Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 07:19 pm GMT

PDB ID	:	1QJE
Title	:	Isopenicillin N synthase from Aspergillus nidulans (IP1 - Fe complex)
Authors	:	Burzlaff, N.I.; Clifton, I.J.; Rutledge, P.J.; Roach, P.L.; Adlington, R.M.; Baldwin, J.E.
Deposited on	:	1999-06-23
Resolution	:	1.35 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:

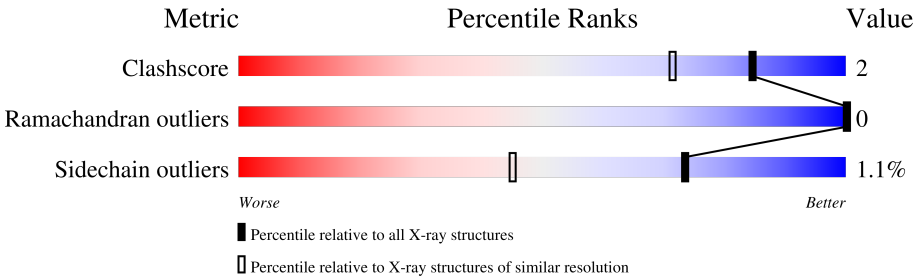
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.35 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))
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)

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%

Mol	Chain	Length	Quality of chain
1	A	331	83% 13%

2 Entry composition (i)

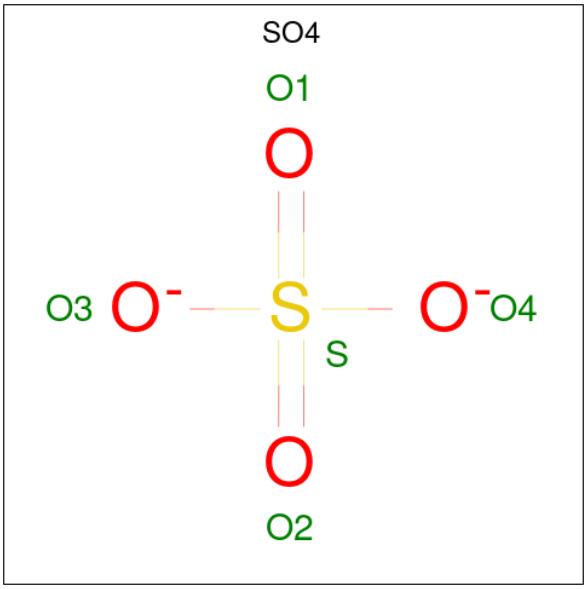
There are 6 unique types of molecules in this entry. The entry contains 3181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ISOPENICILLIN N SYNTHASE.

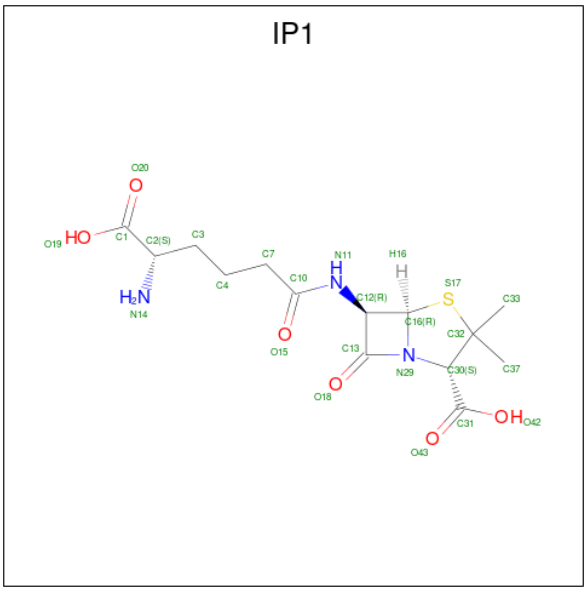
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2635	1684	444	502	5	0	1	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



