Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 06:20 pm GMT

PDB ID	:	6HM2
Title	:	Structure in P1 form of the PBP AgtB in complex with agropinic acid from A.tumefacien R10
Authors	:	Morera, S.; Marty, L.; Vigouroux, A.
Deposited on	:	2018-09-12
Resolution	:	1.74 Å(reported)

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

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

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

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

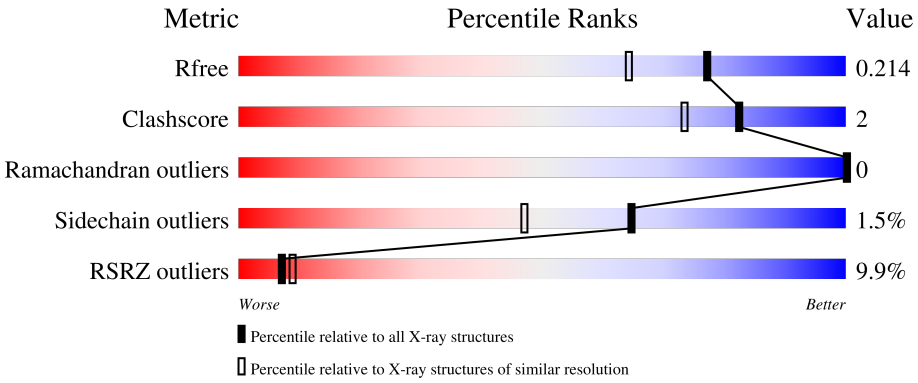
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	341	% 84% 8% 7%
1	B	341	% 83% 10% 7%
1	C	341	86% 5% • 8%
1	D	341	87% 5% 8%
1	E	341	44% 87% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13234 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 Agropine permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2426	1556	400	462	8			
1	B	317	Total	C	N	O	S	0	0	0
			2435	1561	402	464	8			
1	C	314	Total	C	N	O	S	0	0	0
			2410	1547	396	459	8			
1	D	314	Total	C	N	O	S	0	0	0
			2410	1547	396	459	8			
1	E	312	Total	C	N	O	S	0	0	0
			2394	1537	394	457	6			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP W8FRA6
A	9	GLY	-	expression tag	UNP W8FRA6
A	10	SER	-	expression tag	UNP W8FRA6
A	11	SER	-	expression tag	UNP W8FRA6
A	12	HIS	-	expression tag	UNP W8FRA6
A	13	HIS	-	expression tag	UNP W8FRA6
A	14	HIS	-	expression tag	UNP W8FRA6
A	15	HIS	-	expression tag	UNP W8FRA6
A	16	HIS	-	expression tag	UNP W8FRA6
A	17	HIS	-	expression tag	UNP W8FRA6
A	18	SER	-	expression tag	UNP W8FRA6
A	19	SER	-	expression tag	UNP W8FRA6
A	20	GLY	-	expression tag	UNP W8FRA6
A	21	LEU	-	expression tag	UNP W8FRA6
A	22	VAL	-	expression tag	UNP W8FRA6
A	23	PRO	-	expression tag	UNP W8FRA6
A	24	ARG	-	expression tag	UNP W8FRA6
A	25	GLY	-	expression tag	UNP W8FRA6
A	26	SER	-	expression tag	UNP W8FRA6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	HIS	-	expression tag	UNP W8FRA6
A	28	MET	-	expression tag	UNP W8FRA6
A	29	MET	-	expression tag	UNP W8FRA6
A	343	HIS	-	expression tag	UNP W8FRA6
A	344	HIS	-	expression tag	UNP W8FRA6
A	345	HIS	-	expression tag	UNP W8FRA6
A	346	HIS	-	expression tag	UNP W8FRA6
A	347	HIS	-	expression tag	UNP W8FRA6
A	348	HIS	-	expression tag	UNP W8FRA6
B	8	MET	-	initiating methionine	UNP W8FRA6
B	9	GLY	-	expression tag	UNP W8FRA6
B	10	SER	-	expression tag	UNP W8FRA6
B	11	SER	-	expression tag	UNP W8FRA6
B	12	HIS	-	expression tag	UNP W8FRA6
B	13	HIS	-	expression tag	UNP W8FRA6
B	14	HIS	-	expression tag	UNP W8FRA6
B	15	HIS	-	expression tag	UNP W8FRA6
B	16	HIS	-	expression tag	UNP W8FRA6
B	17	HIS	-	expression tag	UNP W8FRA6
B	18	SER	-	expression tag	UNP W8FRA6
B	19	SER	-	expression tag	UNP W8FRA6
B	20	GLY	-	expression tag	UNP W8FRA6
B	21	LEU	-	expression tag	UNP W8FRA6
B	22	VAL	-	expression tag	UNP W8FRA6
B	23	PRO	-	expression tag	UNP W8FRA6
B	24	ARG	-	expression tag	UNP W8FRA6
B	25	GLY	-	expression tag	UNP W8FRA6
B	26	SER	-	expression tag	UNP W8FRA6
B	27	HIS	-	expression tag	UNP W8FRA6
B	28	MET	-	expression tag	UNP W8FRA6
B	29	MET	-	expression tag	UNP W8FRA6
B	343	HIS	-	expression tag	UNP W8FRA6
B	344	HIS	-	expression tag	UNP W8FRA6
B	345	HIS	-	expression tag	UNP W8FRA6
B	346	HIS	-	expression tag	UNP W8FRA6
B	347	HIS	-	expression tag	UNP W8FRA6
B	348	HIS	-	expression tag	UNP W8FRA6
C	8	MET	-	initiating methionine	UNP W8FRA6
C	9	GLY	-	expression tag	UNP W8FRA6
C	10	SER	-	expression tag	UNP W8FRA6
C	11	SER	-	expression tag	UNP W8FRA6
C	12	HIS	-	expression tag	UNP W8FRA6

Continued on next page...

Continued from previous page...

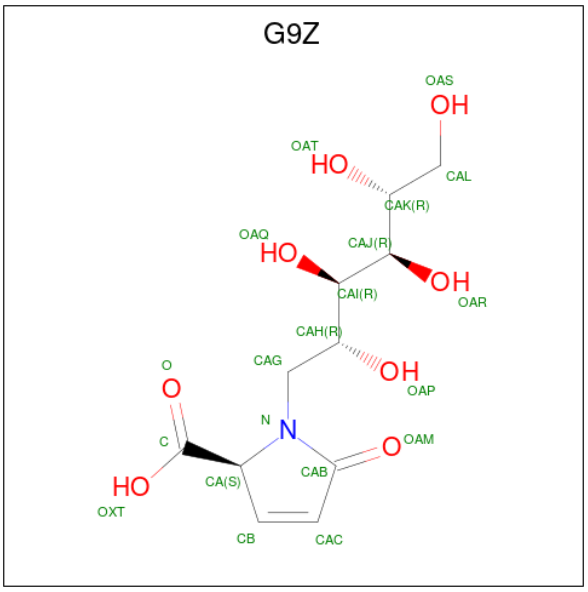
Chain	Residue	Modelled	Actual	Comment	Reference
C	13	HIS	-	expression tag	UNP W8FRA6
C	14	HIS	-	expression tag	UNP W8FRA6
C	15	HIS	-	expression tag	UNP W8FRA6
C	16	HIS	-	expression tag	UNP W8FRA6
C	17	HIS	-	expression tag	UNP W8FRA6
C	18	SER	-	expression tag	UNP W8FRA6
C	19	SER	-	expression tag	UNP W8FRA6
C	20	GLY	-	expression tag	UNP W8FRA6
C	21	LEU	-	expression tag	UNP W8FRA6
C	22	VAL	-	expression tag	UNP W8FRA6
C	23	PRO	-	expression tag	UNP W8FRA6
C	24	ARG	-	expression tag	UNP W8FRA6
C	25	GLY	-	expression tag	UNP W8FRA6
C	26	SER	-	expression tag	UNP W8FRA6
C	27	HIS	-	expression tag	UNP W8FRA6
C	28	MET	-	expression tag	UNP W8FRA6
C	29	MET	-	expression tag	UNP W8FRA6
C	343	HIS	-	expression tag	UNP W8FRA6
C	344	HIS	-	expression tag	UNP W8FRA6
C	345	HIS	-	expression tag	UNP W8FRA6
C	346	HIS	-	expression tag	UNP W8FRA6
C	347	HIS	-	expression tag	UNP W8FRA6
C	348	HIS	-	expression tag	UNP W8FRA6
D	8	MET	-	initiating methionine	UNP W8FRA6
D	9	GLY	-	expression tag	UNP W8FRA6
D	10	SER	-	expression tag	UNP W8FRA6
D	11	SER	-	expression tag	UNP W8FRA6
D	12	HIS	-	expression tag	UNP W8FRA6
D	13	HIS	-	expression tag	UNP W8FRA6
D	14	HIS	-	expression tag	UNP W8FRA6
D	15	HIS	-	expression tag	UNP W8FRA6
D	16	HIS	-	expression tag	UNP W8FRA6
D	17	HIS	-	expression tag	UNP W8FRA6
D	18	SER	-	expression tag	UNP W8FRA6
D	19	SER	-	expression tag	UNP W8FRA6
D	20	GLY	-	expression tag	UNP W8FRA6
D	21	LEU	-	expression tag	UNP W8FRA6
D	22	VAL	-	expression tag	UNP W8FRA6
D	23	PRO	-	expression tag	UNP W8FRA6
D	24	ARG	-	expression tag	UNP W8FRA6
D	25	GLY	-	expression tag	UNP W8FRA6
D	26	SER	-	expression tag	UNP W8FRA6

Continued on next page...

