Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 04:15 PM JST

PDB ID	:	5WQH
Title	:	Structure of fungal meroterpenoid isomerase Trt14 complexed with substrate analog and endo-terretonin D
Authors	:	Mori, T.; Matsuda, Y.; Abe, I.
Deposited on	:	2016-11-26
Resolution	:	2.10 Å(reported)

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

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

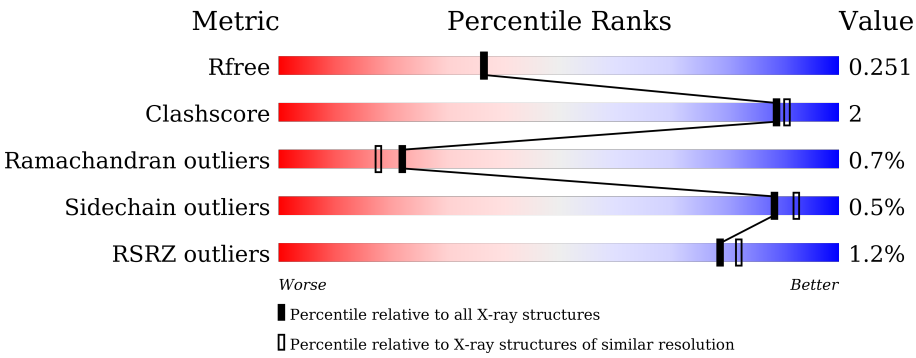
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	162	.% 83% • 14%
1	B	162	82% • 14%
1	C	162	83% • 14%
1	D	162	2% 79% 7% 14%
1	E	162	2% 80% 6% 14%
1	F	162	.% 80% 7% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7301 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 Isomerase trt14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	140	1119	707	188	219	5	0	0	0
1	B	140	1119	707	188	219	5	0	0	0
1	C	140	1119	707	188	219	5	0	0	0
1	D	140	1119	707	188	219	5	0	0	0
1	E	140	1119	707	188	219	5	0	0	0
1	F	140	1119	707	188	219	5	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q0C8A2
A	-18	GLY	-	expression tag	UNP Q0C8A2
A	-17	SER	-	expression tag	UNP Q0C8A2
A	-16	SER	-	expression tag	UNP Q0C8A2
A	-15	HIS	-	expression tag	UNP Q0C8A2
A	-14	HIS	-	expression tag	UNP Q0C8A2
A	-13	HIS	-	expression tag	UNP Q0C8A2
A	-12	HIS	-	expression tag	UNP Q0C8A2
A	-11	HIS	-	expression tag	UNP Q0C8A2
A	-10	HIS	-	expression tag	UNP Q0C8A2
A	-9	SER	-	expression tag	UNP Q0C8A2
A	-8	SER	-	expression tag	UNP Q0C8A2
A	-7	GLY	-	expression tag	UNP Q0C8A2
A	-6	LEU	-	expression tag	UNP Q0C8A2
A	-5	VAL	-	expression tag	UNP Q0C8A2
A	-4	PRO	-	expression tag	UNP Q0C8A2
A	-3	ARG	-	expression tag	UNP Q0C8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q0C8A2
A	-1	SER	-	expression tag	UNP Q0C8A2
A	0	HIS	-	expression tag	UNP Q0C8A2
B	-19	MET	-	expression tag	UNP Q0C8A2
B	-18	GLY	-	expression tag	UNP Q0C8A2
B	-17	SER	-	expression tag	UNP Q0C8A2
B	-16	SER	-	expression tag	UNP Q0C8A2
B	-15	HIS	-	expression tag	UNP Q0C8A2
B	-14	HIS	-	expression tag	UNP Q0C8A2
B	-13	HIS	-	expression tag	UNP Q0C8A2
B	-12	HIS	-	expression tag	UNP Q0C8A2
B	-11	HIS	-	expression tag	UNP Q0C8A2
B	-10	HIS	-	expression tag	UNP Q0C8A2
B	-9	SER	-	expression tag	UNP Q0C8A2
B	-8	SER	-	expression tag	UNP Q0C8A2
B	-7	GLY	-	expression tag	UNP Q0C8A2
B	-6	LEU	-	expression tag	UNP Q0C8A2
B	-5	VAL	-	expression tag	UNP Q0C8A2
B	-4	PRO	-	expression tag	UNP Q0C8A2
B	-3	ARG	-	expression tag	UNP Q0C8A2
B	-2	GLY	-	expression tag	UNP Q0C8A2
B	-1	SER	-	expression tag	UNP Q0C8A2
B	0	HIS	-	expression tag	UNP Q0C8A2
C	-19	MET	-	expression tag	UNP Q0C8A2
C	-18	GLY	-	expression tag	UNP Q0C8A2
C	-17	SER	-	expression tag	UNP Q0C8A2
C	-16	SER	-	expression tag	UNP Q0C8A2
C	-15	HIS	-	expression tag	UNP Q0C8A2
C	-14	HIS	-	expression tag	UNP Q0C8A2
C	-13	HIS	-	expression tag	UNP Q0C8A2
C	-12	HIS	-	expression tag	UNP Q0C8A2
C	-11	HIS	-	expression tag	UNP Q0C8A2
C	-10	HIS	-	expression tag	UNP Q0C8A2
C	-9	SER	-	expression tag	UNP Q0C8A2
C	-8	SER	-	expression tag	UNP Q0C8A2
C	-7	GLY	-	expression tag	UNP Q0C8A2
C	-6	LEU	-	expression tag	UNP Q0C8A2
C	-5	VAL	-	expression tag	UNP Q0C8A2
C	-4	PRO	-	expression tag	UNP Q0C8A2
C	-3	ARG	-	expression tag	UNP Q0C8A2
C	-2	GLY	-	expression tag	UNP Q0C8A2
C	-1	SER	-	expression tag	UNP Q0C8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q0C8A2
D	-19	MET	-	expression tag	UNP Q0C8A2
D	-18	GLY	-	expression tag	UNP Q0C8A2
D	-17	SER	-	expression tag	UNP Q0C8A2
D	-16	SER	-	expression tag	UNP Q0C8A2
D	-15	HIS	-	expression tag	UNP Q0C8A2
D	-14	HIS	-	expression tag	UNP Q0C8A2
D	-13	HIS	-	expression tag	UNP Q0C8A2
D	-12	HIS	-	expression tag	UNP Q0C8A2
D	-11	HIS	-	expression tag	UNP Q0C8A2
D	-10	HIS	-	expression tag	UNP Q0C8A2
D	-9	SER	-	expression tag	UNP Q0C8A2
D	-8	SER	-	expression tag	UNP Q0C8A2
D	-7	GLY	-	expression tag	UNP Q0C8A2
D	-6	LEU	-	expression tag	UNP Q0C8A2
D	-5	VAL	-	expression tag	UNP Q0C8A2
D	-4	PRO	-	expression tag	UNP Q0C8A2
D	-3	ARG	-	expression tag	UNP Q0C8A2
D	-2	GLY	-	expression tag	UNP Q0C8A2
D	-1	SER	-	expression tag	UNP Q0C8A2
D	0	HIS	-	expression tag	UNP Q0C8A2
E	-19	MET	-	expression tag	UNP Q0C8A2
E	-18	GLY	-	expression tag	UNP Q0C8A2
E	-17	SER	-	expression tag	UNP Q0C8A2
E	-16	SER	-	expression tag	UNP Q0C8A2
E	-15	HIS	-	expression tag	UNP Q0C8A2
E	-14	HIS	-	expression tag	UNP Q0C8A2
E	-13	HIS	-	expression tag	UNP Q0C8A2
E	-12	HIS	-	expression tag	UNP Q0C8A2
E	-11	HIS	-	expression tag	UNP Q0C8A2
E	-10	HIS	-	expression tag	UNP Q0C8A2
E	-9	SER	-	expression tag	UNP Q0C8A2
E	-8	SER	-	expression tag	UNP Q0C8A2
E	-7	GLY	-	expression tag	UNP Q0C8A2
E	-6	LEU	-	expression tag	UNP Q0C8A2
E	-5	VAL	-	expression tag	UNP Q0C8A2
E	-4	PRO	-	expression tag	UNP Q0C8A2
E	-3	ARG	-	expression tag	UNP Q0C8A2
E	-2	GLY	-	expression tag	UNP Q0C8A2
E	-1	SER	-	expression tag	UNP Q0C8A2
E	0	HIS	-	expression tag	UNP Q0C8A2
F	-19	MET	-	expression tag	UNP Q0C8A2