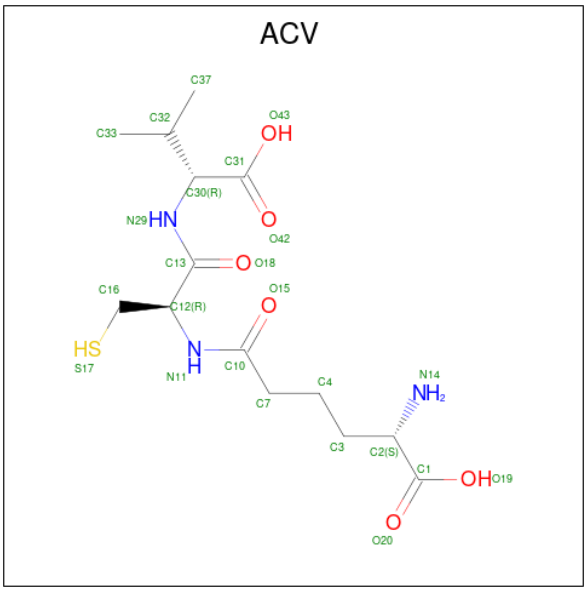
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0

- Molecule 3 is ISOPENICILLIN N (three-letter code: IP1) (formula: $C_{14}H_{21}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	14	3	6	1		

- Molecule 4 is L-D-(A-AMINOADIPOYL)-L-CYSTEINYL-D-VALINE (three-letter code: ACV) (formula: $C_{14}H_{25}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			24	14	3	6	1		

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe 1 1	0	0

- Molecule 6 is water.

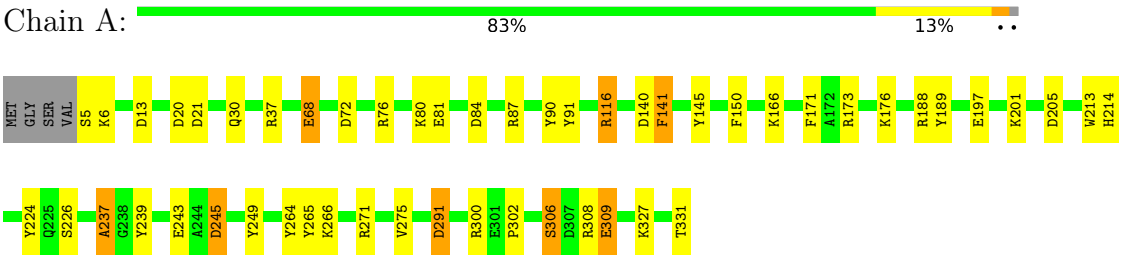
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	492	Total O 492 492	0	0

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. 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. 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: ISOPENICILLIN N SYNTHASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.67Å 71.91Å 101.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.35 23.34 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.2 (25.00-1.35) 91.2 (23.34-1.35)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.35Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.131 , 0.187 0.370 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 81.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	3181	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: ACV, SO4, FE2, IP1

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	1.04	3/2715 (0.1%)	1.84	64/3694 (1.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	GLU	CD-OE2	7.31	1.33	1.25
1	A	331	THR	C-OXT	7.27	1.37	1.23
1	A	306	SER	CB-OG	-5.61	1.34	1.42