Continued from previous page...

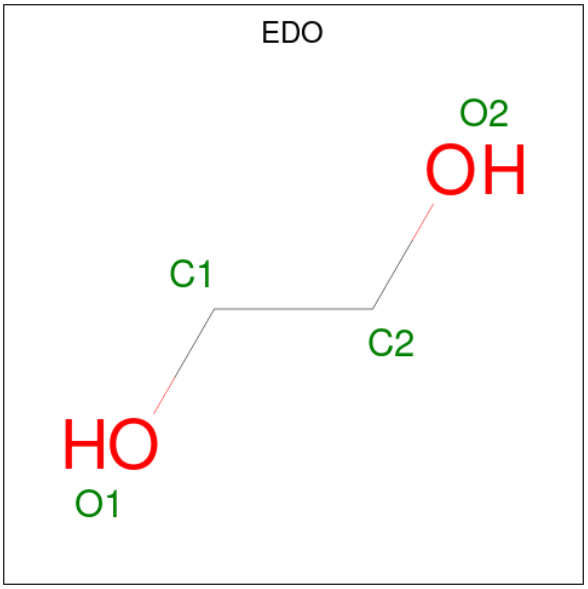
Chain	Residue	Modelled	Actual	Comment	Reference
D	27	HIS	-	expression tag	UNP W8FRA6
D	28	MET	-	expression tag	UNP W8FRA6
D	29	MET	-	expression tag	UNP W8FRA6
D	343	HIS	-	expression tag	UNP W8FRA6
D	344	HIS	-	expression tag	UNP W8FRA6
D	345	HIS	-	expression tag	UNP W8FRA6
D	346	HIS	-	expression tag	UNP W8FRA6
D	347	HIS	-	expression tag	UNP W8FRA6
D	348	HIS	-	expression tag	UNP W8FRA6
E	8	MET	-	initiating methionine	UNP W8FRA6
E	9	GLY	-	expression tag	UNP W8FRA6
E	10	SER	-	expression tag	UNP W8FRA6
E	11	SER	-	expression tag	UNP W8FRA6
E	12	HIS	-	expression tag	UNP W8FRA6
E	13	HIS	-	expression tag	UNP W8FRA6
E	14	HIS	-	expression tag	UNP W8FRA6
E	15	HIS	-	expression tag	UNP W8FRA6
E	16	HIS	-	expression tag	UNP W8FRA6
E	17	HIS	-	expression tag	UNP W8FRA6
E	18	SER	-	expression tag	UNP W8FRA6
E	19	SER	-	expression tag	UNP W8FRA6
E	20	GLY	-	expression tag	UNP W8FRA6
E	21	LEU	-	expression tag	UNP W8FRA6
E	22	VAL	-	expression tag	UNP W8FRA6
E	23	PRO	-	expression tag	UNP W8FRA6
E	24	ARG	-	expression tag	UNP W8FRA6
E	25	GLY	-	expression tag	UNP W8FRA6
E	26	SER	-	expression tag	UNP W8FRA6
E	27	HIS	-	expression tag	UNP W8FRA6
E	28	MET	-	expression tag	UNP W8FRA6
E	29	MET	-	expression tag	UNP W8FRA6
E	343	HIS	-	expression tag	UNP W8FRA6
E	344	HIS	-	expression tag	UNP W8FRA6
E	345	HIS	-	expression tag	UNP W8FRA6
E	346	HIS	-	expression tag	UNP W8FRA6
E	347	HIS	-	expression tag	UNP W8FRA6
E	348	HIS	-	expression tag	UNP W8FRA6

- Molecule 2 is agropinic acid (three-letter code: G9Z) (formula: $C_{11}H_{17}NO_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 20 11 1 8	0	0
2	B	1	Total C N O 20 11 1 8	0	0
2	C	1	Total C N O 20 11 1 8	0	0
2	D	1	Total C N O 20 11 1 8	0	0
2	E	1	Total C N O 20 11 1 8	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

- Molecule 5 is water.

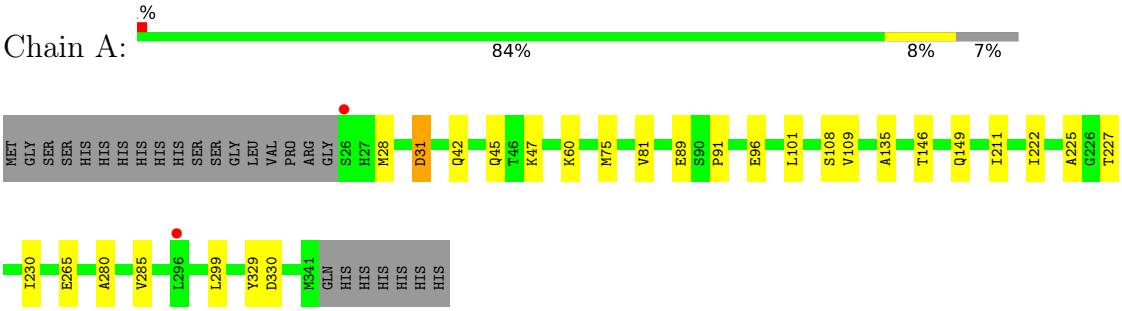
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	263	Total O 263 263	0	0
5	B	250	Total O 250 250	0	0
5	C	229	Total O 229 229	0	0
5	D	256	Total O 256 256	0	0
5	E	21	Total O 21 21	0	0

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.

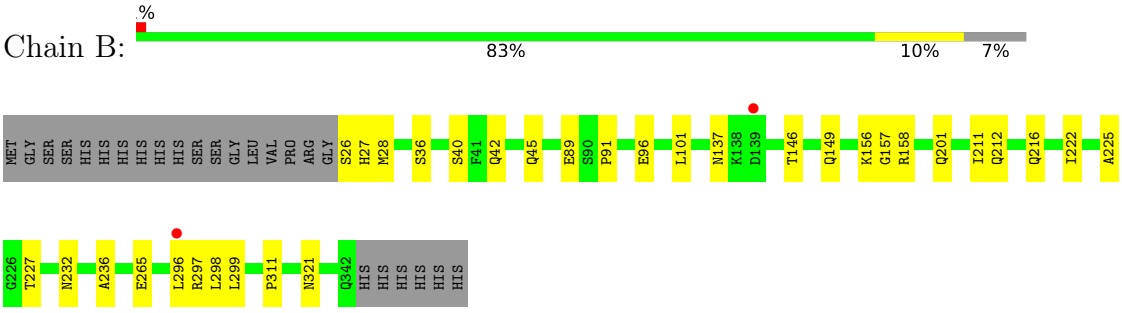
• Molecule 1: Agropine permease

Chain A:



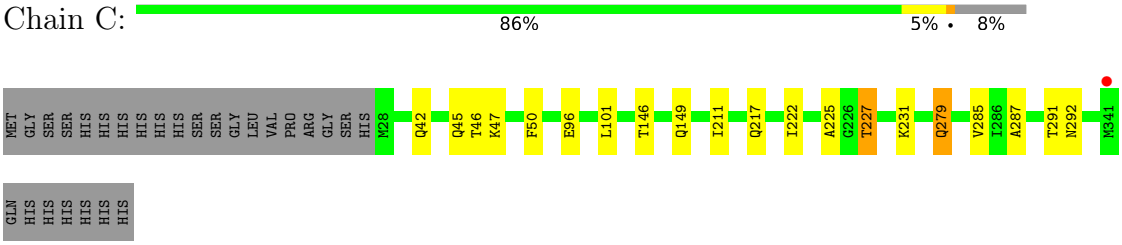
• Molecule 1: Agropine permease

Chain B:



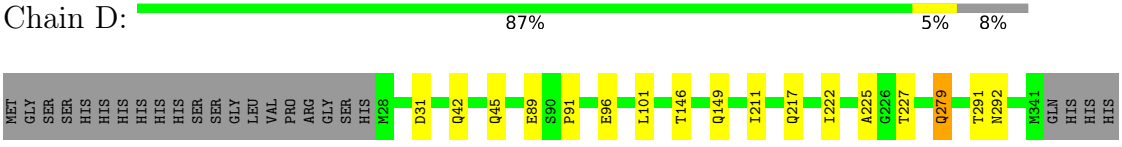
• Molecule 1: Agropine permease

Chain C:



• Molecule 1: Agropine permease

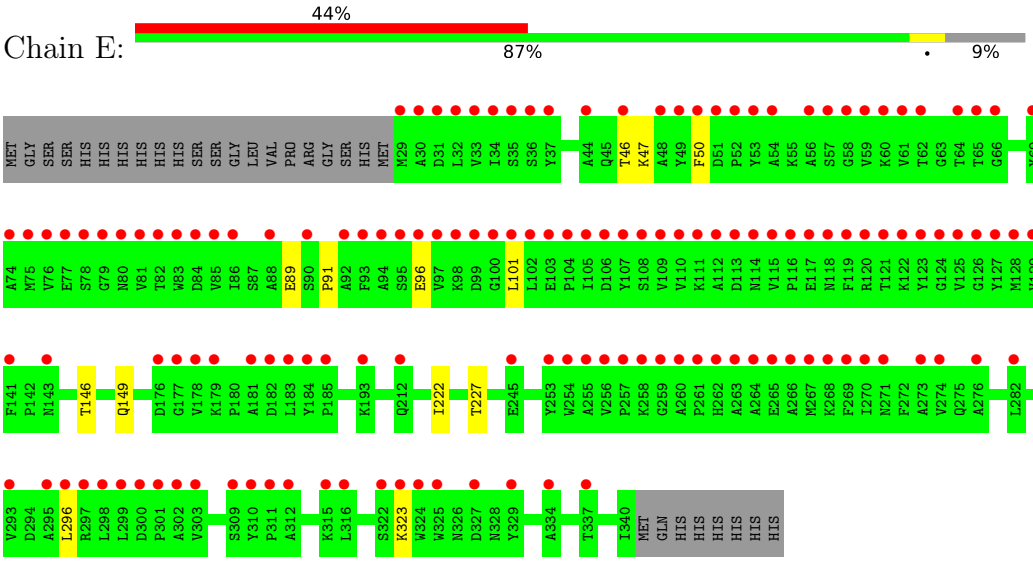
Chain D:



HIS
HIS
HIS

• Molecule 1: Agropine permease

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.57Å 86.31Å 106.52Å 71.14° 81.00° 76.32°	Depositor
Resolution (Å)	49.73 – 1.74 49.73 – 1.74	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.73-1.74) 95.6 (49.73-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.74Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.201 0.186 , 0.214	Depositor DCC
R_{free} test set	6483 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.083 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13234	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.29% 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: G9Z, NA, EDO

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	0.51	0/2488	0.60	0/3388
1	B	0.53	0/2497	0.62	0/3400
1	C	0.52	0/2471	0.60	0/3365
1	D	0.53	0/2471	0.60	0/3365
1	E	0.40	0/2455	0.58	0/3345
All	All	0.50	0/12382	0.60	0/16863

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	2426	0	2373	15	0
1	B	2435	0	2381	21	0
1	C	2410	0	2361	13	0
1	D	2410	0	2361	7	0
1	E	2394	0	2343	6	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	20	0	0	0	0
2	E	20	0	0	0	0
3	A	8	0	12	2	0
3	B	8	0	12	2	0
3	C	8	0	12	0	0
3	D	12	0	18	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	263	0	0	0	0
5	B	250	0	0	0	0
5	C	229	0	0	0	0
5	D	256	0	0	0	0
5	E	21	0	0	0	0
All	All	13234	0	11873	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (59) 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:C:227:THR:HG22	1:C:231:LYS:HE2	1.44	0.99
1:C:231:LYS:HE3	1:C:287:ALA:CB	2.12	0.79
1:B:156:LYS:HA	1:B:201:GLN:HE22	1.49	0.77
1:D:279:GLN:HE22	1:D:291:THR:H	1.34	0.74
1:C:279:GLN:HE22	1:C:291:THR:H	1.36	0.72
1:A:146:THR:H	1:A:149:GLN:HE21	1.41	0.69
1:B:146:THR:H	1:B:149:GLN:HE21	1.40	0.69
1:C:146:THR:H	1:C:149:GLN:HE21	1.40	0.67
1:D:146:THR:H	1:D:149:GLN:HE21	1.43	0.66
1:D:42:GLN:HA	1:D:45:GLN:HE21	1.64	0.62
1:A:28:MET:SD	1:A:265:GLU:HG3	2.39	0.62
1:C:231:LYS:HE3	1:C:287:ALA:HB1	1.80	0.62
1:E:146:THR:H	1:E:149:GLN:HE21	1.44	0.62
1:C:42:GLN:HA	1:C:45:GLN:HE21	1.66	0.61
1:B:26:SER:HB3	1:B:27:HIS:HA	1.85	0.58
1:A:329:TYR:HB3	3:A:403:EDO:H12	1.86	0.58
1:A:42:GLN:HA	1:A:45:GLN:HE21	1.70	0.56
1:A:47:LYS:HD3	1:A:285:VAL:HG11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:LYS:HD3	1:E:285:VAL:HG11	1.86	0.56
1:B:212:GLN:HE21	1:B:216:GLN:NE2	2.04	0.56
1:C:227:THR:HG22	1:C:231:LYS:CE	2.29	0.55
1:B:296:LEU:HA	1:B:299:LEU:HD12	1.88	0.54
1:D:279:GLN:NE2	1:D:292:ASN:H	2.05	0.54
1:C:279:GLN:NE2	1:C:292:ASN:H	2.06	0.54
1:A:31:ASP:HB3	1:A:60:LYS:HG2	1.89	0.53
1:B:42:GLN:HA	1:B:45:GLN:HE21	1.73	0.53
1:B:26:SER:CB	1:B:27:HIS:HA	2.39	0.52
1:B:216:GLN:HE21	1:B:236:ALA:HB3	1.76	0.49
1:C:231:LYS:HE3	1:C:287:ALA:HB3	1.90	0.49
1:A:109:VAL:HG22	1:B:297:ARG:NH1	2.28	0.48
1:D:89:GLU:HG3	1:D:91:PRO:HD2	1.96	0.48
1:B:311:PRO:HB3	3:B:402:EDO:H12	1.96	0.47
1:B:89:GLU:HG3	1:B:91:PRO:HD2	1.96	0.47
1:A:89:GLU:HG3	1:A:91:PRO:HD2	1.97	0.46
1:B:40:SER:HB2	1:B:232:ASN:HD22	1.80	0.46
1:E:89:GLU:HG3	1:E:91:PRO:HD2	1.97	0.46
1:B:158:ARG:NH1	1:E:71:LYS:HG2	2.30	0.46
1:B:216:GLN:NE2	1:B:236:ALA:HB3	2.31	0.46
1:D:96:GLU:HA	1:D:101:LEU:HD12	1.97	0.45
1:B:36:SER:CB	1:B:45:GLN:HE22	2.28	0.45
1:B:321:ASN:HB2	3:B:403:EDO:H11	1.98	0.45
1:D:211:ILE:HG21	1:D:225:ALA:HB2	1.99	0.45
1:E:46:THR:HA	1:E:50:PHE:HB2	1.98	0.45
1:C:96:GLU:HA	1:C:101:LEU:HD12	2.00	0.43
1:A:211:ILE:HG21	1:A:225:ALA:HB2	2.00	0.43
1:E:96:GLU:HA	1:E:101:LEU:HD12	1.99	0.43
1:B:157:GLY:H	1:B:201:GLN:NE2	2.16	0.42
1:A:75:MET:HG2	1:A:81:VAL:HA	2.01	0.42
1:A:135:ALA:HB2	1:A:230:ILE:HD13	2.02	0.42
1:C:47:LYS:HD3	1:C:285:VAL:HG11	2.02	0.42
1:C:46:THR:HA	1:C:50:PHE:HB2	2.02	0.41
1:A:108:SER:HB2	1:B:298:LEU:HD11	2.03	0.41
1:A:330:ASP:CG	3:A:403:EDO:H11	2.40	0.41
1:B:96:GLU:HA	1:B:101:LEU:HD12	2.01	0.41
1:C:211:ILE:HG21	1:C:225:ALA:HB2	2.02	0.41
1:B:211:ILE:HG21	1:B:225:ALA:HB2	2.03	0.41
1:A:96:GLU:HA	1:A:101:LEU:HD12	2.01	0.41
1:B:28:MET:SD	1:B:265:GLU:HG3	2.60	0.41
1:A:280:ALA:O	1:A:299:LEU:HD21	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/341 (92%)	309 (98%)	5 (2%)	0	100	100
1	B	315/341 (92%)	309 (98%)	6 (2%)	0	100	100
1	C	312/341 (92%)	307 (98%)	5 (2%)	0	100	100
1	D	312/341 (92%)	306 (98%)	6 (2%)	0	100	100
1	E	310/341 (91%)	304 (98%)	6 (2%)	0	100	100
All	All	1563/1705 (92%)	1535 (98%)	28 (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	248/270 (92%)	245 (99%)	3 (1%)	71	56
1	B	249/270 (92%)	246 (99%)	3 (1%)	71	56
1	C	246/270 (91%)	242 (98%)	4 (2%)	62	44
1	D	246/270 (91%)	241 (98%)	5 (2%)	55	33
1	E	244/270 (90%)	240 (98%)	4 (2%)	62	44
All	All	1233/1350 (91%)	1214 (98%)	19 (2%)	65	47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	222	ILE
1	A	227	THR
1	B	137	ASN
1	B	222	ILE
1	B	227	THR
1	C	217	GLN
1	C	222	ILE
1	C	227	THR
1	C	279	GLN
1	D	31	ASP
1	D	217	GLN
1	D	222	ILE
1	D	227	THR
1	D	279	GLN
1	E	222	ILE
1	E	227	THR
1	E	296	LEU
1	E	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	149	GLN
1	A	262	HIS
1	A	275	GLN
1	A	326	ASN
1	A	328	ASN
1	B	45	GLN
1	B	137	ASN
1	B	149	GLN
1	B	201	GLN
1	B	216	GLN
1	B	232	ASN
1	B	262	HIS
1	B	326	ASN
1	C	45	GLN
1	C	133	ASN
1	C	149	GLN
1	C	279	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	45	GLN
1	D	133	ASN
1	D	149	GLN
1	D	279	GLN
1	D	326	ASN
1	E	45	GLN
1	E	149	GLN
1	E	275	GLN
1	E	328	ASN

