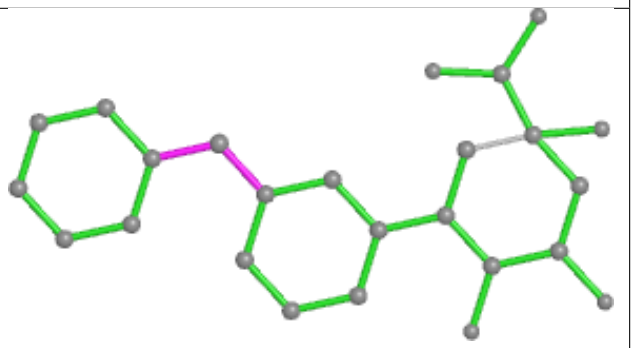


Rings

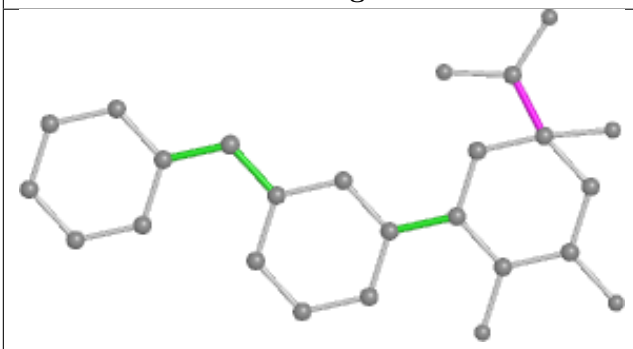
Ligand RP4 A 1151



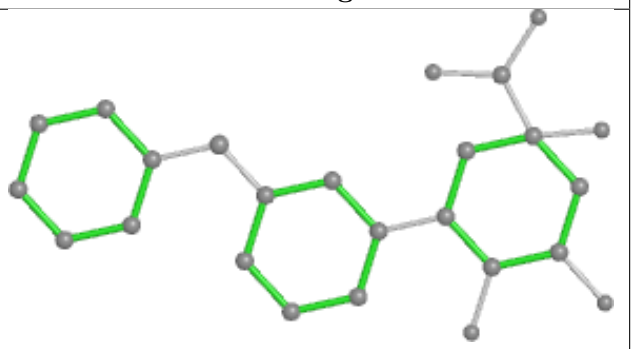
Bond lengths



Bond angles

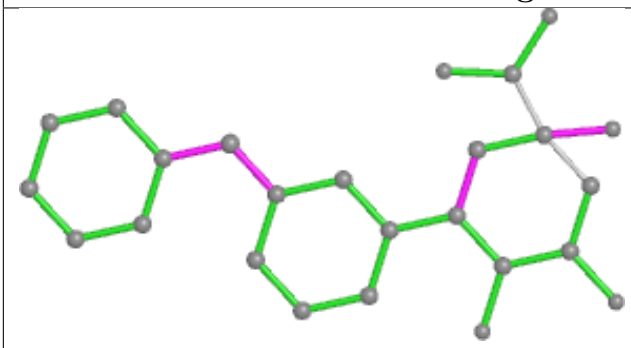


Torsions

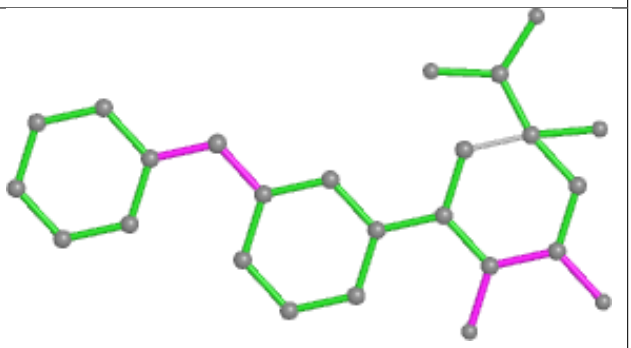


Rings

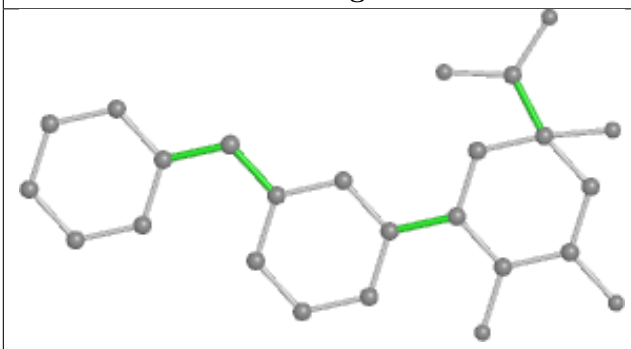
Ligand RP4 G 2351



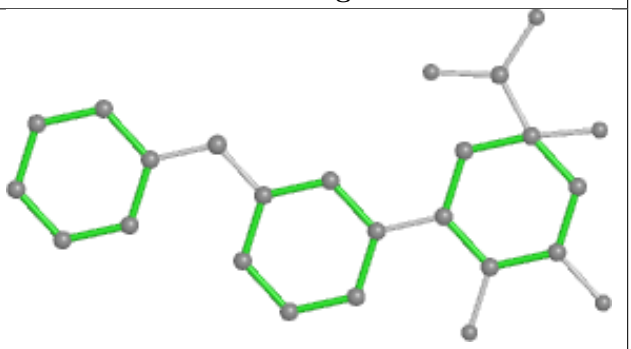
Bond lengths



Bond angles

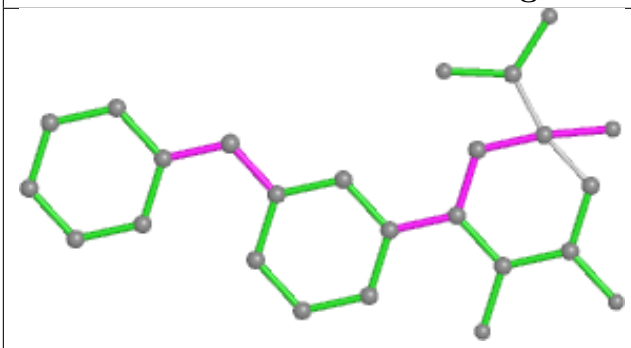


Torsions

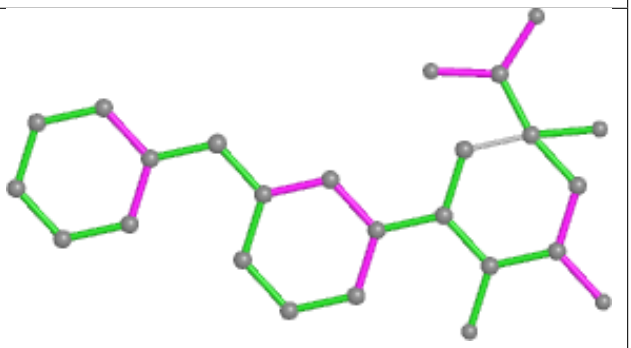


Rings

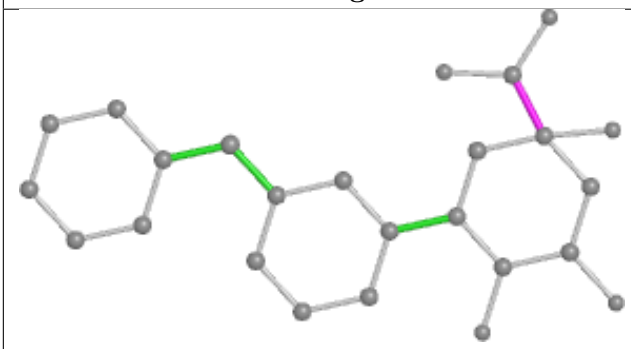
Ligand RP4 L 3351



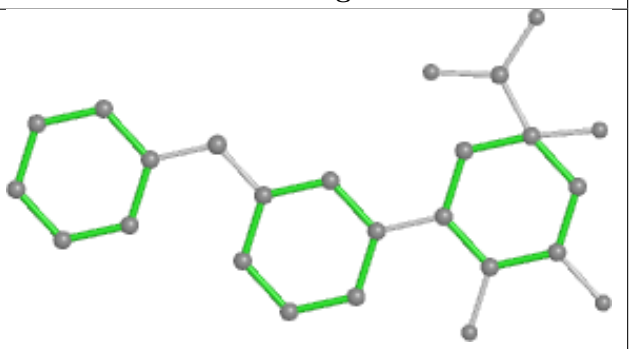
Bond lengths



Bond angles

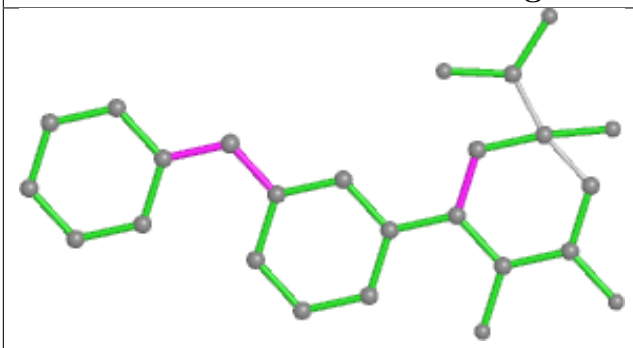


Torsions

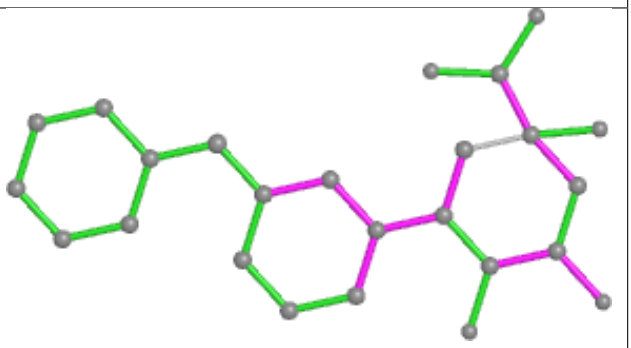


Rings

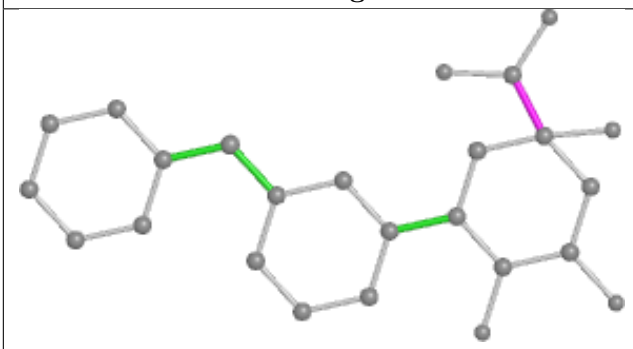
Ligand RP4 I 2751



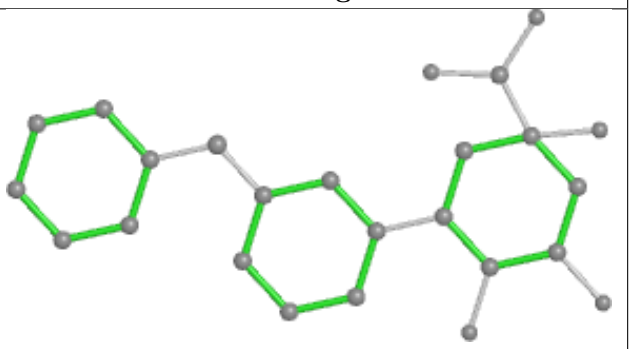
Bond lengths