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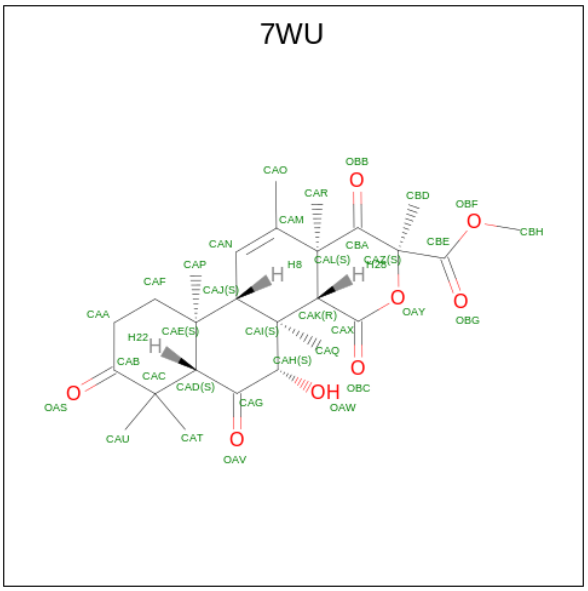
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP Q0C8A2
F	-17	SER	-	expression tag	UNP Q0C8A2
F	-16	SER	-	expression tag	UNP Q0C8A2
F	-15	HIS	-	expression tag	UNP Q0C8A2
F	-14	HIS	-	expression tag	UNP Q0C8A2
F	-13	HIS	-	expression tag	UNP Q0C8A2
F	-12	HIS	-	expression tag	UNP Q0C8A2
F	-11	HIS	-	expression tag	UNP Q0C8A2
F	-10	HIS	-	expression tag	UNP Q0C8A2
F	-9	SER	-	expression tag	UNP Q0C8A2
F	-8	SER	-	expression tag	UNP Q0C8A2
F	-7	GLY	-	expression tag	UNP Q0C8A2
F	-6	LEU	-	expression tag	UNP Q0C8A2
F	-5	VAL	-	expression tag	UNP Q0C8A2
F	-4	PRO	-	expression tag	UNP Q0C8A2
F	-3	ARG	-	expression tag	UNP Q0C8A2
F	-2	GLY	-	expression tag	UNP Q0C8A2
F	-1	SER	-	expression tag	UNP Q0C8A2
F	0	HIS	-	expression tag	UNP Q0C8A2

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

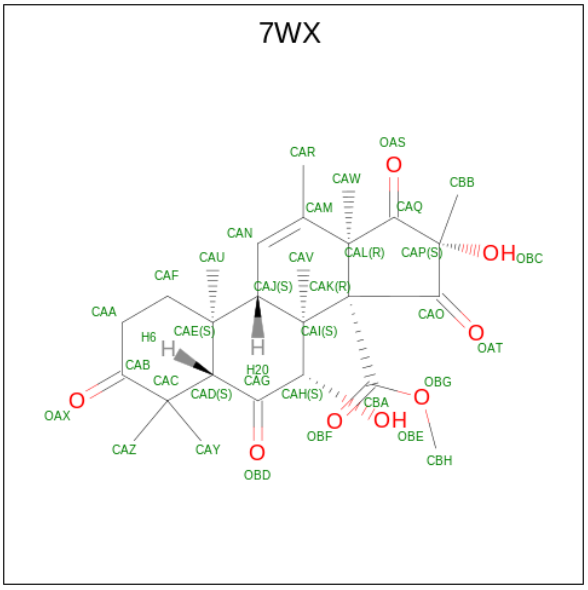
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	3	3	3	0	0
			Total	Ca		
2	B	1	1	1	0	0
			Total	Ca		
2	E	1	1	1	0	0
			Total	Ca		
2	F	2	2	2	0	0

- Molecule 3 is methyl (2S,4aR,4bS,5S,6aS,10aS,10bS,12aS)-2,4b,7,7,10a,12,12a-heptamethyl-5-oxidanyl-1,4,6,8-tetrakis(oxidanylidene)-4a,5,6a,9,10,10b-hexahydronaphtho[1,2-h]isochromene-2-carboxylate (three-letter code: 7WU) (formula: $C_{26}H_{34}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	34	26	8	0	0
			Total	C	O		
3	B	1	34	26	8	0	0
			Total	C	O		
3	C	1	34	26	8	0	0
			Total	C	O		
3	F	1	34	26	8	0	0

- Molecule 4 is methyl (5S,7S,8S,9S,10S,13R,14R,16S)-4,4,8,10,12,13,16-heptamethyl-7,16-bis(oxidanyl)-3,6,15,17-tetrakis(oxidanylidene)-2,5,7,9-tetrahydro-1H-cyclopenta[a]phenanthrene-14-carboxylate (three-letter code: 7WX) (formula: $C_{26}H_{34}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	D	1	34	26	8	0	0
			Total	C	O		
4	E	1	34	26	8	0	0

- Molecule 5 is water.

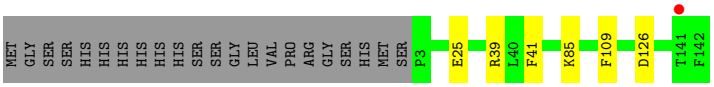
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	88	88	88	0	0
			Total	O		
5	B	98	98	98	0	0
			Total	O		
5	C	55	55	55	0	0
			Total	O		
5	D	50	50	50	0	0
			Total	O		
5	E	32	32	32	0	0
			Total	O		
5	F	53	53	53	0	0

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.

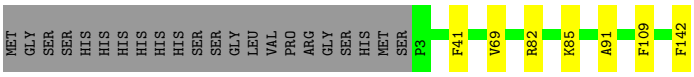
- Molecule 1: Isomerase trt14

Chain A:



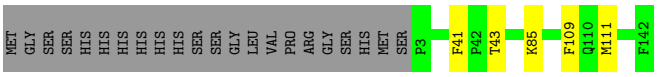
- Molecule 1: Isomerase trt14

Chain B:



- Molecule 1: Isomerase trt14

Chain C:

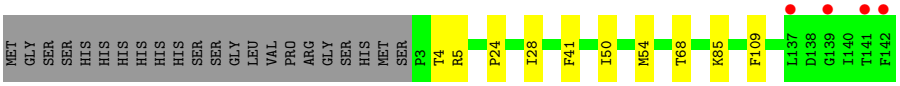


- Molecule 1: Isomerase trt14

Chain D:

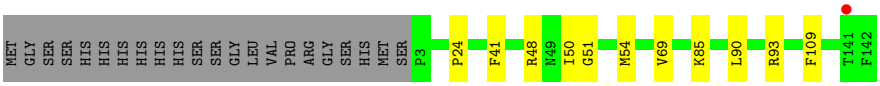
- Molecule 1: Isomerase trt14

Chain E:



- Molecule 1: Isomerase trt14

Chain F:


MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
LEU
VAL
PRO
ARG
GLY
SER
HIS
MET
SER
P3
P24
F41
R48
N49
I50
G51
M54
V69
K85
L90
R93
F109
T141
F142

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.34Å 47.23Å 121.09Å 90.00° 107.95° 90.00°	Depositor
Resolution (Å)	47.25 – 2.10 47.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.25-2.10) 98.5 (47.25-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.250 0.198 , 0.251	Depositor DCC
R_{free} test set	3105 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7301	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: 7WX, CA, 7WU

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	0.39	0/1140	0.56	0/1541
1	B	0.38	0/1140	0.56	0/1541
1	C	0.36	0/1140	0.52	0/1541
1	D	0.39	0/1140	0.57	1/1541 (0.1%)
1	E	0.36	0/1140	0.53	0/1541
1	F	0.35	0/1140	0.54	0/1541
All	All	0.37	0/6840	0.55	1/9246 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	90	LEU	CA-CB-CG	5.68	128.36	115.30

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	1119	0	1094	3	1
1	B	1119	0	1094	3	1
1	C	1119	0	1094	2	0
1	D	1119	0	1094	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1119	0	1094	8	0
1	F	1119	0	1094	5	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
3	A	34	0	0	1	0
3	B	34	0	0	0	0
3	C	34	0	0	1	0
3	F	34	0	0	1	0
4	D	34	0	0	2	0
4	E	34	0	0	0	0
5	A	88	0	0	0	0
5	B	98	0	0	0	0
5	C	55	0	0	0	0
5	D	50	0	0	0	0
5	E	32	0	0	0	0
5	F	53	0	0	0	0
All	All	7301	0	6564	26	1