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 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
3	EDO	A	403	-	3,3,3	0.49	0	2,2,2	0.37	0
2	G9Z	A	401	4	19,20,20	2.79	3 (15%)	21,28,28	2.38	4 (19%)
2	G9Z	E	401	-	19,20,20	2.91	4 (21%)	21,28,28	3.08	4 (19%)
2	G9Z	D	401	4	19,20,20	2.79	4 (21%)	21,28,28	3.06	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	A	402	-	3,3,3	0.55	0	2,2,2	0.26	0
3	EDO	B	403	-	3,3,3	0.69	0	2,2,2	0.02	0
3	EDO	D	404	-	3,3,3	0.58	0	2,2,2	0.15	0
2	G9Z	B	401	4	19,20,20	2.27	3 (15%)	21,28,28	2.77	5 (23%)
3	EDO	D	402	-	3,3,3	0.49	0	2,2,2	0.39	0
3	EDO	B	402	-	3,3,3	0.66	0	2,2,2	0.13	0
3	EDO	C	402	-	3,3,3	0.82	0	2,2,2	0.21	0
3	EDO	C	403	-	3,3,3	0.69	0	2,2,2	0.11	0
2	G9Z	C	401	4	19,20,20	2.94	3 (15%)	21,28,28	2.68	5 (23%)
3	EDO	D	403	-	3,3,3	0.55	0	2,2,2	0.27	0

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
3	EDO	A	403	-	-	0/1/1/1	-
2	G9Z	A	401	4	-	3/22/35/35	0/1/1/1
2	G9Z	E	401	-	-	3/22/35/35	0/1/1/1
2	G9Z	D	401	4	-	2/22/35/35	0/1/1/1
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	D	404	-	-	1/1/1/1	-
2	G9Z	B	401	4	-	2/22/35/35	0/1/1/1
3	EDO	D	402	-	-	0/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
3	EDO	C	403	-	-	0/1/1/1	-
2	G9Z	C	401	4	-	2/22/35/35	0/1/1/1
3	EDO	D	403	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	G9Z	CAC-CB	10.90	1.55	1.33
2	D	401	G9Z	CAC-CB	9.72	1.53	1.33
2	E	401	G9Z	CAC-CB	9.50	1.52	1.33
2	A	401	G9Z	CAC-CB	9.12	1.51	1.33
2	B	401	G9Z	CAC-CB	7.14	1.47	1.33
2	E	401	G9Z	CA-C	-5.20	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	G9Z	CAC-CAB	-4.89	1.39	1.48
2	E	401	G9Z	CAC-CAB	-4.76	1.39	1.48
2	D	401	G9Z	CA-C	-4.41	1.44	1.53
2	A	401	G9Z	CA-C	-4.32	1.44	1.53
2	D	401	G9Z	CAC-CAB	-4.18	1.40	1.48
2	B	401	G9Z	CA-C	-4.07	1.45	1.53
2	B	401	G9Z	CAC-CAB	-3.88	1.41	1.48
2	C	401	G9Z	CA-C	-3.56	1.46	1.53
2	C	401	G9Z	CAC-CAB	-3.40	1.42	1.48
2	E	401	G9Z	CAG-N	2.33	1.51	1.47
2	D	401	G9Z	CAJ-CAI	2.08	1.57	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	G9Z	CAC-CAB-N	11.76	113.78	106.37
2	D	401	G9Z	CAC-CAB-N	11.03	113.31	106.37
2	B	401	G9Z	CAC-CAB-N	10.34	112.88	106.37
2	C	401	G9Z	CAC-CAB-N	9.60	112.41	106.37
2	A	401	G9Z	CAC-CAB-N	8.24	111.56	106.37
2	D	401	G9Z	CB-CAC-CAB	-5.68	106.03	110.09
2	C	401	G9Z	CB-CAC-CAB	-5.12	106.43	110.09
2	E	401	G9Z	CA-N-CAB	-4.50	109.89	113.31
2	E	401	G9Z	CB-CAC-CAB	-4.35	106.98	110.09
2	B	401	G9Z	CB-CAC-CAB	-4.25	107.06	110.09
2	A	401	G9Z	CA-N-CAB	-3.86	110.37	113.31
2	D	401	G9Z	CAG-N-CAB	3.37	126.86	123.75
2	E	401	G9Z	OAM-CAB-CAC	-3.34	122.32	128.56
2	A	401	G9Z	CAG-N-CAB	3.30	126.80	123.75
2	B	401	G9Z	CA-N-CAB	-3.30	110.80	113.31
2	A	401	G9Z	OAM-CAB-CAC	-3.28	122.44	128.56
2	D	401	G9Z	OAM-CAB-CAC	-3.25	122.50	128.56
2	D	401	G9Z	CA-N-CAB	-3.16	110.90	113.31
2	B	401	G9Z	OAM-CAB-CAC	-3.10	122.78	128.56
2	C	401	G9Z	OAM-CAB-CAC	-2.79	123.35	128.56
2	C	401	G9Z	CA-N-CAB	-2.74	111.22	113.31
2	C	401	G9Z	CAG-N-CAB	2.68	126.23	123.75
2	B	401	G9Z	C-CA-N	2.07	116.14	110.59

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	G9Z	CAG-CAH-CAI-CAJ
2	B	401	G9Z	CAG-CAH-CAI-CAJ
2	C	401	G9Z	CAG-CAH-CAI-CAJ
2	D	401	G9Z	CAG-CAH-CAI-CAJ
2	E	401	G9Z	CAG-CAH-CAI-CAJ
2	A	401	G9Z	OAP-CAH-CAI-CAJ
2	B	401	G9Z	OAP-CAH-CAI-CAJ
2	E	401	G9Z	OAP-CAH-CAI-CAJ
3	A	402	EDO	O1-C1-C2-O2
2	D	401	G9Z	OAP-CAH-CAI-CAJ
3	B	403	EDO	O1-C1-C2-O2
3	D	404	EDO	O1-C1-C2-O2
2	C	401	G9Z	OAP-CAH-CAI-CAJ
2	E	401	G9Z	OAP-CAH-CAI-OAQ
3	B	402	EDO	O1-C1-C2-O2
2	A	401	G9Z	OAP-CAH-CAI-OAQ

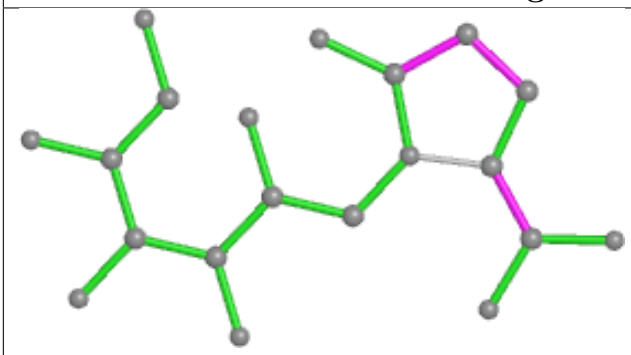
There are no ring outliers.

3 monomers are involved in 4 short contacts:

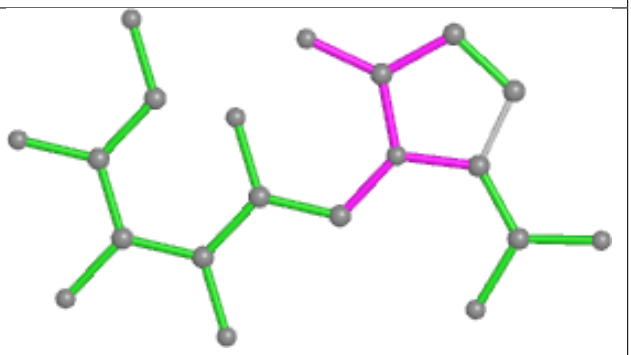
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	EDO	2	0
3	B	403	EDO	1	0
3	B	402	EDO	1	0

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.