Bond angles

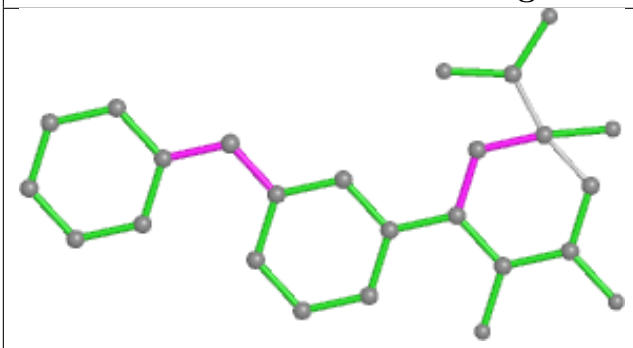


Torsions

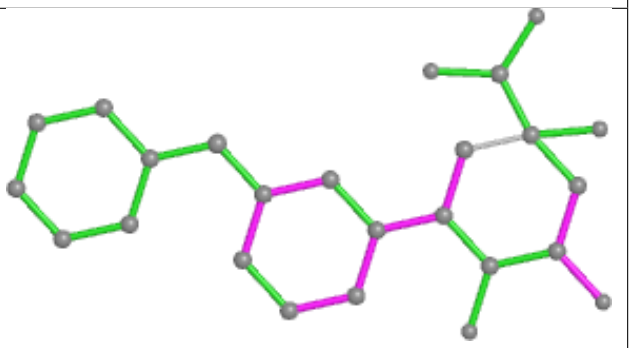


Rings

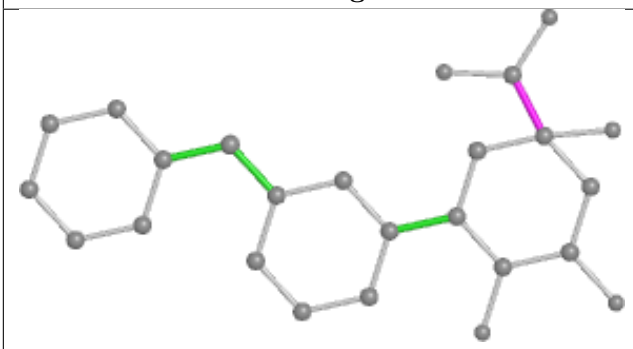
Ligand RP4 C 1551



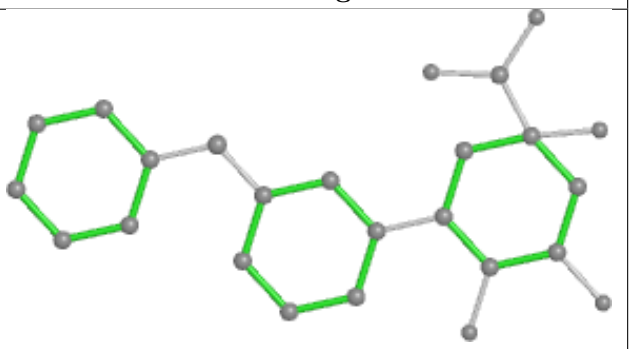
Bond lengths



Bond angles

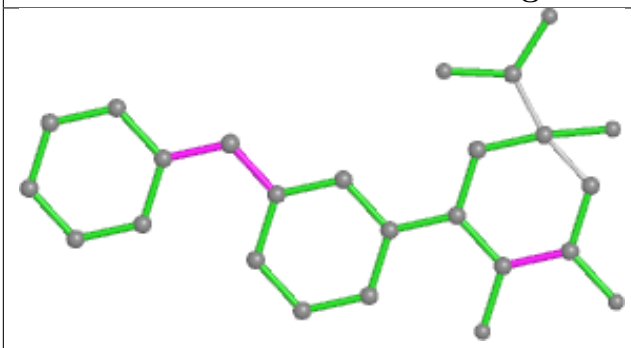


Torsions

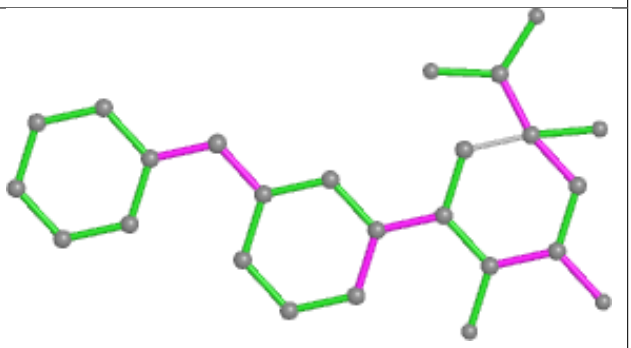


Rings

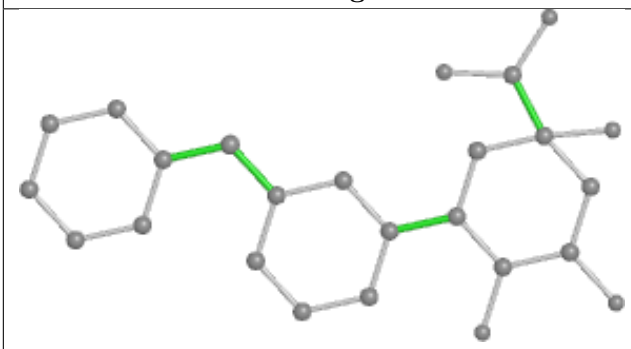
Ligand RP4 J 2951



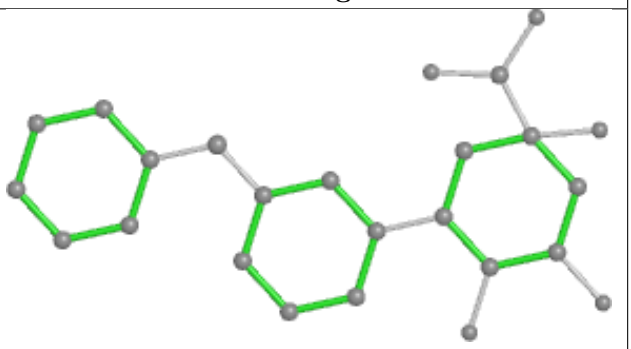
Bond lengths



Bond angles

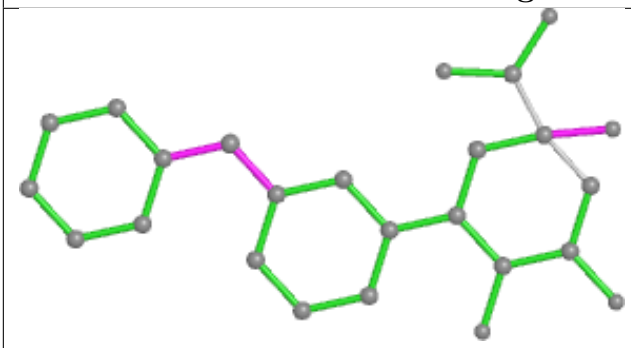


Torsions

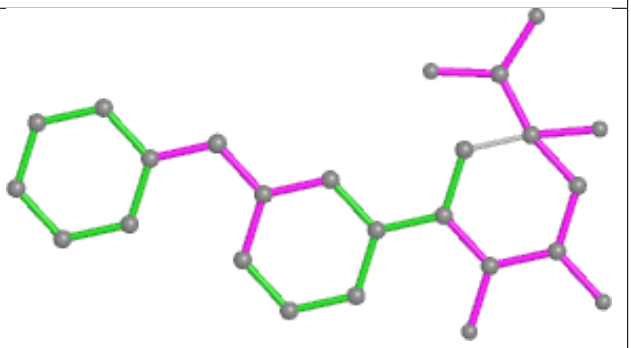


Rings

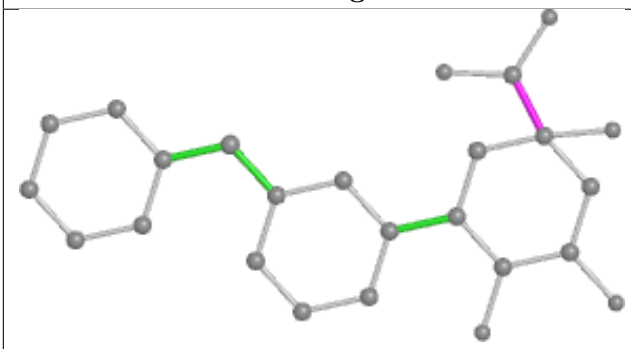
Ligand RP4 K 3151



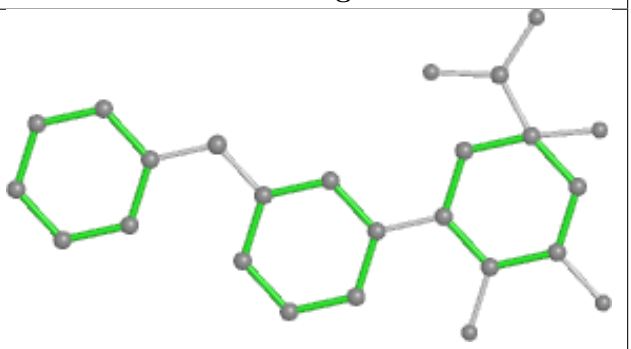
Bond lengths



Bond angles



Torsions



Rings

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	149/157 (94%)	0.31	1 (0%) 87 92	7, 20, 42, 51	0
1	B	149/157 (94%)	0.42	0 100 100	11, 21, 39, 48	0