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ARG	CD-NE-CZ	26.79	161.10	123.60
1	A	300	ARG	CD-NE-CZ	19.52	150.93	123.60
1	A	116	ARG	NE-CZ-NH2	-15.96	112.32	120.30
1	A	308	ARG	NE-CZ-NH1	13.06	126.83	120.30
1	A	308	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	A	249	TYR	OH-CZ-CE2	12.07	152.70	120.10
1	A	72	ASP	CB-CG-OD1	12.04	129.13	118.30
1	A	249	TYR	CB-CG-CD1	12.00	128.20	121.00
1	A	76	ARG	NE-CZ-NH1	11.87	126.23	120.30
1	A	141	PHE	CB-CG-CD1	-10.67	113.33	120.80
1	A	141	PHE	CB-CG-CD2	10.10	127.87	120.80
1	A	249	TYR	CZ-CE2-CD2	9.78	128.60	119.80
1	A	37	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	76	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	173	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	291	ASP	CB-CG-OD1	8.61	126.05	118.30
1	A	249	TYR	CE1-CZ-OH	-8.32	97.62	120.10
1	A	90	TYR	CB-CG-CD1	8.21	125.92	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	LYS	CG-CD-CE	8.19	136.47	111.90
1	A	145	TYR	CB-CG-CD2	7.86	125.72	121.00
1	A	116	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	87	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	275	VAL	CA-CB-CG1	-7.47	99.69	110.90
1	A	68	GLU	OE1-CD-OE2	-7.41	114.41	123.30
1	A	141	PHE	CZ-CE2-CD2	-7.32	111.32	120.10
1	A	188	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	224	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	A	243	GLU	CB-CG-CD	6.92	132.89	114.20
1	A	116	ARG	CD-NE-CZ	-6.89	113.95	123.60
1	A	226	SER	CB-CA-C	-6.86	97.06	110.10
1	A	150	PHE	CG-CD1-CE1	6.64	128.10	120.80
1	A	239	TYR	CG-CD1-CE1	-6.53	116.08	121.30
1	A	81	GLU	OE1-CD-OE2	-6.40	115.62	123.30
1	A	237	ALA	CB-CA-C	-6.39	100.51	110.10
1	A	249	TYR	CE1-CZ-CE2	-6.37	109.62	119.80
1	A	141	PHE	CG-CD2-CE2	6.36	127.79	120.80
1	A	6	LYS	CB-CG-CD	6.31	128.01	111.60
1	A	84	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	309	GLU	CB-CG-CD	6.24	131.05	114.20
1	A	249	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	A	20	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	84	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	72	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	173	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
1	A	245	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	264	TYR	CB-CG-CD1	5.57	124.34	121.00
1	A	68	GLU	CG-CD-OE1	5.53	129.36	118.30
1	A	21	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	265	TYR	CB-CG-CD1	5.51	124.30	121.00
1	A	271	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	176	LYS	CD-CE-NZ	5.46	124.25	111.70
1	A	13	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	171	PHE	CD1-CE1-CZ	-5.37	113.65	120.10
1	A	201	LYS	CD-CE-NZ	5.36	124.02	111.70
1	A	224	TYR	CB-CG-CD2	5.27	124.16	121.00
1	A	197	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	A	239	TYR	CD1-CE1-CZ	5.24	124.52	119.80
1	A	205	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	266	LYS	CD-CE-NZ	5.17	123.60	111.70
1	A	171	PHE	CB-CG-CD2	-5.15	117.19	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	302	PRO	O-C-N	5.10	130.86	122.70
1	A	237	ALA	N-CA-CB	5.08	117.22	110.10
1	A	30	GLN	CG-CD-OE1	-5.07	111.46	121.60
1	A	189	TYR	CD1-CE1-CZ	-5.06	115.25	119.80

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	2635	0	2518	11	0
2	A	5	0	0	1	0
3	A	24	0	19	0	0
4	A	24	0	21	2	0
5	A	1	0	0	0	0
6	A	492	0	0	8	2
All	All	3181	0	2558	12	2