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 (26) 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:E:4:THR:HG22	1:E:5:ARG:N	1.99	0.76
1:E:4:THR:CG2	1:E:5:ARG:N	2.63	0.61
1:F:48:ARG:NH1	3:F:203:7WU:OBC	2.36	0.59
3:A:204:7WU:OAW	3:A:204:7WU:OBC	2.21	0.59
1:D:39:ARG:NH1	4:D:201:7WX:OBE	2.36	0.58
1:F:50:ILE:HD12	1:F:51:GLY:N	2.24	0.53
1:E:4:THR:HG22	1:E:5:ARG:H	1.74	0.51
1:E:28:ILE:HB	1:E:50:ILE:HD12	1.93	0.50
1:E:4:THR:CG2	1:E:5:ARG:H	2.25	0.49
1:F:69:VAL:HG13	1:F:90:LEU:HB3	1.94	0.49
1:C:85:LYS:HA	1:C:109:PHE:O	2.13	0.48
1:E:85:LYS:HA	1:E:109:PHE:O	2.14	0.48
1:F:85:LYS:HA	1:F:109:PHE:O	2.15	0.47
1:F:24:PRO:HB2	1:F:54:MET:HE3	1.97	0.46
1:A:126:ASP:OD2	1:C:43:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:VAL:HG13	1:D:47:THR:HG23	1.98	0.44
1:A:25:GLU:H	1:A:25:GLU:CD	2.21	0.44
1:B:82:ARG:NH1	1:E:68:THR:OG1	2.37	0.44
1:E:24:PRO:O	1:E:54:MET:HG2	2.18	0.43
1:A:85:LYS:HA	1:A:109:PHE:O	2.19	0.43
1:D:19:TYR:HE2	4:D:201:7WX:CBB	2.31	0.42
1:D:85:LYS:HA	1:D:109:PHE:O	2.19	0.42
1:B:85:LYS:HA	1:B:109:PHE:O	2.20	0.42
3:C:201:7WU:OAW	3:C:201:7WU:OBC	2.39	0.41
1:D:78:ILE:HB	1:D:87:VAL:HB	2.02	0.40
1:B:69:VAL:HA	1:B:91:ALA:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:NH2	1:B:142:PHE:O[2_855]	2.17	0.03

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	138/162 (85%)	136 (99%)	1 (1%)	1 (1%)	22	18
1	B	138/162 (85%)	137 (99%)	0	1 (1%)	22	18
1	C	138/162 (85%)	137 (99%)	0	1 (1%)	22	18
1	D	138/162 (85%)	136 (99%)	1 (1%)	1 (1%)	22	18
1	E	138/162 (85%)	135 (98%)	2 (1%)	1 (1%)	22	18
1	F	138/162 (85%)	134 (97%)	3 (2%)	1 (1%)	22	18
All	All	828/972 (85%)	815 (98%)	7 (1%)	6 (1%)	22	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PHE
1	B	41	PHE
1	E	41	PHE
1	F	41	PHE
1	C	41	PHE
1	D	41	PHE

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	124/143 (87%)	124 (100%)	0	100	100
1	B	124/143 (87%)	124 (100%)	0	100	100
1	C	124/143 (87%)	123 (99%)	1 (1%)	81	86
1	D	124/143 (87%)	122 (98%)	2 (2%)	62	69
1	E	124/143 (87%)	124 (100%)	0	100	100
1	F	124/143 (87%)	123 (99%)	1 (1%)	81	86
All	All	744/858 (87%)	740 (100%)	4 (0%)	88	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	111	MET
1	D	120	ARG
1	D	135	SER
1	F	93	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	7WX	E	201	-	32,37,37	4.59	13 (40%)	40,67,67	1.63	6 (15%)
4	7WX	D	201	-	32,37,37	4.47	14 (43%)	40,67,67	1.37	6 (15%)
3	7WU	B	202	-	34,37,37	4.24	12 (35%)	42,65,65	1.55	7 (16%)
3	7WU	C	201	-	34,37,37	4.32	12 (35%)	42,65,65	1.47	7 (16%)
3	7WU	F	203	-	34,37,37	4.36	12 (35%)	42,65,65	1.58	7 (16%)
3	7WU	A	204	-	34,37,37	4.46	12 (35%)	42,65,65	1.50	6 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	7WX	E	201	-	-	2/8/110/110	0/4/4/4
4	7WX	D	201	-	-	3/8/110/110	0/4/4/4
3	7WU	B	202	-	-	0/8/101/101	0/4/4/4
3	7WU	C	201	-	-	0/8/101/101	0/4/4/4
3	7WU	F	203	-	-	2/8/101/101	0/4/4/4
3	7WU	A	204	-	-	2/8/101/101	0/4/4/4