1	C	149/157 (94%)	0.33	1 (0%) 87 92	9, 24, 42, 56	0
1	D	149/157 (94%)	0.41	0 100 100	8, 21, 43, 54	0
1	E	149/157 (94%)	0.41	0 100 100	8, 20, 40, 48	0
1	F	149/157 (94%)	0.48	2 (1%) 77 83	11, 25, 44, 52	0
1	G	149/157 (94%)	0.44	0 100 100	7, 19, 38, 47	0
1	H	149/157 (94%)	0.41	4 (2%) 54 63	12, 25, 42, 55	0
1	I	149/157 (94%)	0.37	1 (0%) 87 92	9, 21, 41, 49	0
1	J	149/157 (94%)	0.41	2 (1%) 77 83	10, 25, 43, 48	0
1	K	149/157 (94%)	0.34	1 (0%) 87 92	8, 22, 43, 51	0
1	L	149/157 (94%)	0.36	0 100 100	11, 20, 42, 56	0
All	All	1788/1884 (94%)	0.39	12 (0%) 87 92	7, 22, 43, 56	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	1802[A]	ARG	3.8
1	I	1605	ALA	3.6
1	H	1406	ASN	2.6
1	H	1404	LEU	2.6
1	A	23	ARG	2.6

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

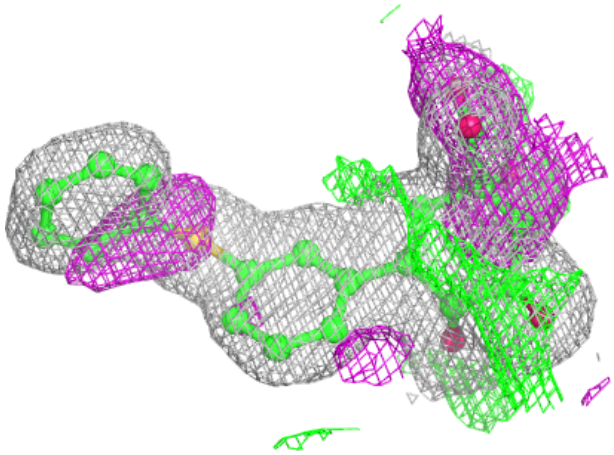
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