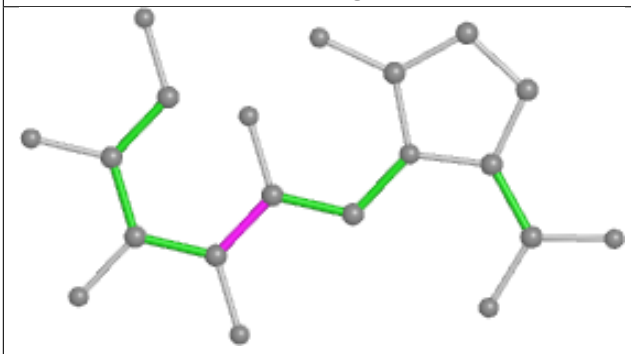
Ligand G9Z A 401



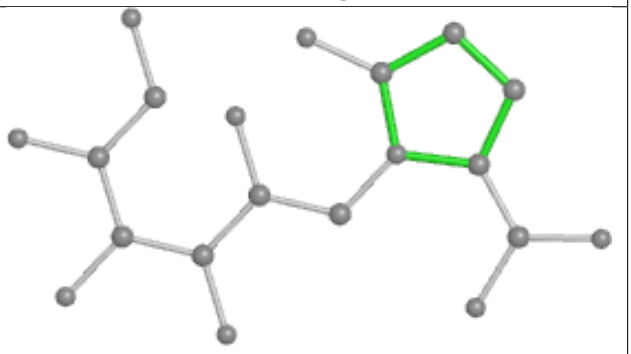
Bond lengths



Bond angles

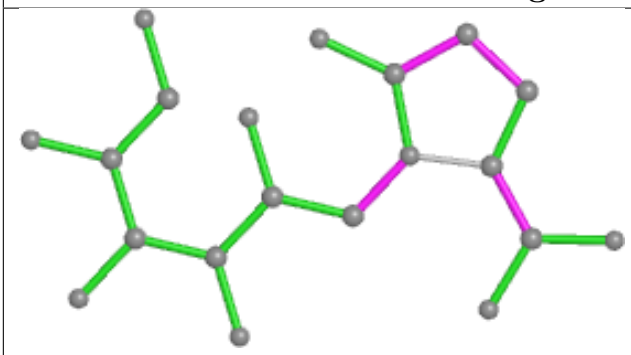


Torsions

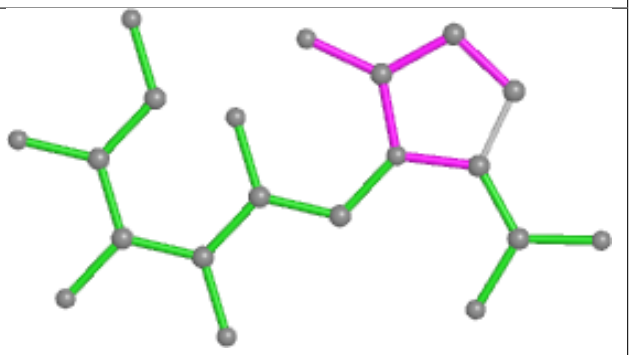


Rings

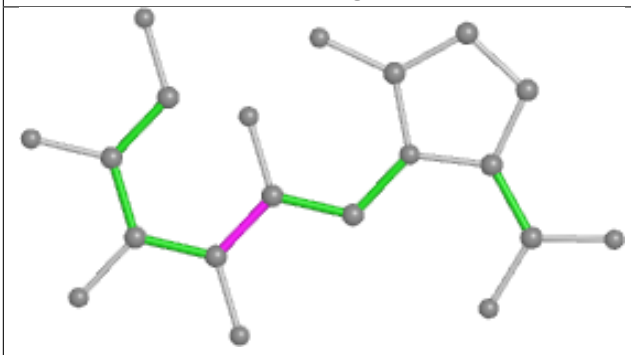
Ligand G9Z E 401



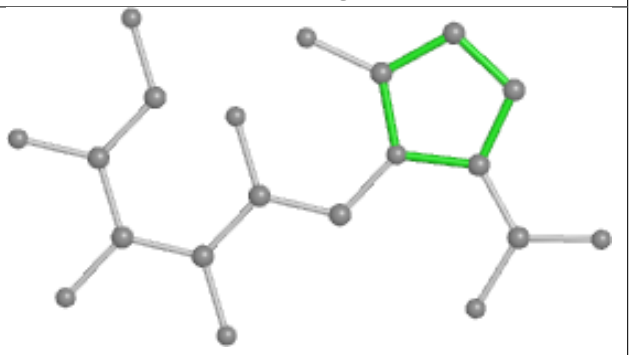
Bond lengths



Bond angles

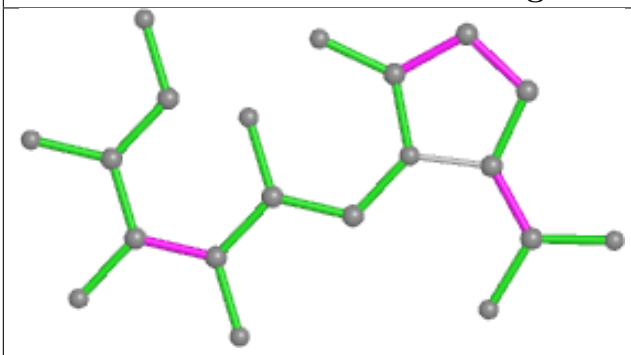


Torsions

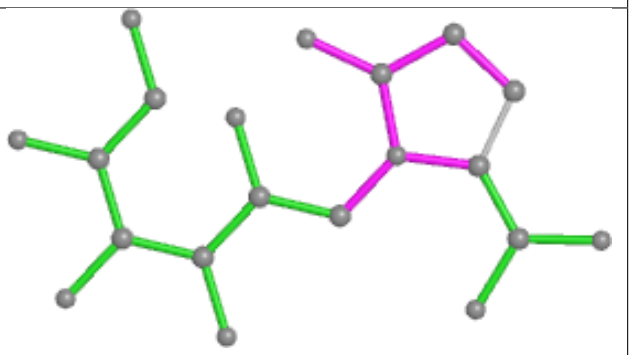


Rings

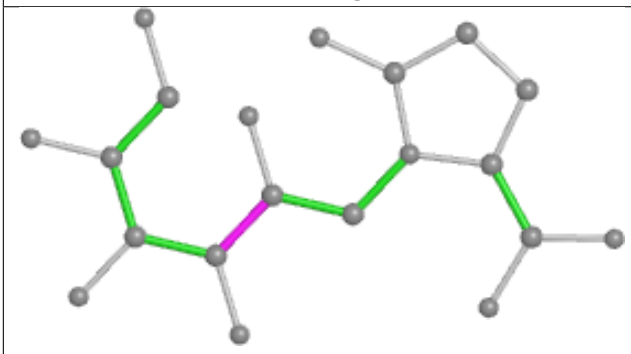
Ligand G9Z D 401



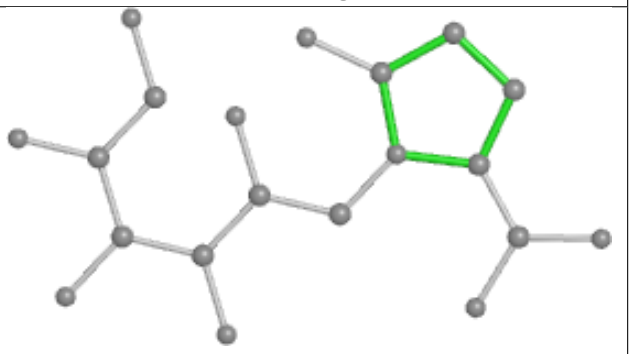
Bond lengths



Bond angles

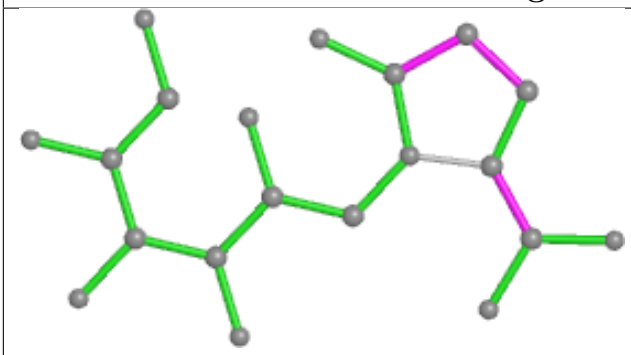


Torsions

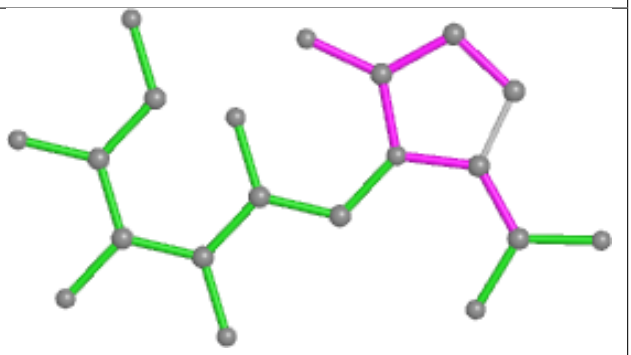


Rings

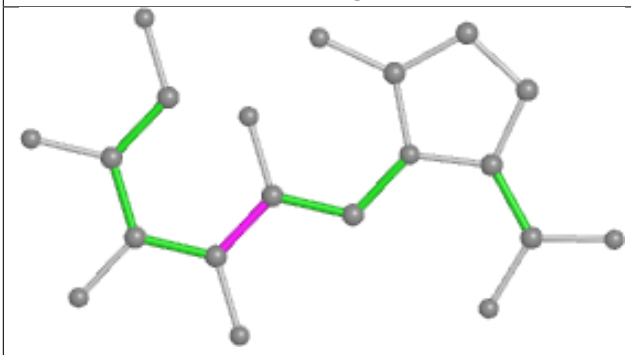
Ligand G9Z B 401



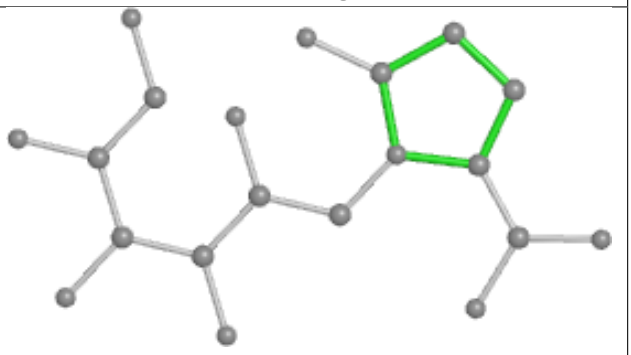
Bond lengths



Bond angles

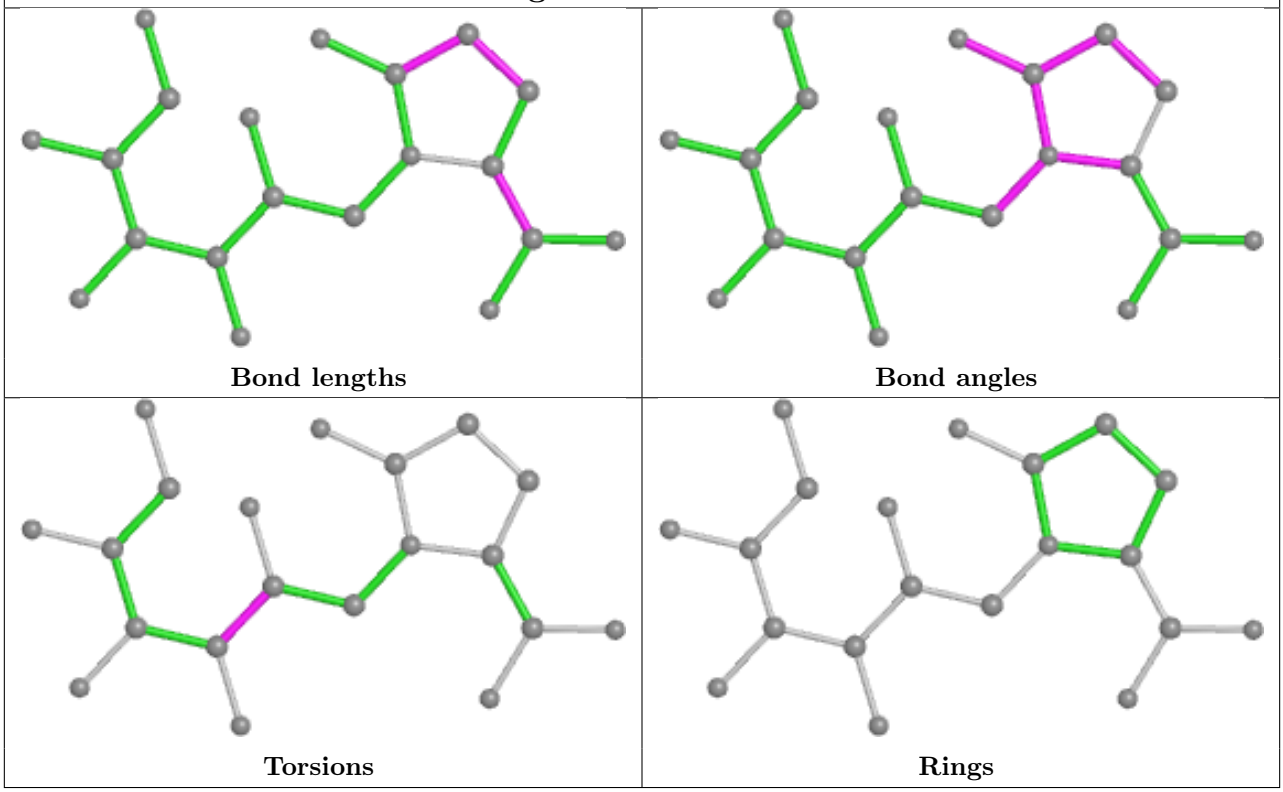


Torsions



Rings

Ligand G9Z C 401



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	316/341 (92%)	-0.34	2 (0%) 89 92	13, 22, 39, 56	3 (0%)
1	B	317/341 (92%)	-0.31	2 (0%) 89 92	14, 22, 40, 69	3 (0%)
1	C	314/341 (92%)	-0.37	1 (0%) 94 95	15, 22, 39, 67	4 (1%)
1	D	314/341 (92%)	-0.44	0 100 100	15, 21, 37, 70	4 (1%)
1	E	312/341 (91%)	2.85	150 (48%) 0 0	30, 78, 183, 214	3 (0%)
All	All	1573/1705 (92%)	0.27	155 (9%) 7 9	13, 24, 119, 214	17 (1%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	30	ALA	18.6
1	E	266	ALA	17.0
1	E	125	VAL	15.5
1	E	104	PRO	13.6
1	E	107	TYR	13.4
1	E	56	ALA	12.1
1	E	103	GLU	11.9
1	E	32	LEU	11.9
1	E	76	VAL	11.6
1	E	100	GLY	11.3
1	E	33	VAL	11.3
1	E	257	PRO	11.3
1	E	61	VAL	11.0
1	E	123	TYR	11.0
1	E	60	LYS	10.2
1	E	59	VAL	9.4
1	E	105	ILE	9.3
1	E	102	LEU	9.0
1	E	85	VAL	8.9
1	E	31	ASP	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	101	LEU	8.5
1	E	93	PHE	8.4
1	E	110	VAL	8.0
1	E	97	VAL	7.9
1	E	108	SER	7.8
1	E	84	ASP	7.5
1	E	264	ALA	7.4
1	E	29	MET	7.2
1	E	269	PHE	7.1
1	E	99	ASP	7.0
1	E	316	LEU	6.9
1	E	79	GLY	6.9
1	E	255	ALA	6.8
1	E	263	ALA	6.8
1	E	119	PHE	6.7
1	E	120	ARG	6.7
1	E	54	ALA	6.7
1	E	86	ILE	6.6
1	E	274	VAL	6.3
1	E	83	TRP	6.3
1	E	57	SER	6.2
1	E	34	ILE	6.2
1	E	311	PRO	6.1
1	E	261	PRO	6.0
1	E	52	PRO	5.9
1	E	260	ALA	5.7
1	E	109	VAL	5.6
1	E	62	THR	5.5
1	E	298	LEU	5.3
1	E	256	VAL	5.2
1	E	88	ALA	5.2
1	E	35	SER	5.1
1	E	310	TYR	5.0
1	E	69	TYR	4.9
1	E	265	GLU	4.9
1	E	262	HIS	4.7