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	7WU	CAZ-CBA	-12.89	1.40	1.54
3	A	204	7WU	CAZ-CBA	-12.30	1.41	1.54
3	B	202	7WU	CAZ-CBA	-12.20	1.41	1.54
3	F	203	7WU	CAZ-CBA	-11.72	1.42	1.54
3	A	204	7WU	CAL-CBA	-11.25	1.43	1.53
4	D	201	7WX	CAL-CAQ	-10.99	1.41	1.54
3	F	203	7WU	CAL-CBA	-10.97	1.43	1.53
3	C	201	7WU	CAL-CBA	-9.99	1.44	1.53
3	B	202	7WU	CAL-CBA	-9.99	1.44	1.53
4	E	201	7WX	CAL-CAQ	-9.98	1.42	1.54
3	A	204	7WU	CAC-CAB	-9.66	1.39	1.52
4	E	201	7WX	CAH-CAG	-9.47	1.38	1.52
4	D	201	7WX	CAJ-CAN	-9.38	1.39	1.50
3	F	203	7WU	CAC-CAB	-9.28	1.39	1.52
3	C	201	7WU	CAC-CAB	-9.14	1.39	1.52
4	E	201	7WX	CAJ-CAN	-9.12	1.39	1.50
4	E	201	7WX	CAC-CAB	-9.03	1.40	1.52
3	B	202	7WU	CAH-CAG	-8.87	1.39	1.52
4	E	201	7WX	CAP-CAQ	-8.69	1.40	1.54
4	D	201	7WX	CAP-CAO	-8.67	1.40	1.54
3	C	201	7WU	CAH-CAG	-8.38	1.40	1.52
4	D	201	7WX	CAC-CAB	-8.33	1.41	1.52
3	F	203	7WU	CAJ-CAN	-8.29	1.40	1.50
3	B	202	7WU	CAC-CAB	-8.29	1.41	1.52
3	A	204	7WU	CAJ-CAN	-8.27	1.40	1.50
3	A	204	7WU	CAH-CAG	-8.21	1.40	1.52
3	F	203	7WU	CAH-CAG	-7.95	1.40	1.52
4	D	201	7WX	CAH-CAG	-7.93	1.40	1.52
4	E	201	7WX	CAP-CAO	-7.76	1.41	1.54
3	C	201	7WU	CAJ-CAN	-7.69	1.41	1.50
3	B	202	7WU	CAJ-CAN	-7.08	1.42	1.50
3	A	204	7WU	CAD-CAG	-6.95	1.39	1.51
4	D	201	7WX	CAP-CAQ	-6.60	1.43	1.54
4	E	201	7WX	CAA-CAB	-6.50	1.40	1.50
4	D	201	7WX	CAA-CAB	-6.49	1.40	1.50
3	F	203	7WU	CAD-CAG	-6.49	1.40	1.51
3	B	202	7WU	CAA-CAB	-6.38	1.40	1.50
4	E	201	7WX	CAD-CAG	-6.32	1.40	1.51
3	C	201	7WU	CAD-CAG	-6.29	1.41	1.51
4	D	201	7WX	CAR-CAM	-6.00	1.38	1.50
4	D	201	7WX	CAD-CAG	-5.87	1.41	1.51
3	F	203	7WU	CAA-CAB	-5.81	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	204	7WU	CAA-CAB	-5.78	1.41	1.50
3	C	201	7WU	CAO-CAM	-5.51	1.39	1.50
3	B	202	7WU	CAD-CAG	-5.29	1.42	1.51
3	B	202	7WU	CAN-CAM	5.11	1.41	1.33
4	E	201	7WX	CAK-CAI	5.00	1.64	1.58
3	F	203	7WU	CAO-CAM	-4.97	1.40	1.50
3	A	204	7WU	CAO-CAM	-4.96	1.40	1.50
4	E	201	7WX	CAR-CAM	-4.93	1.40	1.50
3	F	203	7WU	CAN-CAM	4.91	1.40	1.33
3	C	201	7WU	CAA-CAB	-4.88	1.42	1.50
3	A	204	7WU	CAN-CAM	4.88	1.40	1.33
3	B	202	7WU	CAO-CAM	-4.87	1.40	1.50
3	C	201	7WU	CAN-CAM	4.78	1.40	1.33
3	B	202	7WU	CAK-CAX	-4.43	1.40	1.50
4	E	201	7WX	CAN-CAM	4.24	1.39	1.33
4	E	201	7WX	OBG-CBA	4.07	1.41	1.33
4	D	201	7WX	OBG-CBA	3.81	1.40	1.33
3	C	201	7WU	CAK-CAX	-3.75	1.42	1.50
4	D	201	7WX	CAK-CAI	3.71	1.62	1.58
3	F	203	7WU	CAK-CAX	-3.25	1.43	1.50
4	D	201	7WX	CAN-CAM	3.19	1.38	1.33
4	E	201	7WX	CAK-CBA	-2.66	1.46	1.51
3	A	204	7WU	CAK-CAX	-2.60	1.44	1.50
4	D	201	7WX	OBC-CAP	2.54	1.46	1.42
4	D	201	7WX	CAK-CBA	-2.34	1.47	1.51
3	A	204	7WU	CAI-CAK	2.27	1.60	1.56
3	C	201	7WU	OBF-CBE	2.27	1.37	1.33
3	A	204	7WU	CAZ-CBE	-2.26	1.42	1.54
3	F	203	7WU	CAZ-CBE	-2.21	1.42	1.54
3	C	201	7WU	CAZ-CBE	-2.15	1.42	1.54
3	B	202	7WU	CAZ-CBE	-2.12	1.42	1.54
3	B	202	7WU	OBF-CBE	2.05	1.37	1.33
3	F	203	7WU	OBF-CBE	2.00	1.37	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	203	7WU	CBH-OBF-CBE	-5.68	106.36	115.94
4	E	201	7WX	CBH-OBG-CBA	5.23	124.75	115.94
3	C	201	7WU	CBH-OBF-CBE	-4.41	108.50	115.94
3	A	204	7WU	CBH-OBF-CBE	-4.34	108.62	115.94
4	E	201	7WX	CAA-CAF-CAE	-4.09	108.23	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	7WU	OBF-CBE-CAZ	4.06	118.11	110.75
3	C	201	7WU	CAA-CAF-CAE	-3.74	108.68	113.47
3	B	202	7WU	CBH-OBF-CBE	-3.68	109.73	115.94
3	F	203	7WU	CAO-CAM-CAN	-3.34	114.10	121.54
3	A	204	7WU	CAO-CAM-CAN	-3.30	114.18	121.54
3	A	204	7WU	OAV-CAG-CAH	3.03	123.40	120.14
3	B	202	7WU	CAA-CAF-CAE	-2.89	109.76	113.47
4	E	201	7WX	CAR-CAM-CAN	-2.87	115.14	121.54
3	A	204	7WU	CAF-CAE-CAD	-2.75	104.68	108.09
3	A	204	7WU	CAA-CAF-CAE	-2.69	110.02	113.47
3	B	202	7WU	CBD-CAZ-CBE	-2.67	105.13	109.26
3	F	203	7WU	CAF-CAE-CAD	-2.64	104.81	108.09
4	D	201	7WX	OBD-CAG-CAH	2.62	122.97	120.14
4	E	201	7WX	OBG-CBA-CAK	2.59	116.70	110.68
3	B	202	7WU	OBB-CBA-CAZ	-2.58	116.41	119.54
3	B	202	7WU	CAO-CAM-CAN	-2.50	115.97	121.54
3	A	204	7WU	CAO-CAM-CAL	2.49	122.28	117.97
4	E	201	7WX	CAF-CAA-CAB	-2.45	106.73	113.05
3	C	201	7WU	CAO-CAM-CAN	-2.44	116.09	121.54
4	D	201	7WX	CAV-CAI-CAH	-2.43	104.98	109.12
3	F	203	7WU	OBF-CBE-CAZ	2.41	115.12	110.75
4	D	201	7WX	CAA-CAF-CAE	-2.41	110.38	113.47
3	C	201	7WU	OBB-CBA-CAZ	-2.36	116.67	119.54
3	C	201	7WU	OBF-CBE-CAZ	2.34	115.00	110.75
4	E	201	7WX	CAV-CAI-CAH	-2.33	105.14	109.12
4	D	201	7WX	CAV-CAI-CAK	2.27	112.33	109.70
3	B	202	7WU	OAY-CAX-OBC	2.27	123.27	118.33
3	F	203	7WU	CBD-CAZ-CBE	-2.26	105.76	109.26
3	C	201	7WU	CBD-CAZ-CBA	-2.24	107.42	110.42
3	F	203	7WU	CAO-CAM-CAL	2.22	121.81	117.97
3	C	201	7WU	OAY-CAX-OBC	2.16	123.04	118.33
4	D	201	7WX	CAR-CAM-CAN	-2.14	116.78	121.54
3	F	203	7WU	CAA-CAF-CAE	-2.06	110.83	113.47
4	D	201	7WX	CAF-CAE-CAD	-2.01	105.60	108.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	204	7WU	CAZ-CBE-OBF-CBH
3	F	203	7WU	CAZ-CBE-OBF-CBH
4	D	201	7WX	CAK-CBA-OBG-CBH

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Mol	Chain	Res	Type	Atoms
4	E	201	7WX	CAK-CBA-OBG-CBH
4	E	201	7WX	OBF-CBA-OBG-CBH
4	D	201	7WX	OBF-CBA-OBG-CBH
3	F	203	7WU	OBG-CBE-OBF-CBH
3	A	204	7WU	OBG-CBE-OBF-CBH
4	D	201	7WX	CAL-CAK-CBA-OBF

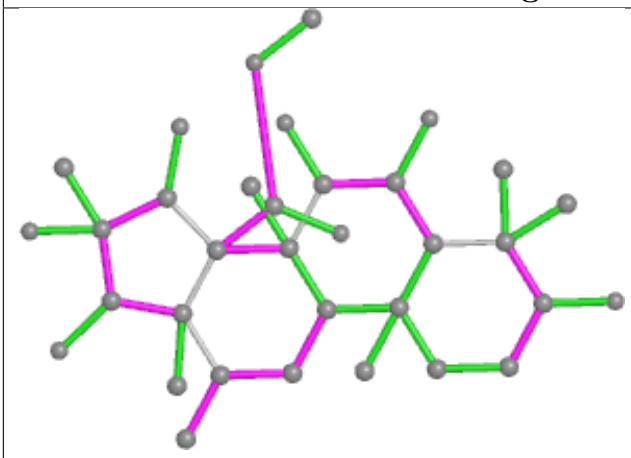
There are no ring outliers.

4 monomers are involved in 5 short contacts:

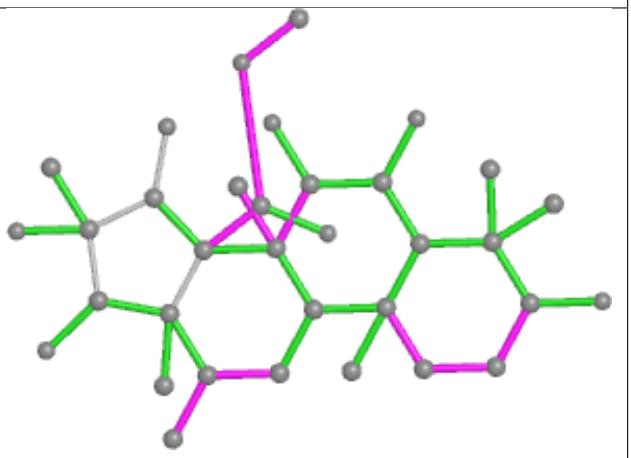
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	201	7WX	2	0
3	C	201	7WU	1	0
3	F	203	7WU	1	0
3	A	204	7WU	1	0

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.