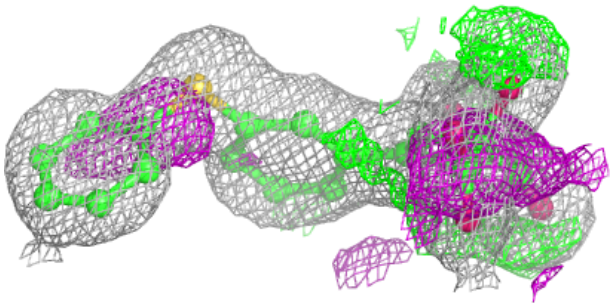
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	F	2153	6/6	0.75	0.33	46,49,49,50	0
3	GOL	D	1753	6/6	0.83	0.27	27,32,33,34	0
3	GOL	L	3352	6/6	0.85	0.19	33,38,41,42	0
3	GOL	H	2552	6/6	0.88	0.25	41,44,49,53	0
2	RP4	G	2351	25/25	0.88	0.17	14,30,33,35	0
2	RP4	I	2751	25/25	0.89	0.17	24,32,35,38	0
3	GOL	J	2954	6/6	0.89	0.26	40,43,47,49	0
3	GOL	A	1152	6/6	0.89	0.26	31,39,42,45	0
3	GOL	K	3152	6/6	0.90	0.25	39,44,45,47	0
2	RP4	E	1951	25/25	0.90	0.17	16,29,38,39	0
2	RP4	J	2951	25/25	0.91	0.17	16,27,37,38	0
2	RP4	D	1751	25/25	0.91	0.15	21,26,28,30	0
3	GOL	G	2353	6/6	0.92	0.12	10,33,34,36	0
3	GOL	K	3153	6/6	0.92	0.20	29,33,36,37	0
3	GOL	J	2955	6/6	0.92	0.26	44,45,46,47	0
2	RP4	B	1351	25/25	0.93	0.16	16,35,39,39	0
5	TRS	B	1353	8/8	0.93	0.12	13,15,18,18	0
3	GOL	E	1952	6/6	0.94	0.14	20,31,35,35	0
2	RP4	C	1551	25/25	0.94	0.14	18,29,32,33	0
2	RP4	F	2151	25/25	0.94	0.13	21,29,32,33	0
2	RP4	A	1151	25/25	0.94	0.15	14,38,45,46	0
4	PO4	J	2952	5/5	0.94	0.18	46,50,52,55	0
2	RP4	H	2551	25/25	0.94	0.14	15,29,37,38	0
5	TRS	D	1752	8/8	0.94	0.12	11,13,15,15	0
4	PO4	B	1352	5/5	0.95	0.11	60,62,64,64	0
2	RP4	K	3151	25/25	0.95	0.13	20,28,34,34	0
3	GOL	B	1354	6/6	0.95	0.20	34,38,39,40	0
2	RP4	L	3351	25/25	0.95	0.13	5,30,35,37	0
4	PO4	F	2152	5/5	0.96	0.15	48,48,53,53	0
5	TRS	I	2752	8/8	0.97	0.13	4,6,9,13	0
4	PO4	G	2352	5/5	0.98	0.14	41,41,42,46	0
5	TRS	J	2953	8/8	0.98	0.11	6,17,19,21	0

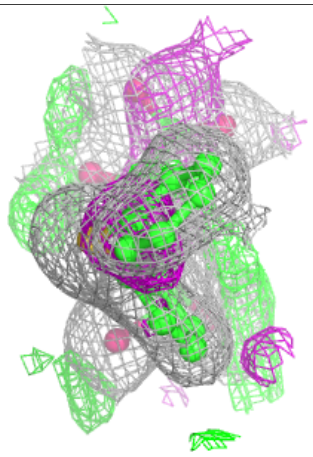
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RP4 G 2351:

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

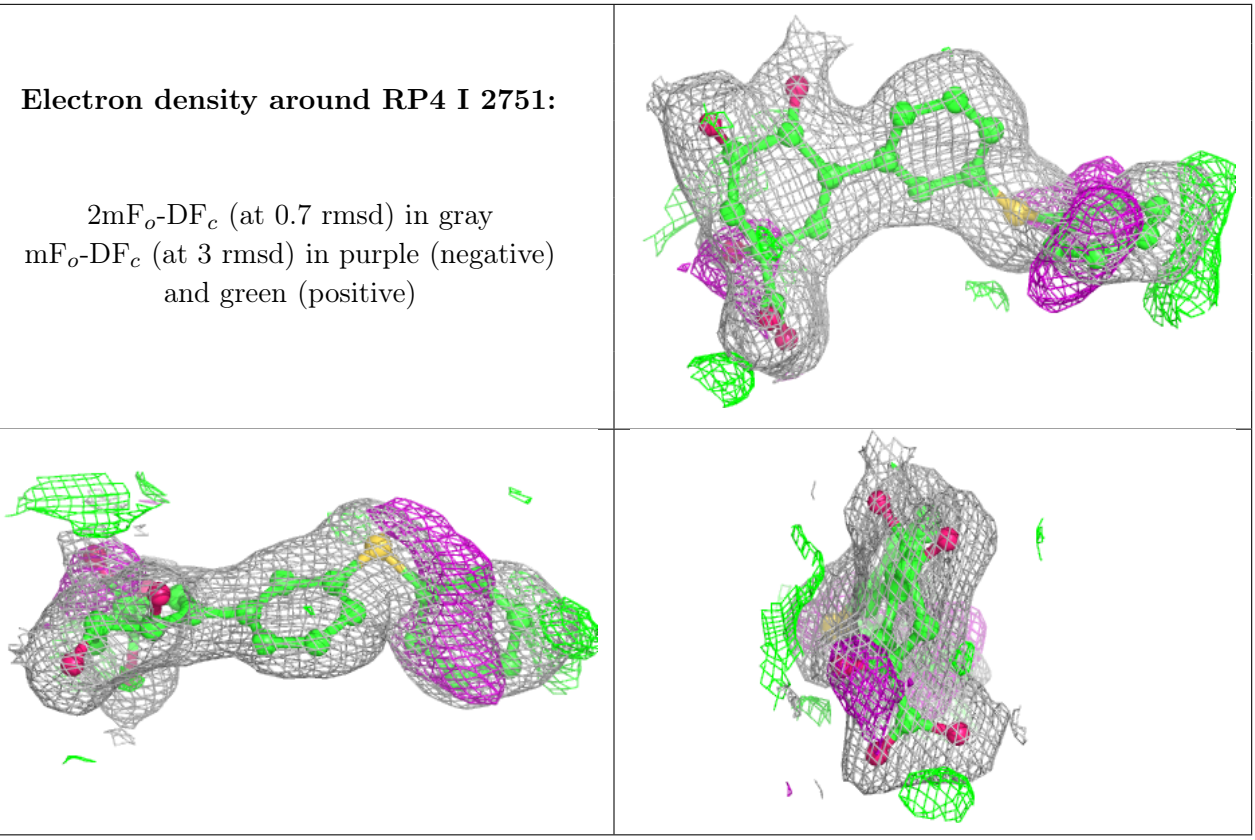






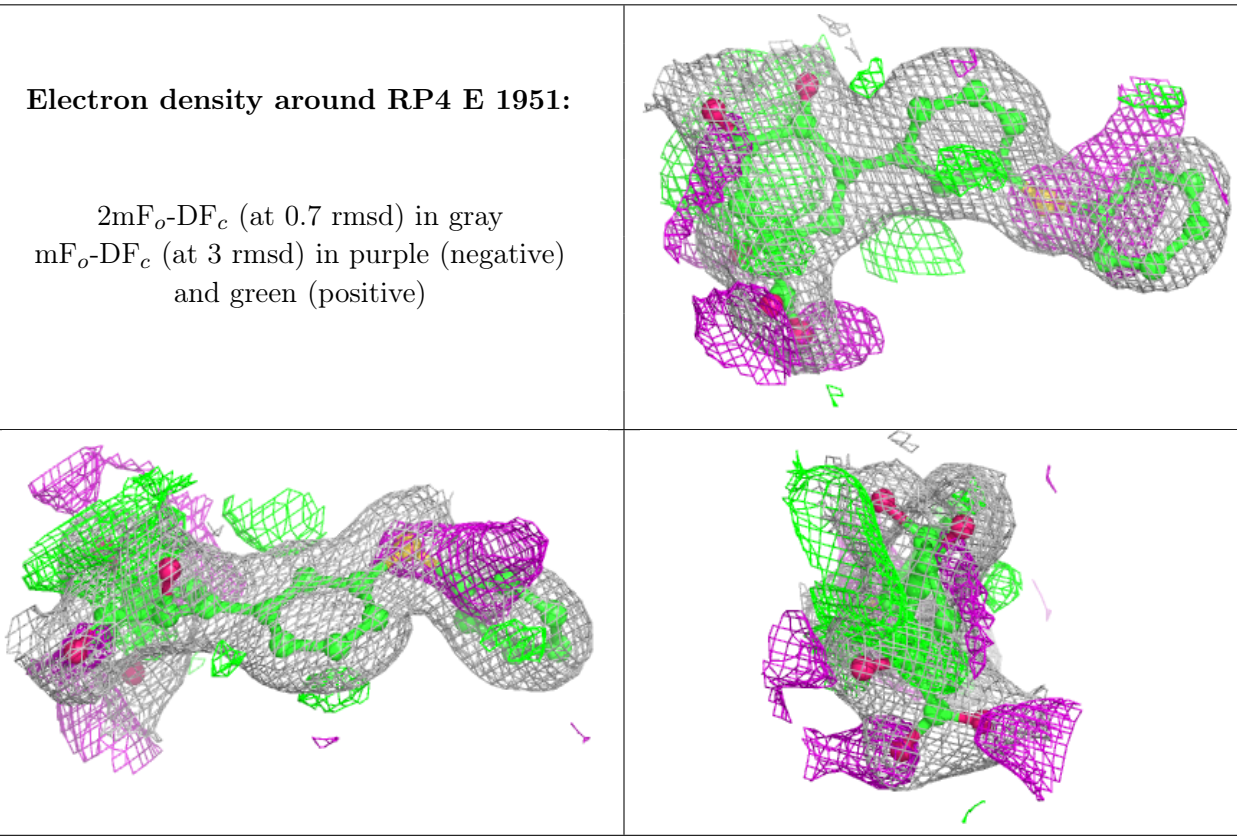
Electron density around RP4 I 2751:

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



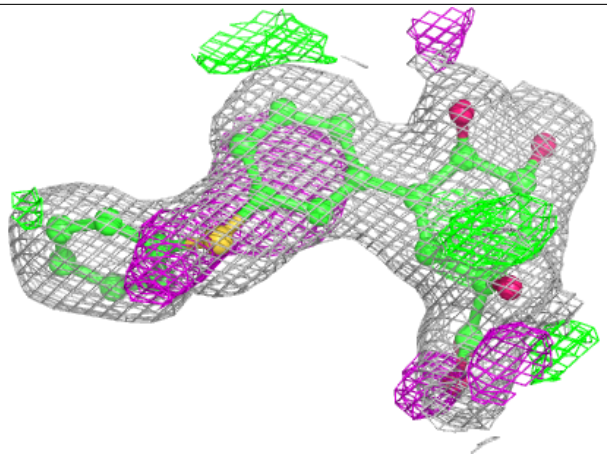
Electron density around RP4 E 1951:

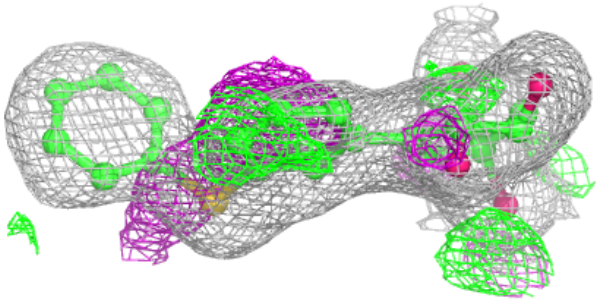
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

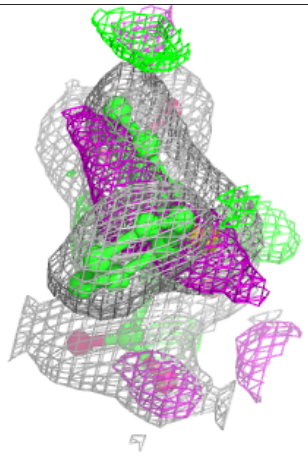


Electron density around RP4 J 2951:

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

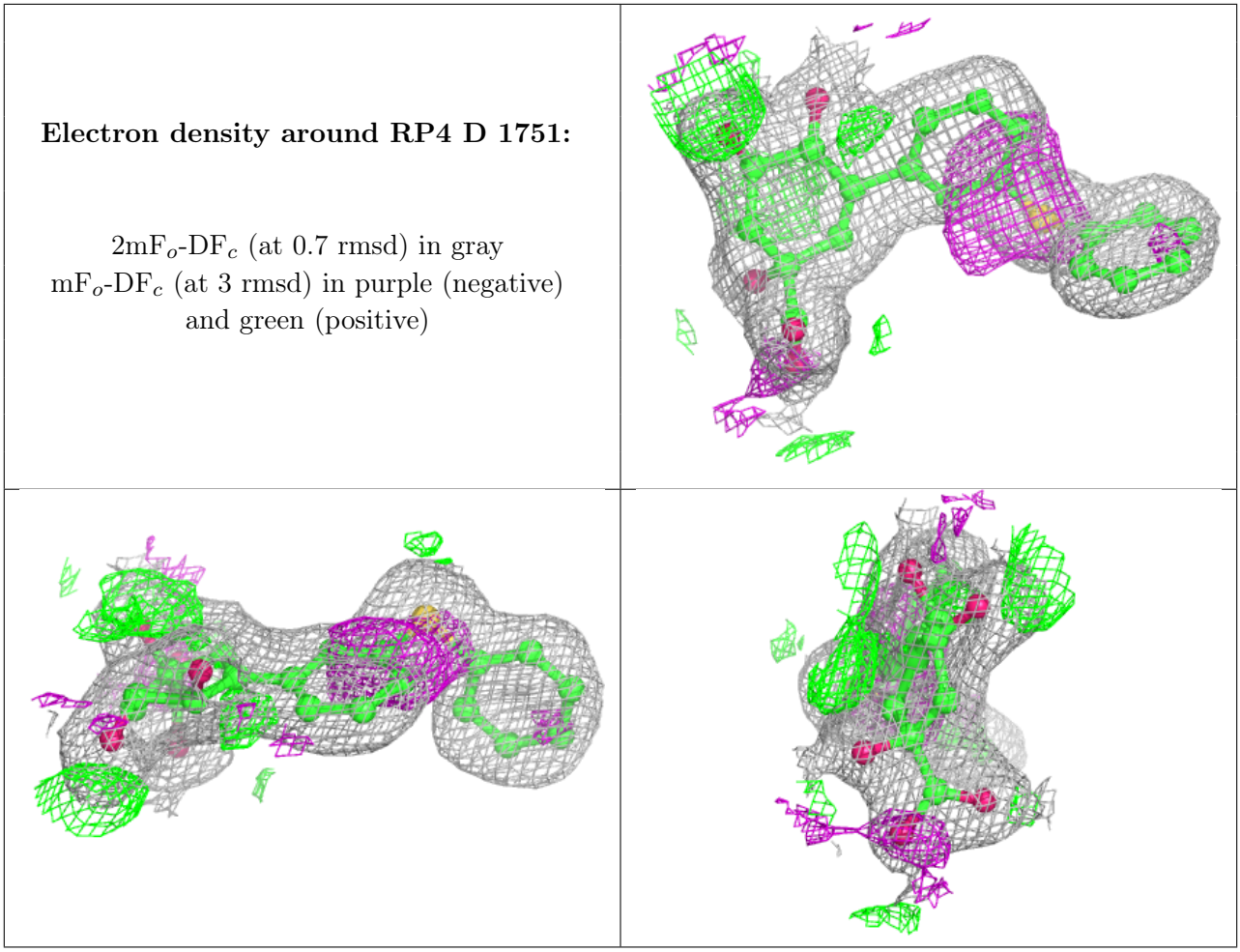






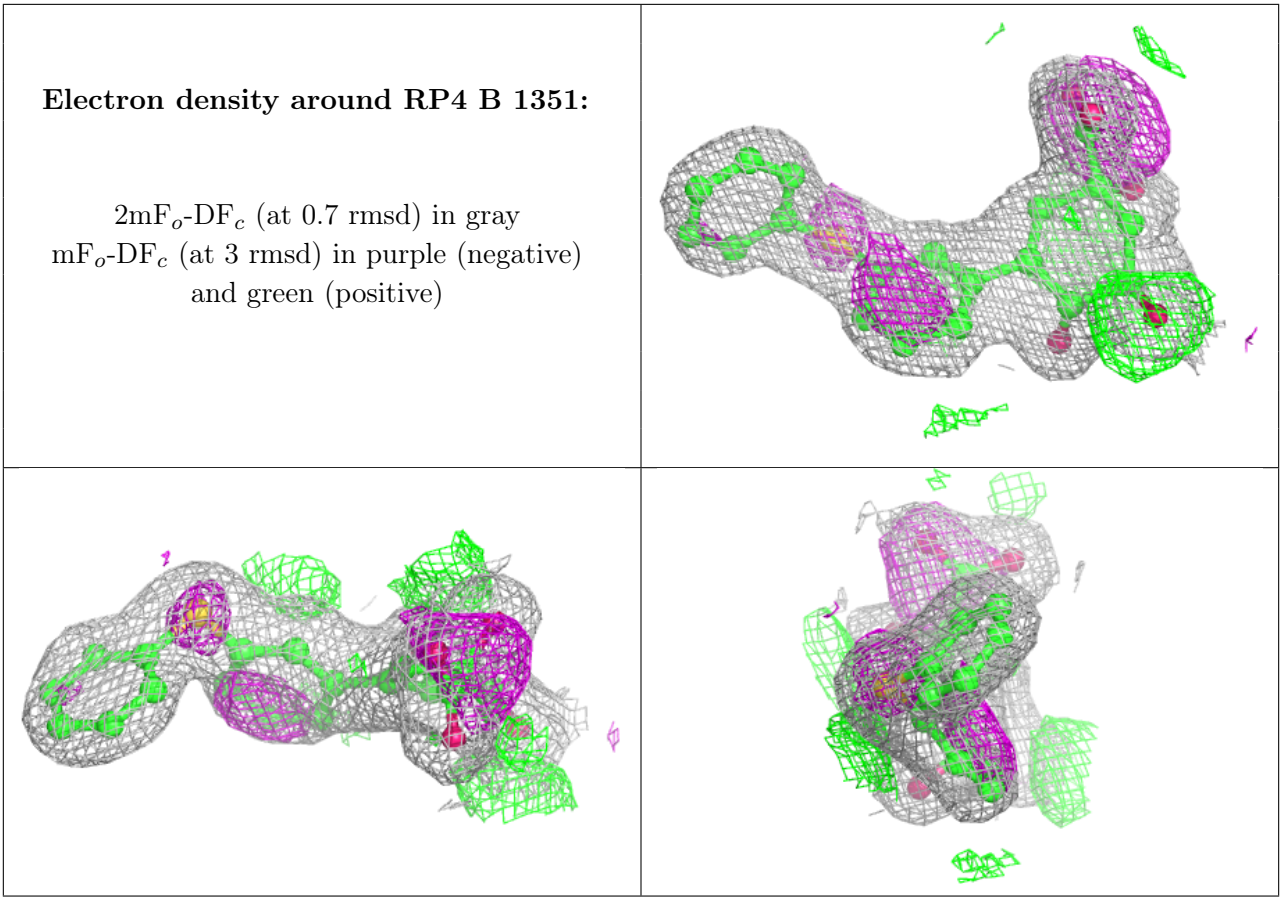
Electron density around RP4 D 1751:

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



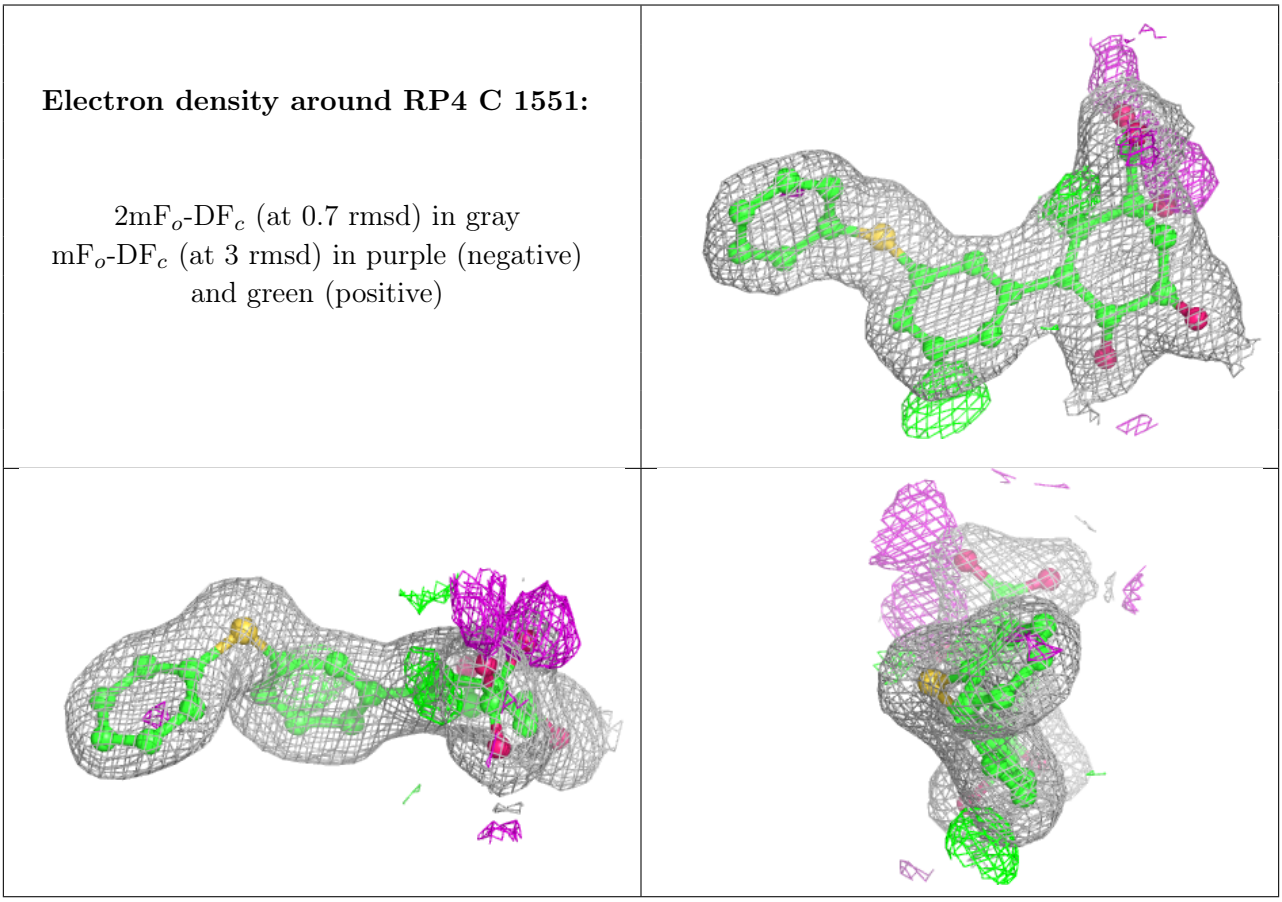
Electron density around RP4 B 1351:

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



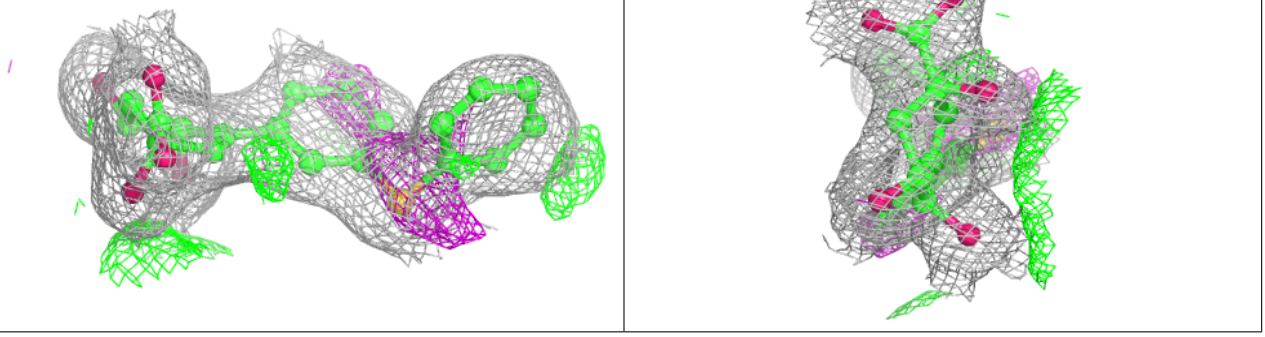
Electron density around RP4 C 1551:

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



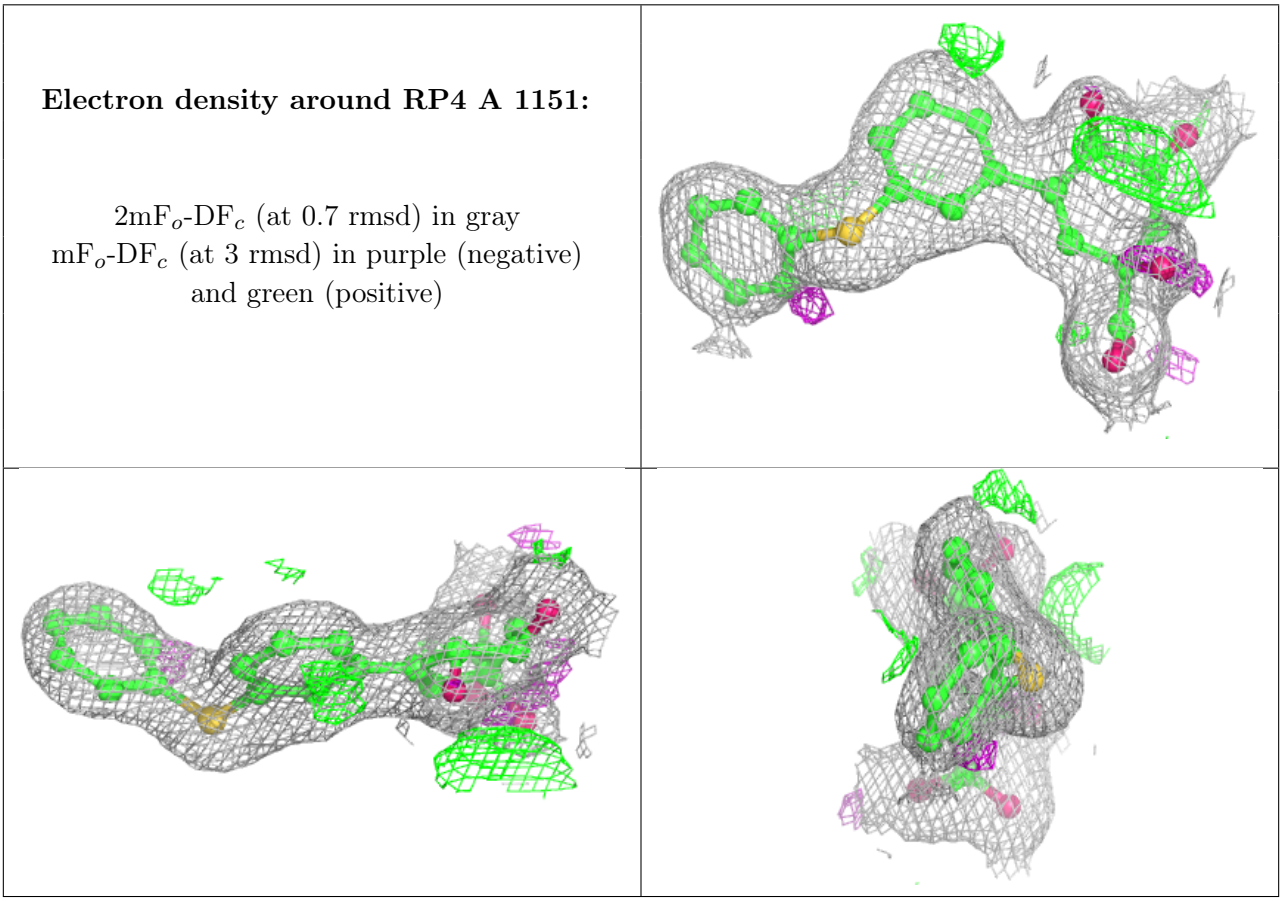
Electron density around RP4 F 2151:

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



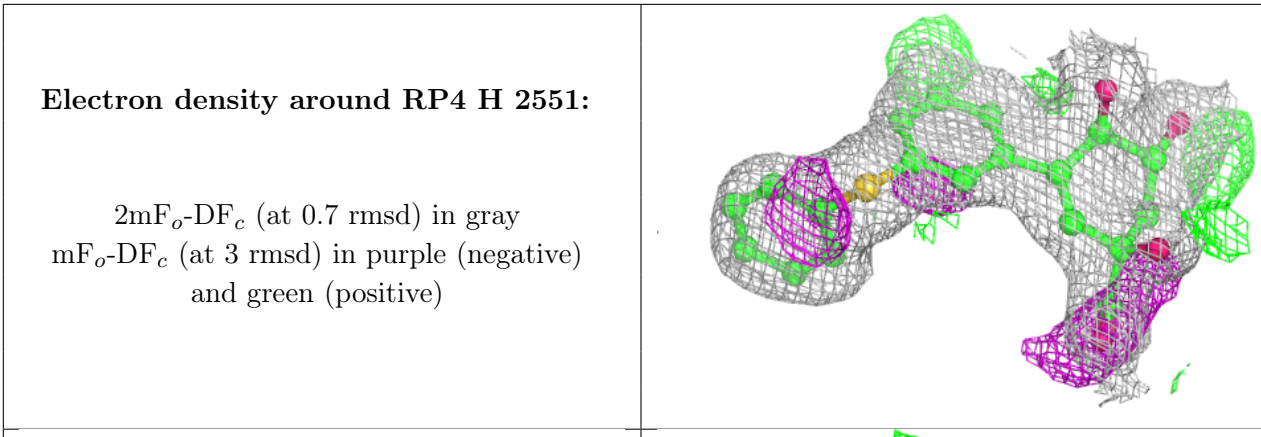
Electron density around RP4 A 1151:

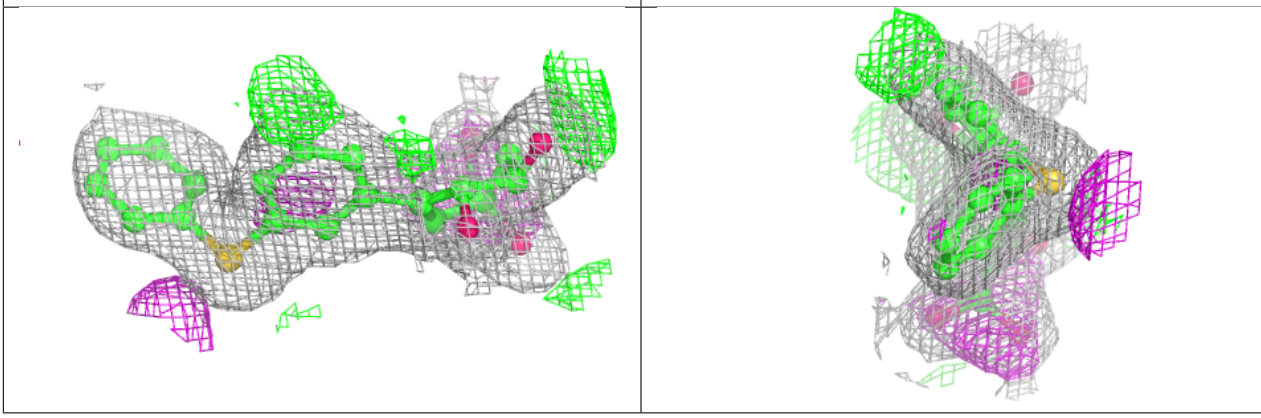
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around RP4 H 2551:

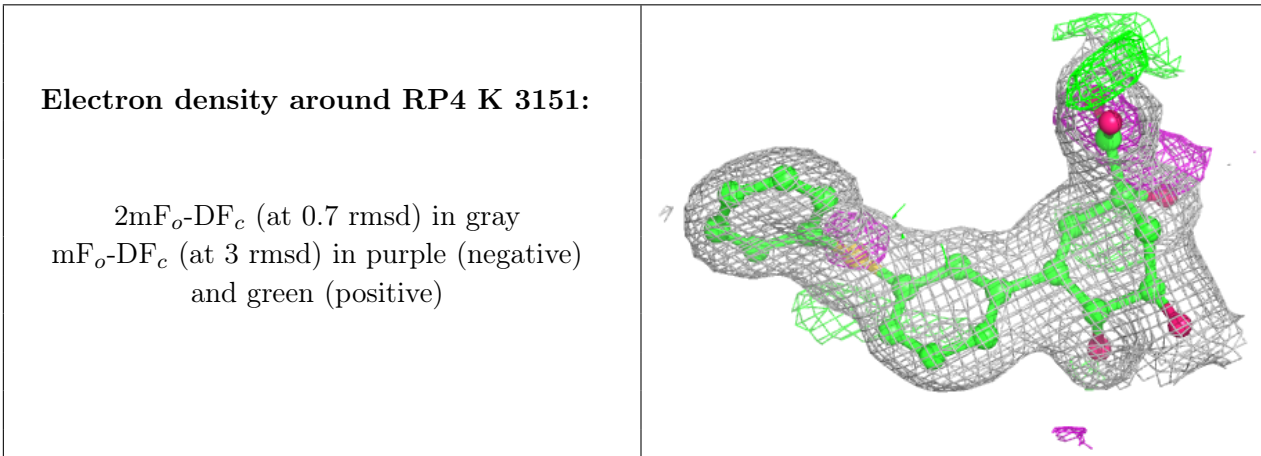
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

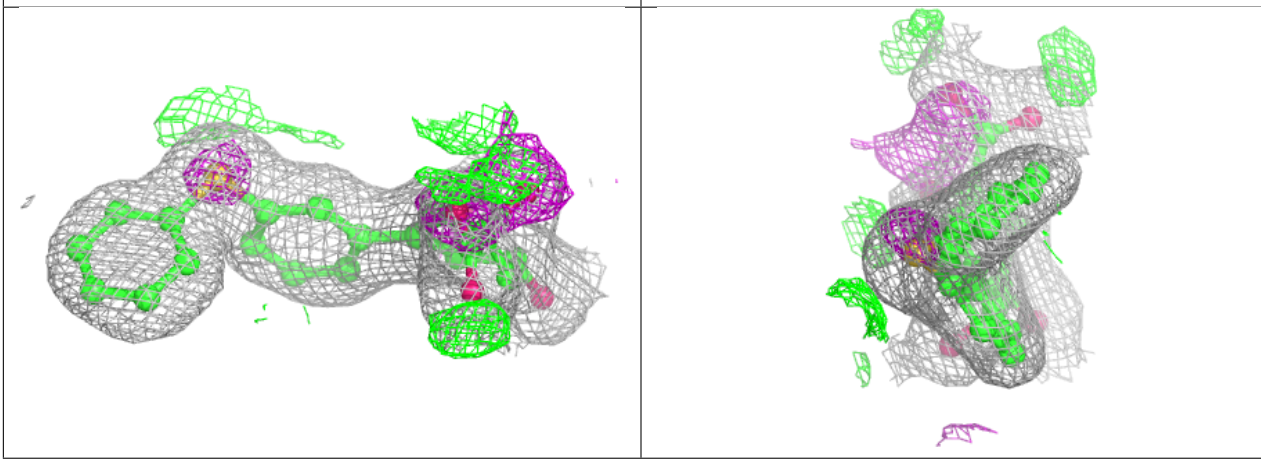




Electron density around RP4 K 3151:

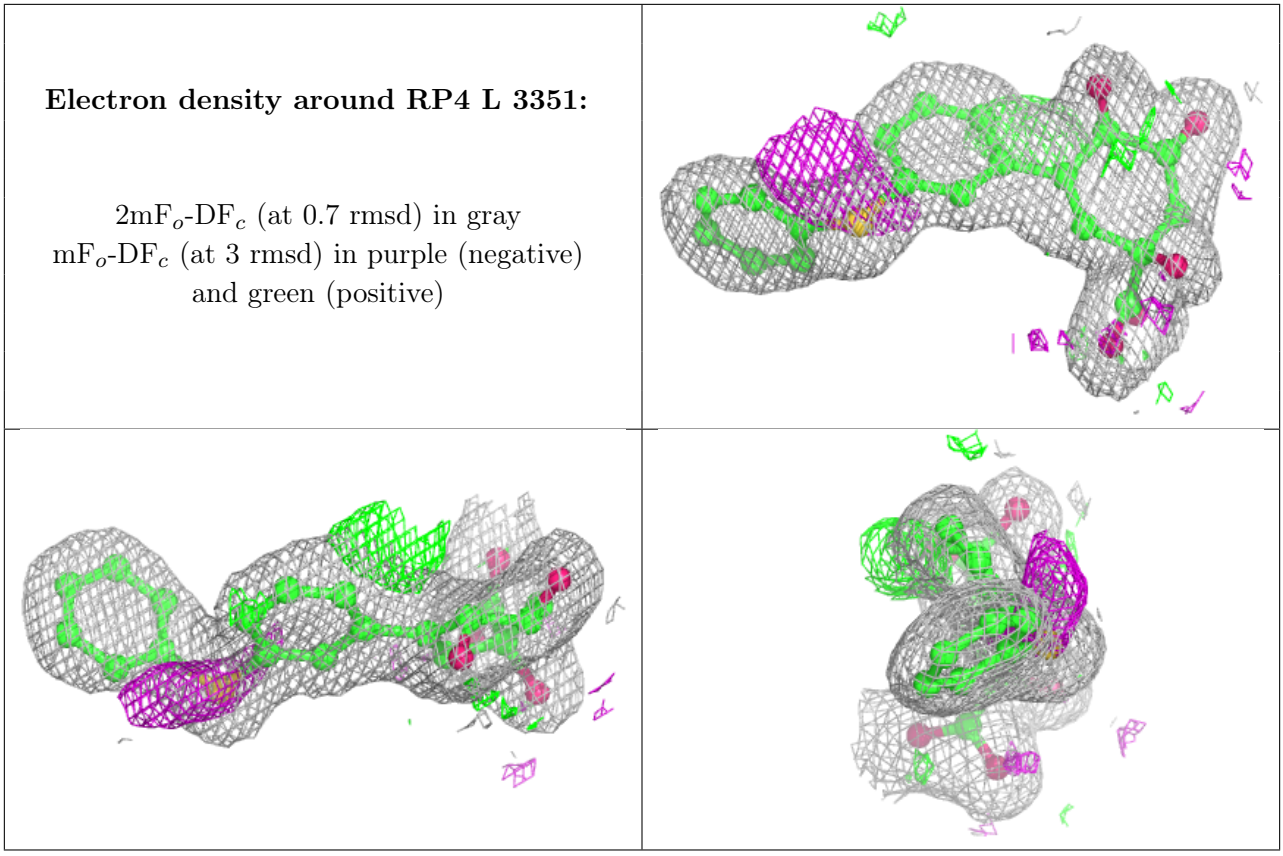
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around RP4 L 3351:

$2mF_o$-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.