1	E	126	GLY	4.6
1	E	121	THR	4.6
1	E	115	VAL	4.6
1	E	111	LYS	4.5
1	E	49	TYR	4.4
1	E	92	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	114	ASN	4.3
1	E	267	MET	4.3
1	E	53	TYR	4.2
1	E	72	VAL	4.2
1	E	106	ASP	4.2
1	E	50	PHE	4.1
1	E	270	ILE	4.1
1	E	117	GLU	4.1
1	E	113	ASP	4.1
1	E	325	TRP	4.0
1	E	75	MET	4.0
1	E	268	LYS	4.0
1	E	94	ALA	4.0
1	E	65	THR	3.9
1	E	273	ALA	3.9
1	E	276	ALA	3.9
1	E	327	ASP	3.9
1	E	78	SER	3.8
1	E	315	LYS	3.8
1	E	184	TYR	3.7
1	E	98	LYS	3.7
1	E	82	THR	3.6
1	E	258	LYS	3.6
1	E	116	PRO	3.6
1	E	181	ALA	3.5
1	E	46	THR	3.5
1	E	74	ALA	3.5
1	E	296	LEU	3.5
1	E	139	ASP	3.4
1	E	81	VAL	3.4
1	E	259	GLY	3.4
1	E	80	ASN	3.4
1	E	183	LEU	3.4
1	E	301	PRO	3.3
1	E	112	ALA	3.3
1	E	58	GLY	3.2
1	E	122	LYS	3.2
1	E	253	TYR	3.2
1	E	323	LYS	3.1
1	E	177	GLY	3.1
1	E	95	SER	3.1
1	E	271	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	64	THR	3.0
1	E	324	TRP	3.0
1	E	138	LYS	3.0
1	E	127	TYR	3.0
1	E	90	SER	2.9
1	E	118	ASN	2.9
1	E	77	GLU	2.9
1	E	71	LYS	2.8
1	E	282	LEU	2.8
1	E	70	ALA	2.8
1	E	37	TYR	2.7
1	E	254	TRP	2.7
1	E	285	VAL	2.7
1	C	341	MET	2.7
1	B	139	ASP	2.6
1	E	51	ASP	2.6
1	B	296	LEU	2.6
1	E	302	ALA	2.6
1	E	245	GLU	2.6
1	E	329	TYR	2.6
1	E	128	MET	2.5
1	E	295	ALA	2.4
1	A	26	SER	2.4
1	E	96	GLU	2.4
1	A	296	LEU	2.4
1	E	176	ASP	2.4
1	E	129	VAL	2.3
1	E	66	GLY	2.3
1	E	178	VAL	2.3
1	E	182	ASP	2.3
1	E	322	SER	2.3
1	E	193	LYS	2.3
1	E	293	VAL	2.3
1	E	303	VAL	2.3
1	E	337	THR	2.3
1	E	300	ASP	2.3
1	E	291	THR	2.2
1	E	299	LEU	2.2
1	E	334	ALA	2.2
1	E	36	SER	2.2
1	E	179	LYS	2.2
1	E	124	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	143	ASN	2.2
1	E	141	PHE	2.2
1	E	312	ALA	2.2
1	E	309	SER	2.2
1	E	185	PRO	2.1
1	E	44	ALA	2.1
1	E	297	ARG	2.1
1	E	48	ALA	2.1
1	E	212	GLN	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
3	EDO	A	403	4/4	0.62	0.28	52,52,52,55	0
3	EDO	B	403	4/4	0.68	0.28	46,48,48,48	0
3	EDO	B	402	4/4	0.71	0.30	38,39,40,41	0
3	EDO	C	402	4/4	0.77	0.18	40,43,45,47	0
3	EDO	D	404	4/4	0.78	0.16	37,41,44,44	0
3	EDO	C	403	4/4	0.83	0.14	48,50,52,53	0
2	G9Z	E	401	20/20	0.86	0.15	36,42,47,50	0
3	EDO	A	402	4/4	0.86	0.13	34,38,41,44	0
3	EDO	D	402	4/4	0.92	0.22	42,45,45,47	0
3	EDO	D	403	4/4	0.94	0.17	36,41,45,48	0
2	G9Z	C	401	20/20	0.96	0.07	10,17,19,21	0
2	G9Z	A	401	20/20	0.97	0.06	12,15,19,20	0
2	G9Z	D	401	20/20	0.97	0.06	13,17,18,19	0
2	G9Z	B	401	20/20	0.98	0.07	11,16,20,21	0