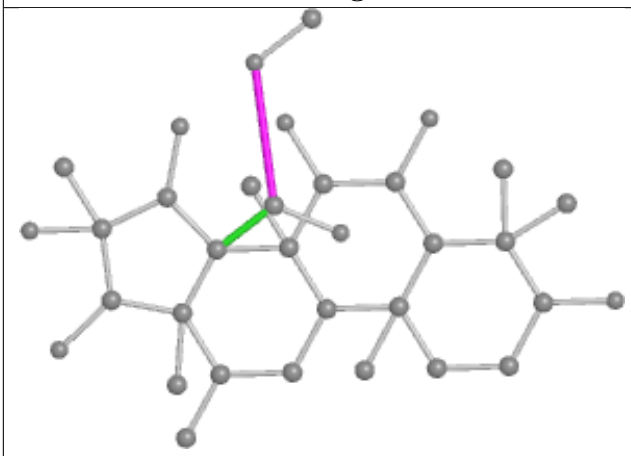
Ligand 7WX E 201



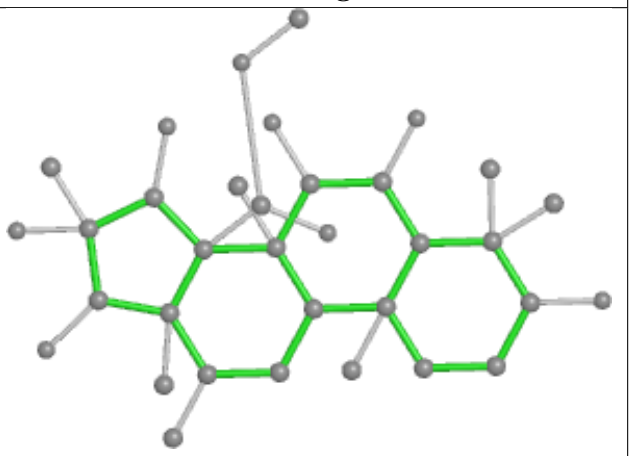
Bond lengths



Bond angles

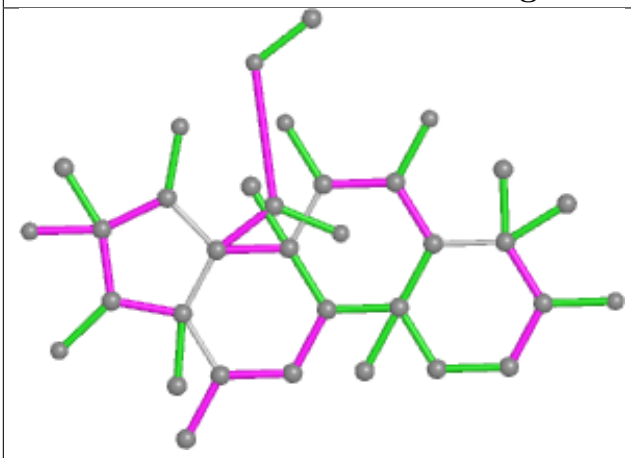


Torsions



Rings

Ligand 7WX D 201



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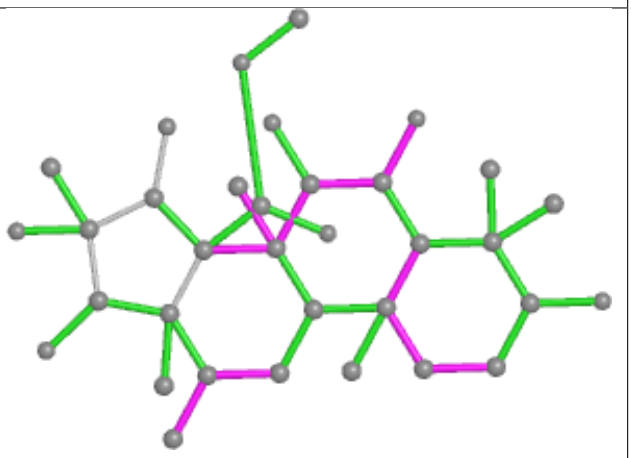
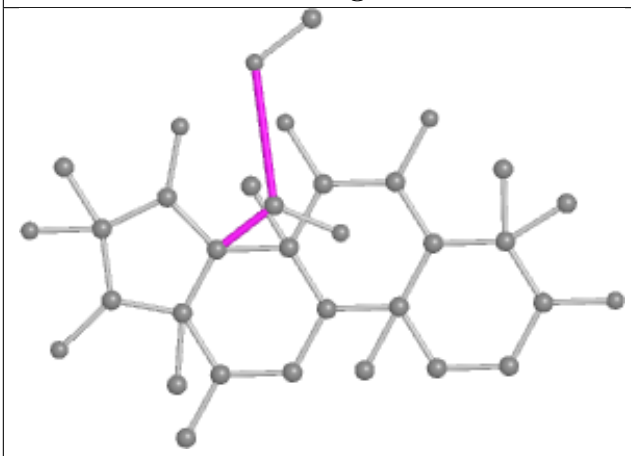
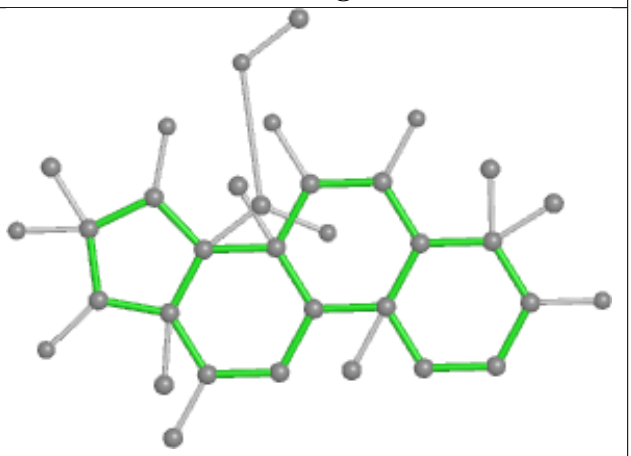