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

All (12) 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:A:237:ALA:HB1	6:A:2380:HOH:O	2.01	0.60
1:A:140:ASP:HB3	6:A:2482:HOH:O	2.09	0.52
4:A:1334[B]:ACV:H331	6:A:2358:HOH:O	2.11	0.50
1:A:309:GLU:HG2	6:A:2454:HOH:O	2.12	0.48
1:A:141:PHE:HA	2:A:1332:SO4:O1	2.15	0.46
1:A:80:LYS:NZ	6:A:2166:HOH:O	2.50	0.45
1:A:116:ARG:NH2	1:A:291:ASP:OD2	2.50	0.44
1:A:213:TRP:CZ2	1:A:327:LYS:HE3	2.54	0.43
1:A:68:GLU:HB3	6:A:2147:HOH:O	2.19	0.43
1:A:166:LYS:NZ	6:A:2303:HOH:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:HB2	6:A:2011:HOH:O	2.20	0.42
1:A:214:HIS:NE2	4:A:1334[B]:ACV:H162	2.36	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2394:HOH:O	6:A:2482:HOH:O[4_455]	1.80	0.40
6:A:2101:HOH:O	6:A:2220:HOH:O[4_455]	1.91	0.29

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	326/331 (98%)	317 (97%)	9 (3%)	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	282/284 (99%)	279 (99%)	3 (1%)	73 45

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	91	TYR
1	A	306	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	230	ASN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	IP1	A	1333[A]	-	24,25,25	1.01	1 (4%)	36,38,38	1.87	12 (33%)
4	ACV	A	1334[B]	5	22,23,23	1.40	1 (4%)	29,30,30	2.10	11 (37%)
2	SO4	A	1332	-	4,4,4	0.46	0	6,6,6	1.19	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	IP1	A	1333[A]	-	-	4/18/49/49	0/2/2/2
4	ACV	A	1334[B]	5	-	6/32/32/32	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1334[B]	ACV	C30-C31	-5.41	1.43	1.52
3	A	1333[A]	IP1	C30-C31	3.33	1.56	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1334[B]	ACV	C16-C12-N11	-5.25	103.80	111.28
4	A	1334[B]	ACV	C32-C30-C31	4.13	120.46	111.05
3	A	1333[A]	IP1	C16-N29-C30	3.92	122.15	117.26
3	A	1333[A]	IP1	S17-C16-N29	-3.76	100.05	105.10
4	A	1334[B]	ACV	O18-C13-C12	3.28	127.35	120.45
4	A	1334[B]	ACV	C31-C30-N29	3.27	117.41	110.28
3	A	1333[A]	IP1	C13-C12-N11	-3.11	106.51	115.38
3	A	1333[A]	IP1	O18-C13-N29	-2.96	127.58	131.75
3	A	1333[A]	IP1	C37-C32-S17	2.93	114.12	109.21
4	A	1334[B]	ACV	C37-C32-C33	2.90	118.70	110.59
4	A	1334[B]	ACV	C12-N11-C10	2.81	128.88	121.65
3	A	1333[A]	IP1	C37-C32-C33	2.60	115.02	110.78
4	A	1334[B]	ACV	C16-C12-C13	-2.53	104.54	109.76
3	A	1333[A]	IP1	C7-C10-N11	2.51	120.19	115.83
3	A	1333[A]	IP1	C32-C30-N29	-2.46	102.77	106.49
3	A	1333[A]	IP1	O43-C31-C30	-2.42	114.93	123.15
4	A	1334[B]	ACV	O15-C10-N11	-2.37	118.95	122.95
4	A	1334[B]	ACV	O18-C13-N29	-2.23	118.79	122.93
3	A	1333[A]	IP1	O18-C13-C12	2.18	142.41	136.31
4	A	1334[B]	ACV	C33-C32-C30	-2.11	105.19	111.16
4	A	1334[B]	ACV	C30-N29-C13	2.04	127.10	121.89
3	A	1333[A]	IP1	C33-C32-C30	-2.03	107.06	111.57
3	A	1333[A]	IP1	C32-S17-C16	-2.01	89.67	94.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1334[B]	ACV	C31-C30-C32-C33
4	A	1334[B]	ACV	C31-C30-C32-C37
3	A	1333[A]	IP1	C13-C12-N11-C10
3	A	1333[A]	IP1	N14-C2-C3-C4
4	A	1334[B]	ACV	N11-C12-C13-N29
4	A	1334[B]	ACV	C32-C30-N29-C13
4	A	1334[B]	ACV	N11-C12-C13-O18
4	A	1334[B]	ACV	C32-C30-C31-O43
3	A	1333[A]	IP1	C32-C30-C31-O42
3	A	1333[A]	IP1	C32-C30-C31-O43