Continued on next page...

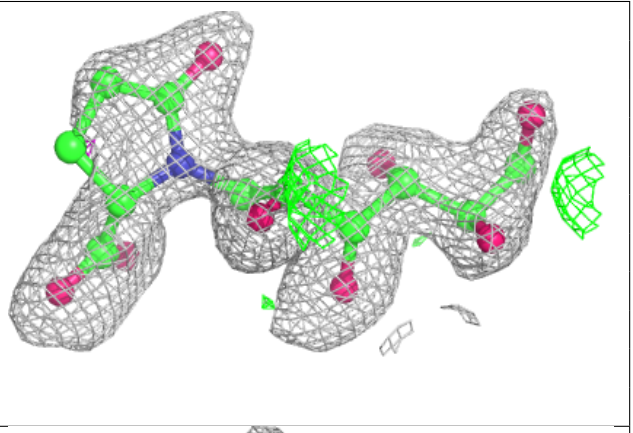
Continued from previous page...

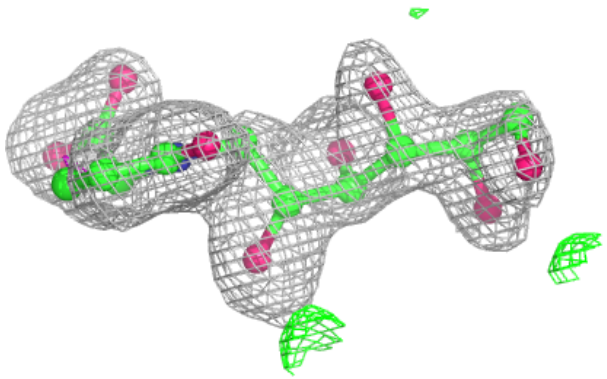
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	B	404	1/1	0.99	0.09	24,24,24,24	0
4	NA	C	404	1/1	0.99	0.04	24,24,24,24	0
4	NA	D	405	1/1	0.99	0.06	23,23,23,23	0
4	NA	A	404	1/1	1.00	0.06	25,25,25,25	0

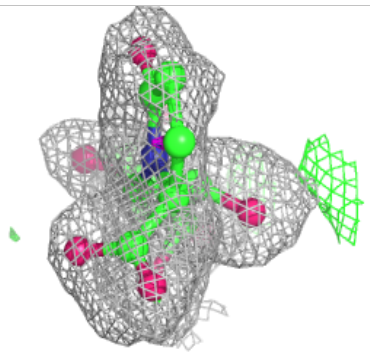
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G9Z E 401:

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

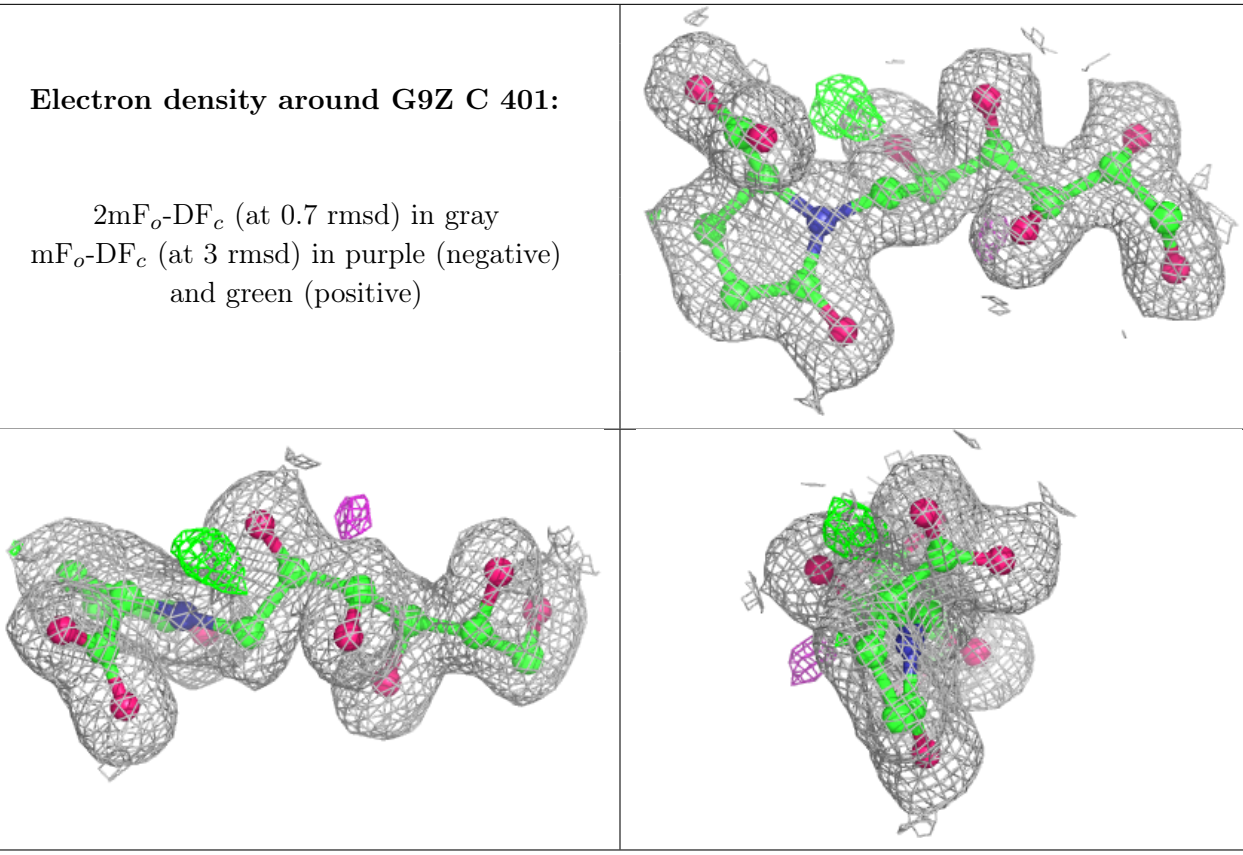






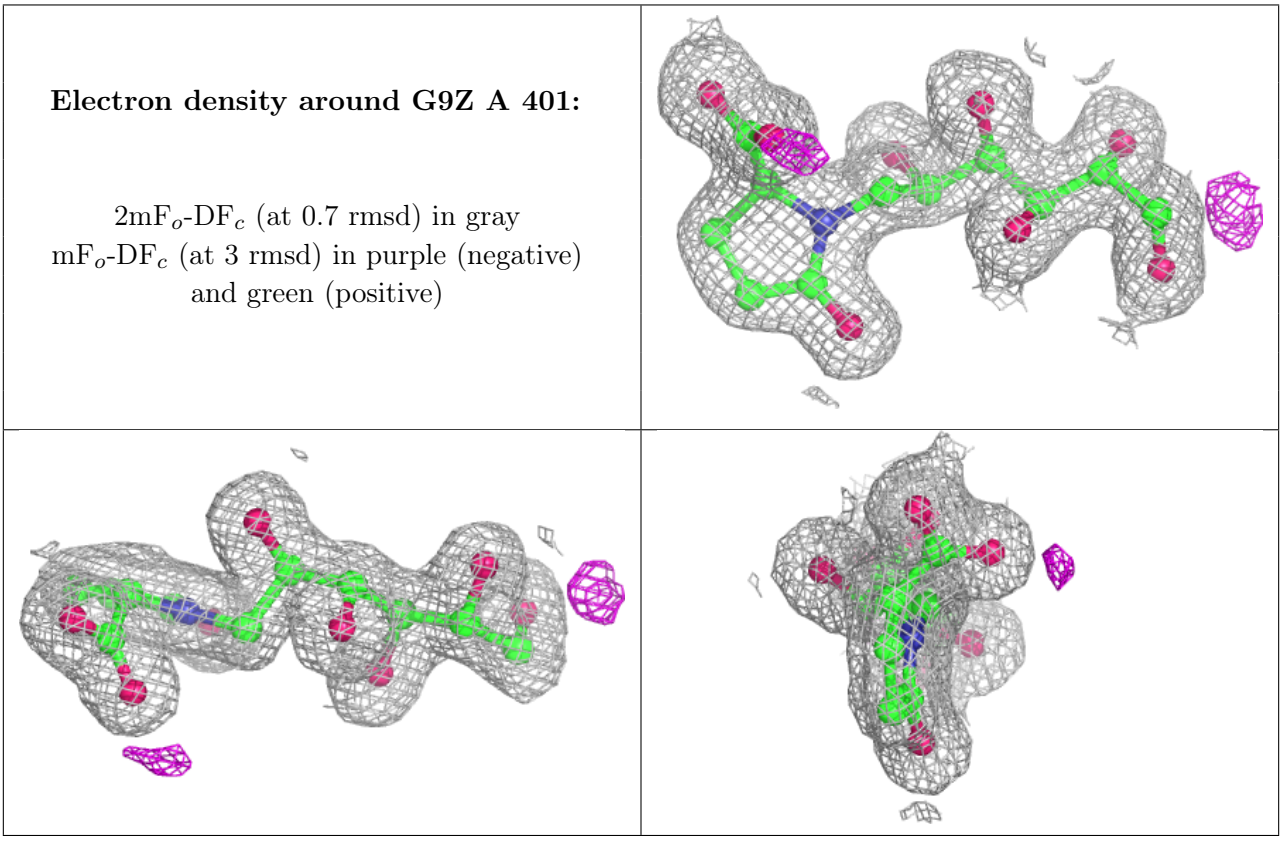
Electron density around G9Z C 401:

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



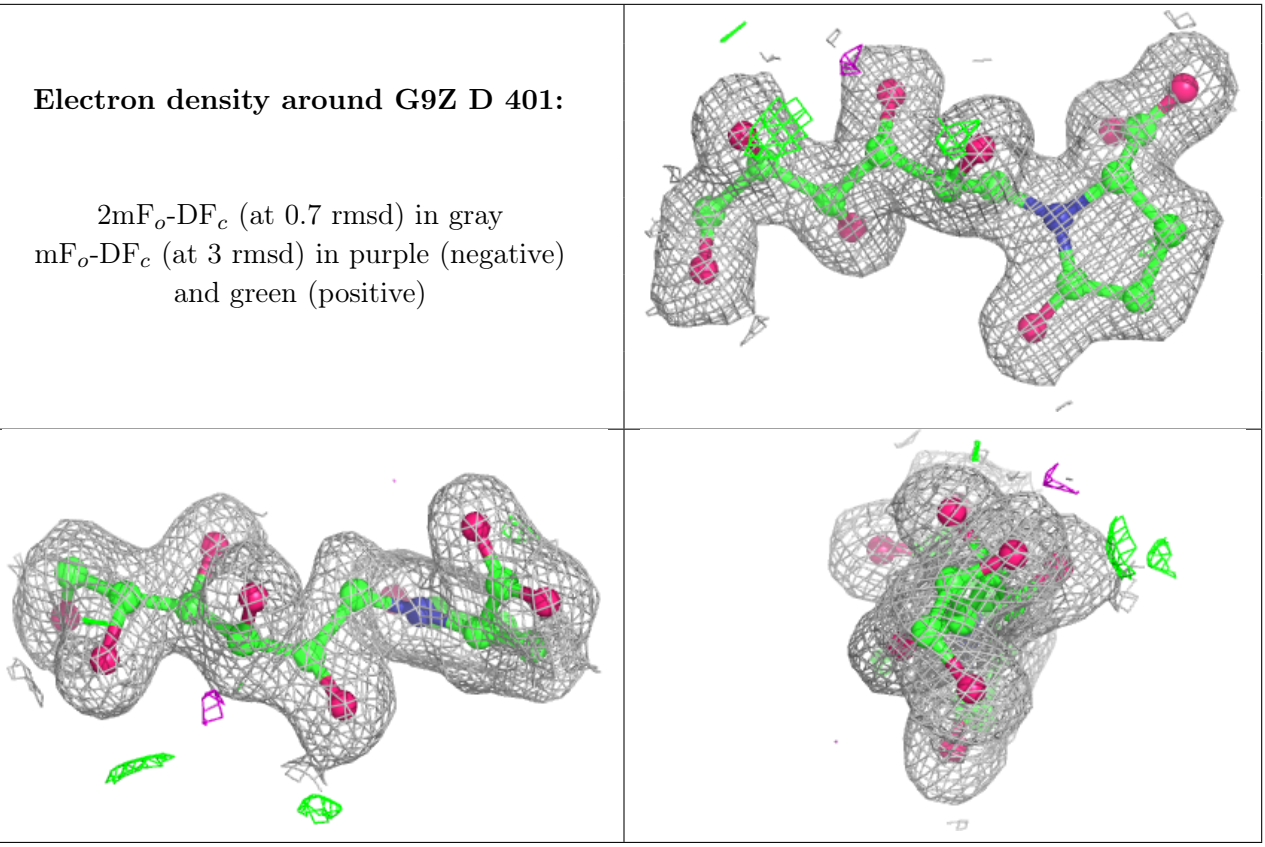
Electron density around G9Z A 401:

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



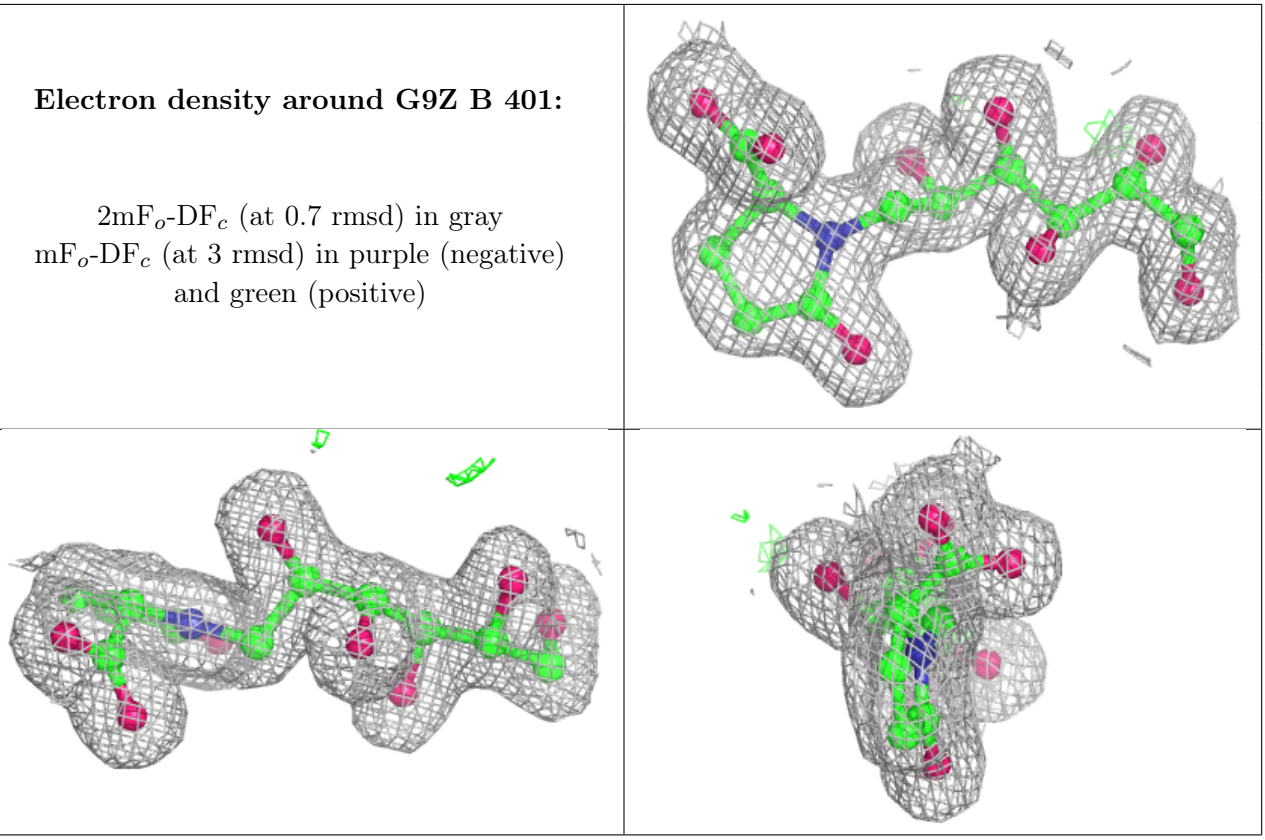
Electron density around G9Z D 401:

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



Electron density around G9Z B 401:

$2mF_o$-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.