Bond angles

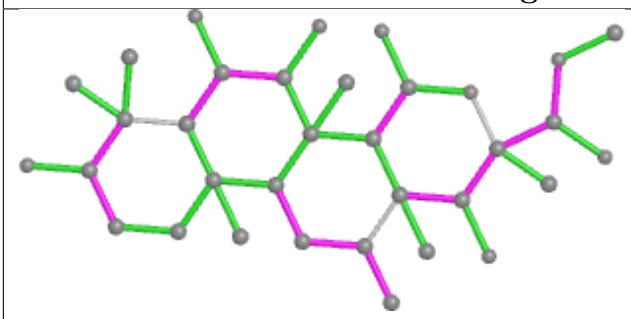


Torsions

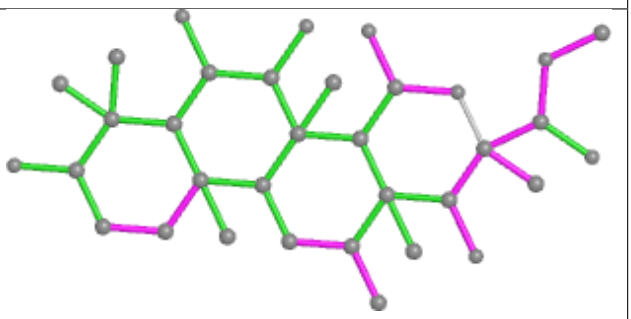


Rings

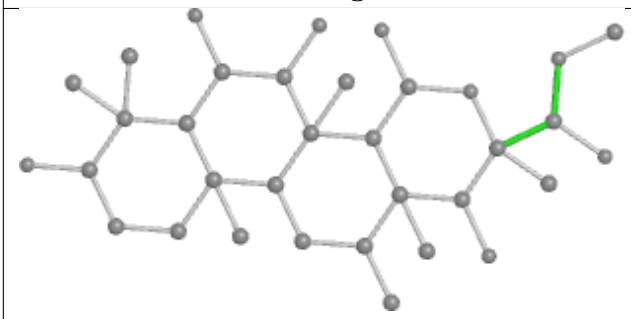
Ligand 7WU B 202



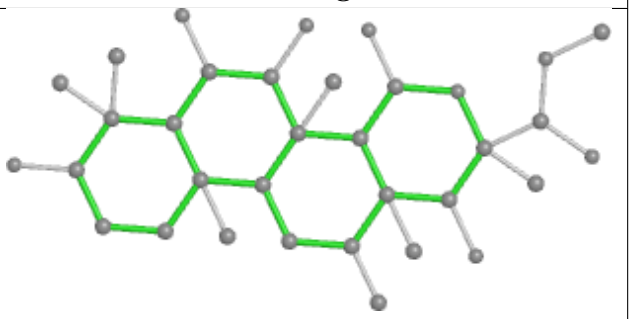
Bond lengths



Bond angles

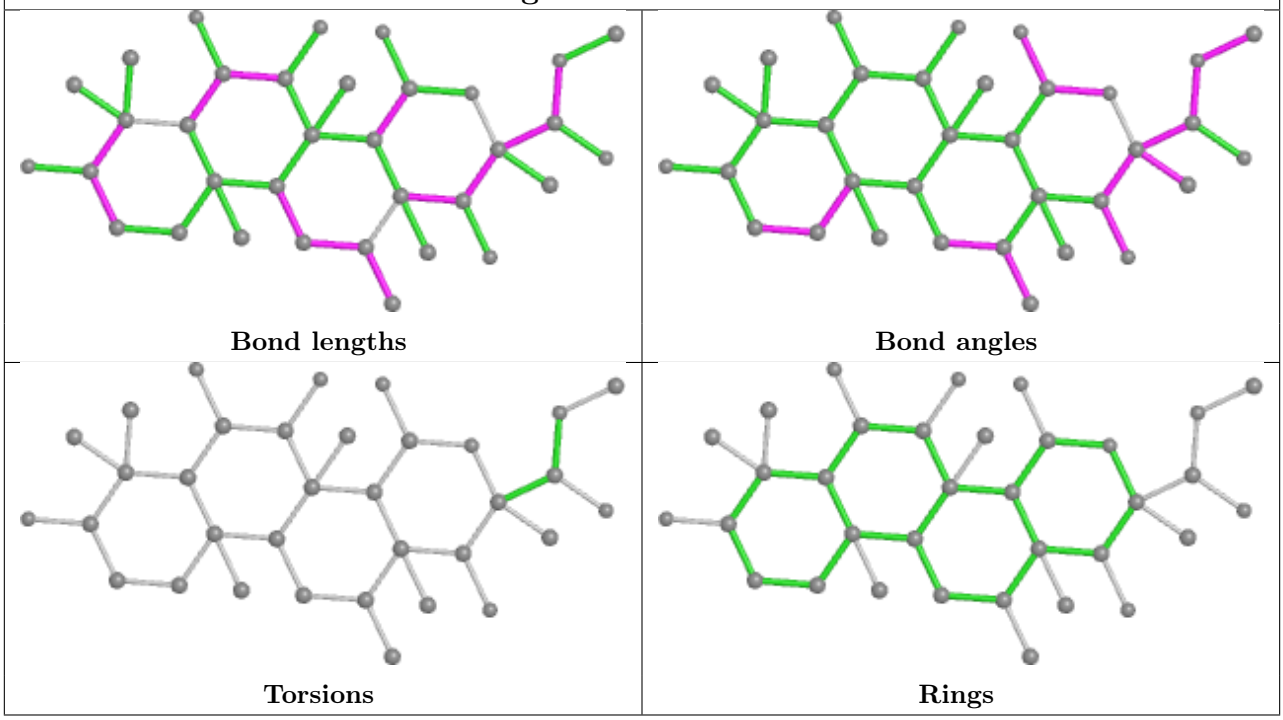


Torsions

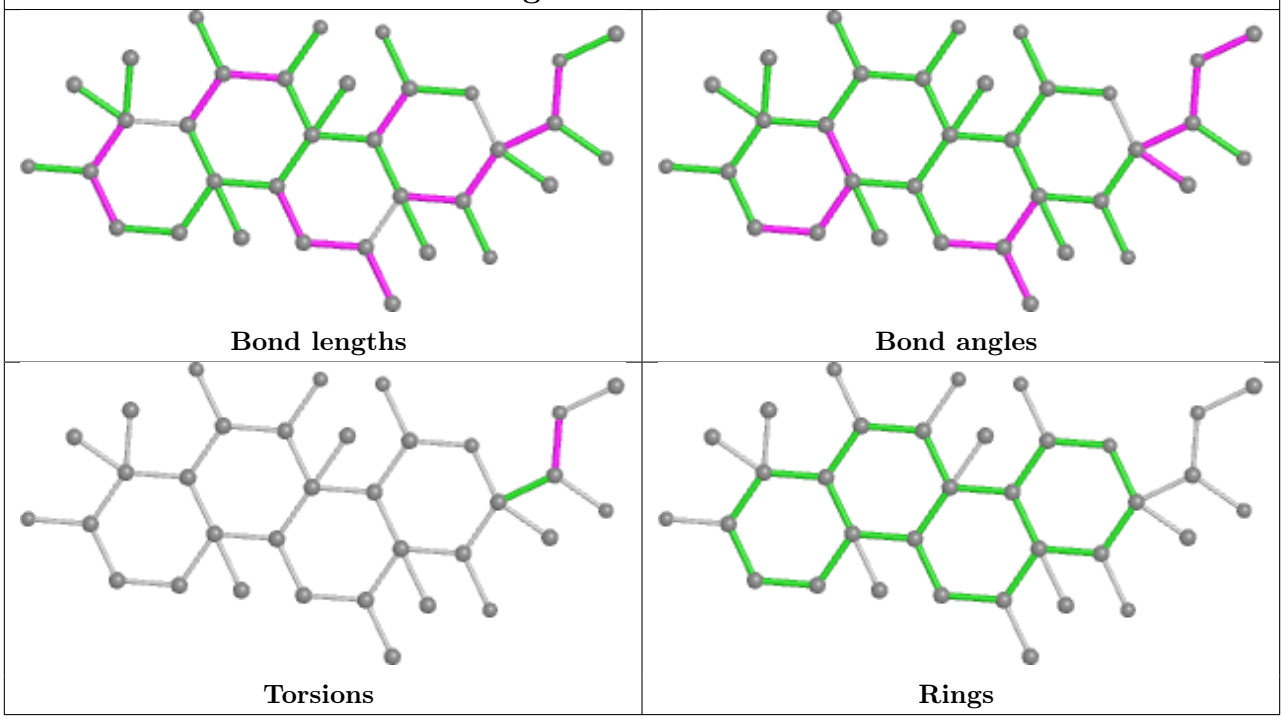


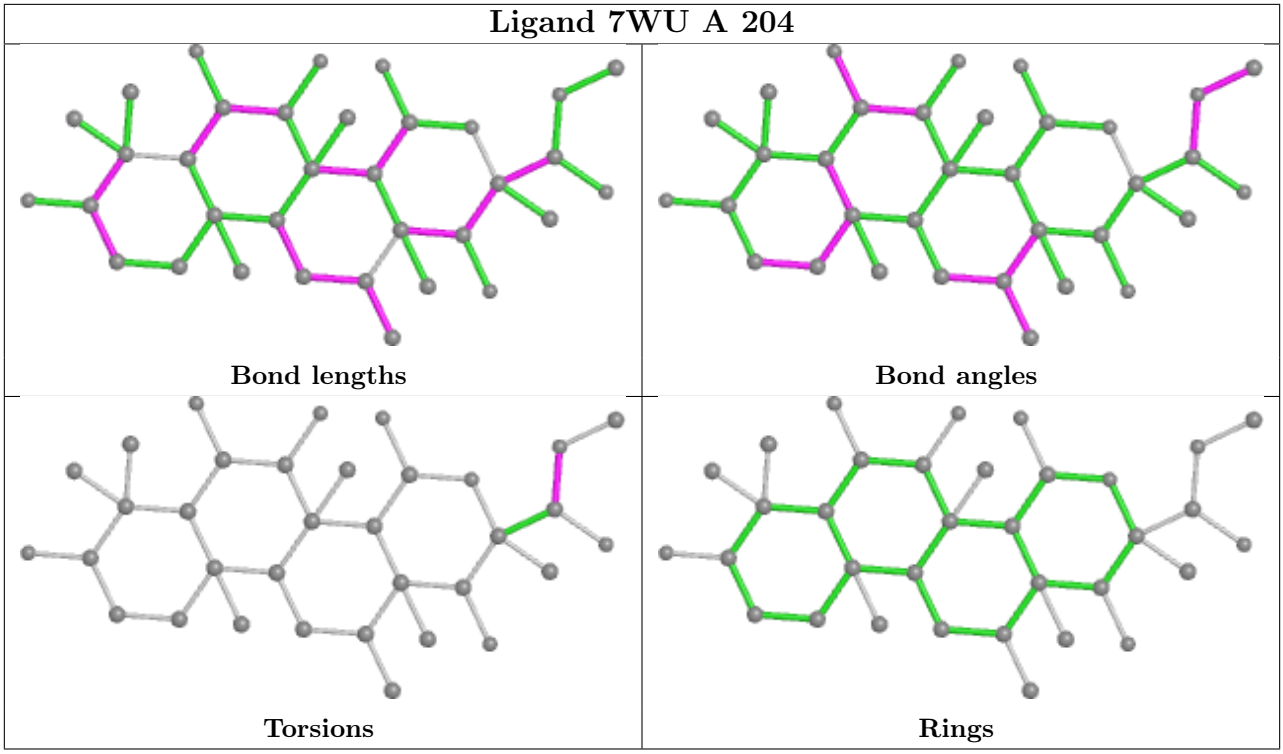
Rings

Ligand 7WU C 201



Ligand 7WU F 203





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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	140/162 (86%)	-0.01	1 (0%)	87	89	26, 35, 50, 59	0
1	B	140/162 (86%)	-0.04	0	100	100	25, 35, 49, 55	0
1	C	140/162 (86%)	-0.12	0	100	100	29, 43, 56, 65	0
1	D	140/162 (86%)	0.01	4 (2%)	51	57	27, 44, 56, 71	0
1	E	140/162 (86%)	0.20	4 (2%)	51	57	33, 47, 58, 62	0
1	F	140/162 (86%)	-0.01	1 (0%)	87	89	33, 44, 58, 67	0
All	All	840/972 (86%)	0.00	10 (1%)	79	82	25, 41, 56, 71	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	142	PHE	4.0
1	A	141	THR	3.2
1	D	93	ARG	2.9
1	F	141	THR	2.8
1	E	139	GLY	2.7
1	D	141	THR	2.7
1	D	142	PHE	2.7
1	E	141	THR	2.4
1	E	137	LEU	2.1
1	D	140	ILE	2.1

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)

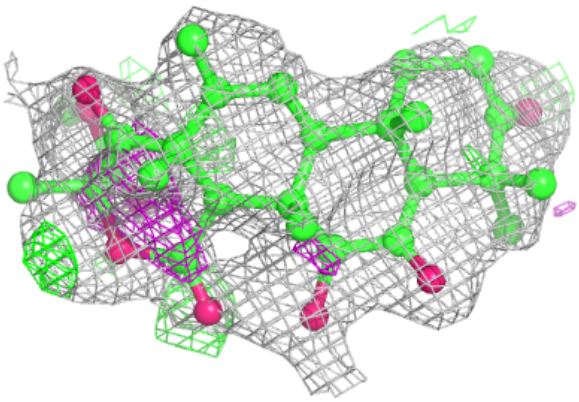
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

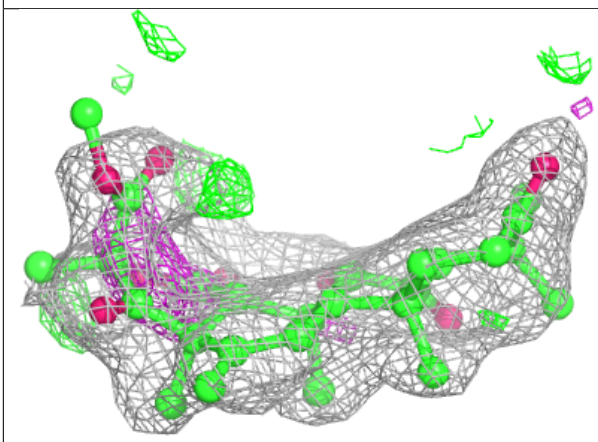
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	7WU	A	204	34/34	0.80	0.25	40,57,71,75	0
3	7WU	F	203	34/34	0.82	0.20	35,52,77,79	0
3	7WU	B	202	34/34	0.83	0.21	36,45,71,76	0
4	7WX	E	201	34/34	0.84	0.23	39,56,76,87	0
4	7WX	D	201	34/34	0.85	0.22	39,58,78,93	0
3	7WU	C	201	34/34	0.88	0.17	32,51,76,79	0
2	CA	A	201	1/1	0.89	0.07	52,52,52,52	0
2	CA	A	203	1/1	0.94	0.06	50,50,50,50	0
2	CA	F	201	1/1	0.95	0.23	74,74,74,74	0
2	CA	E	202	1/1	0.96	0.06	56,56,56,56	0
2	CA	A	202	1/1	0.97	0.17	63,63,63,63	0
2	CA	B	201	1/1	0.98	0.07	46,46,46,46	0
2	CA	F	202	1/1	0.98	0.08	47,47,47,47	0

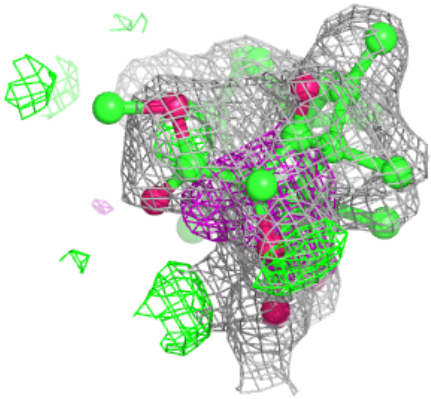
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7WU A 204:

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

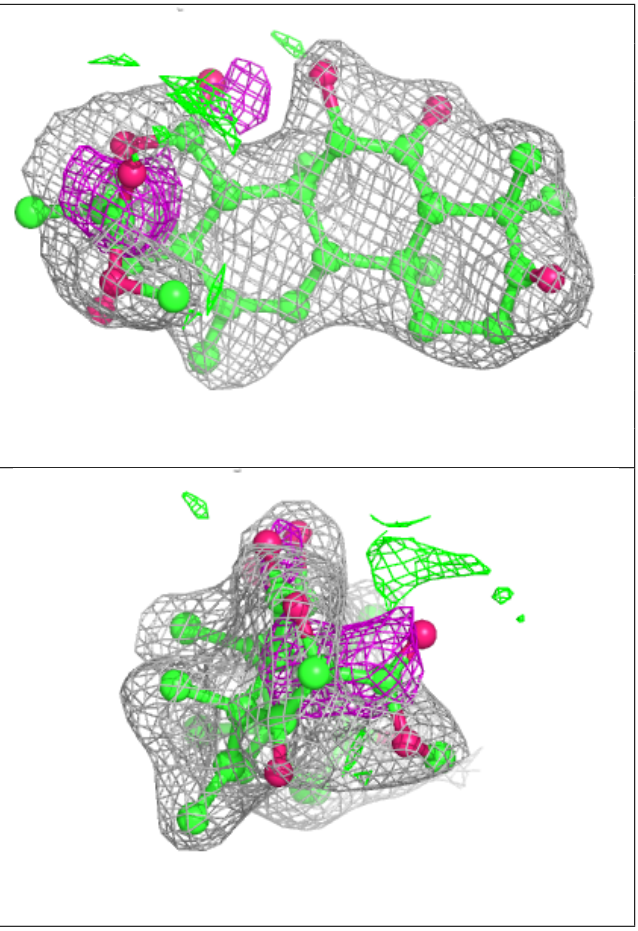


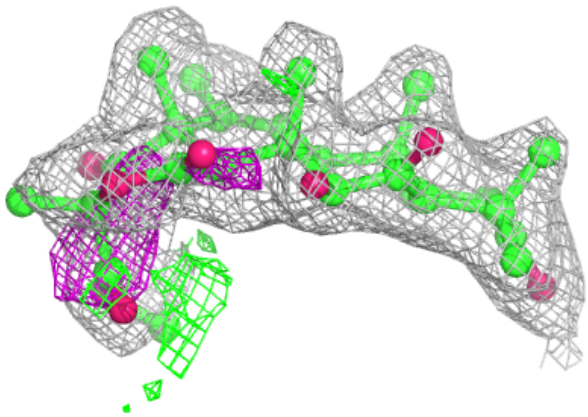




Electron density around 7WU F 203:

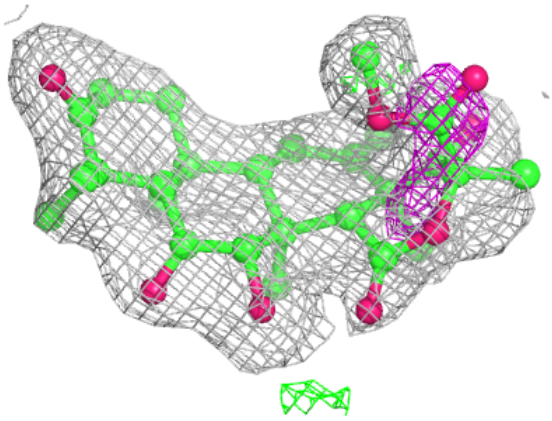
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

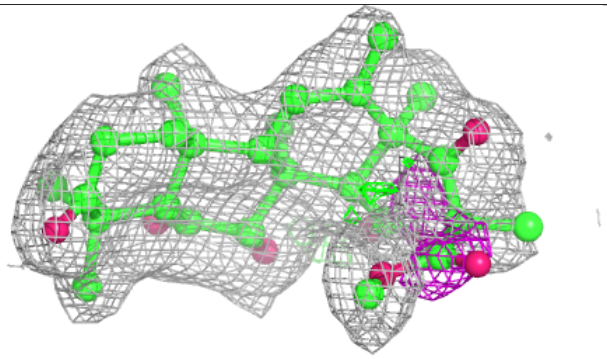


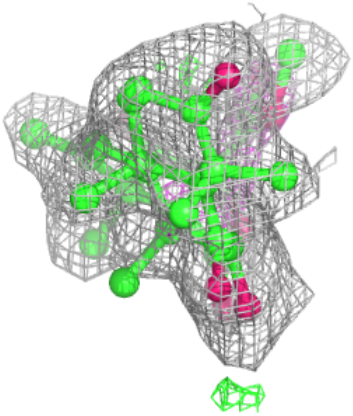


Electron density around 7WU B 202:

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

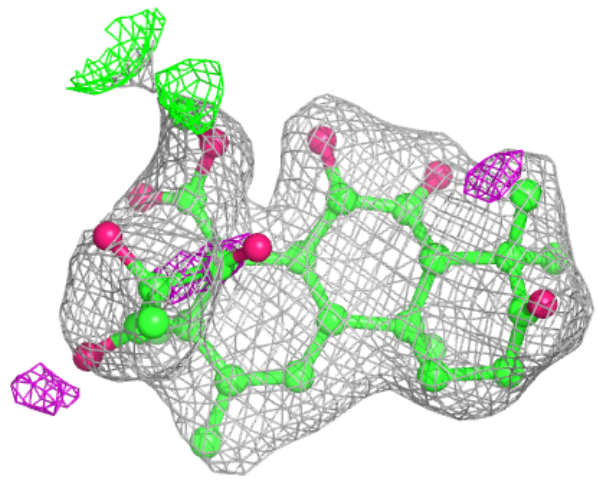


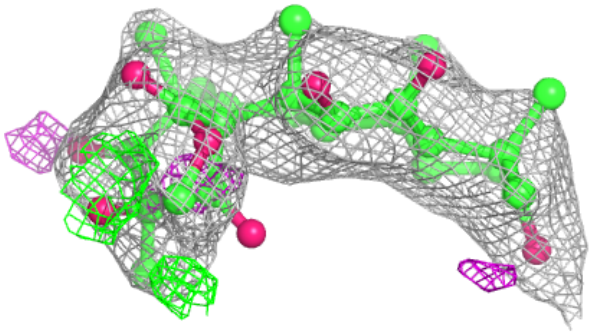


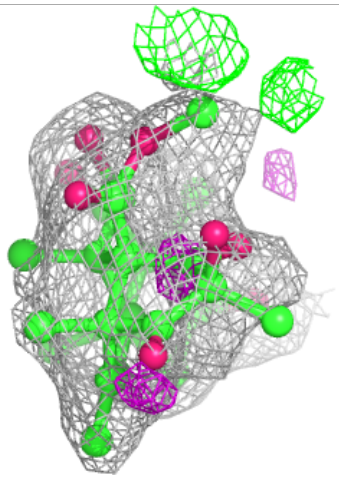


Electron density around 7WX E 201:

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

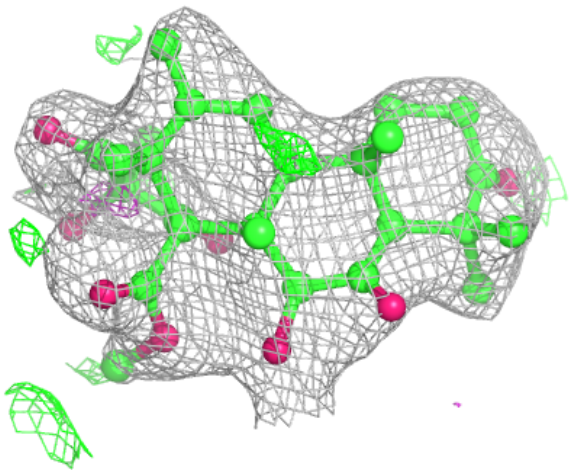


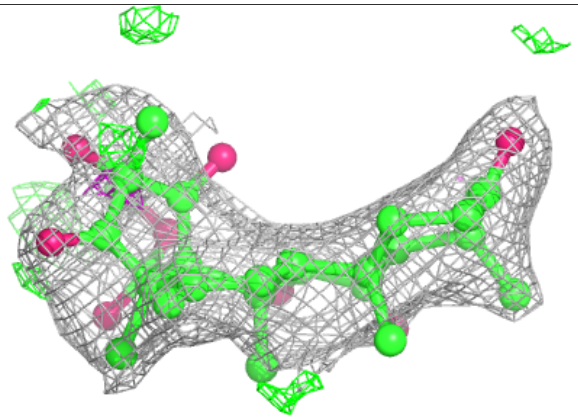


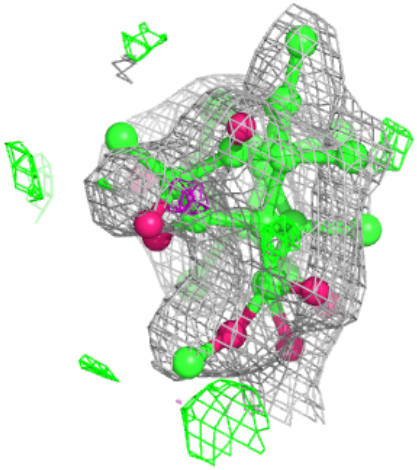


Electron density around 7WX D 201:

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

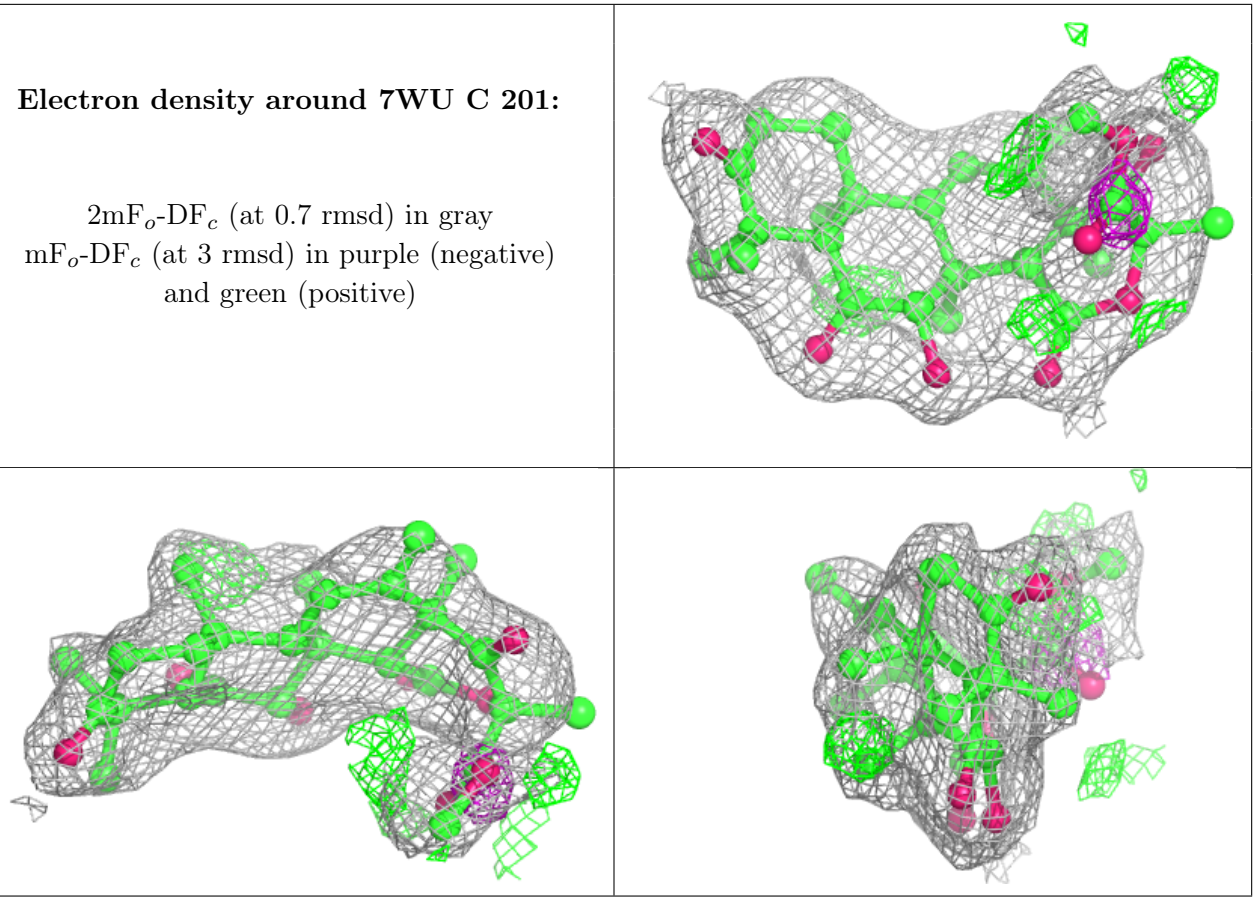






Electron density around 7WU C 201:

$2mF_o$-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.