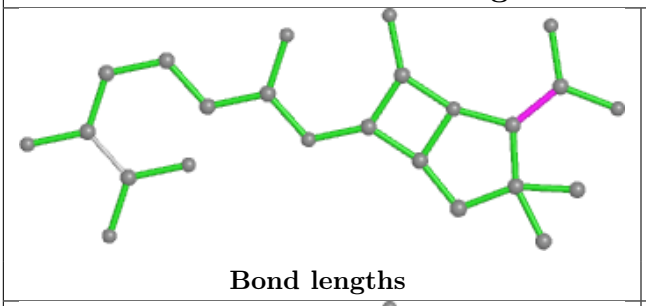
There are no ring outliers.

2 monomers are involved in 3 short contacts:

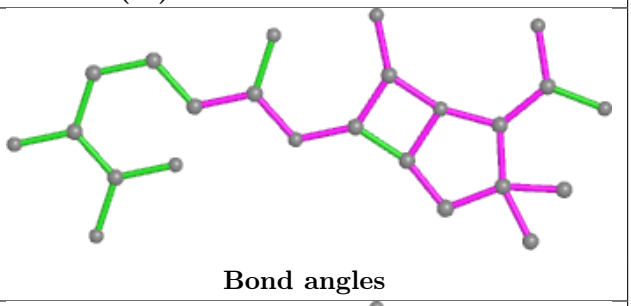
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1334[B]	ACV	2	0
2	A	1332	SO4	1	0

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.

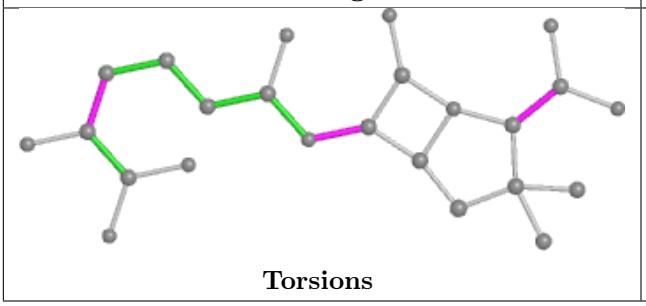
Ligand IP1 A 1333 (A)



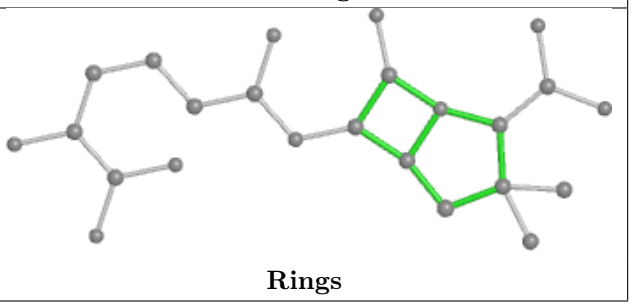
Bond lengths



Bond angles

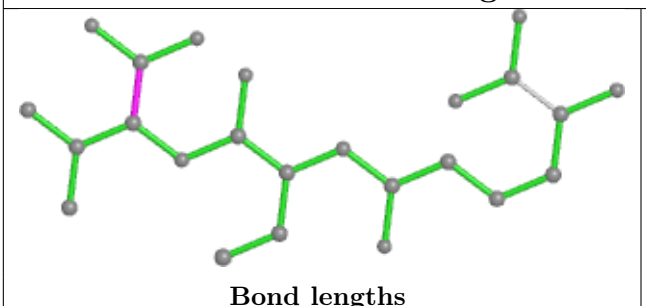


Torsions

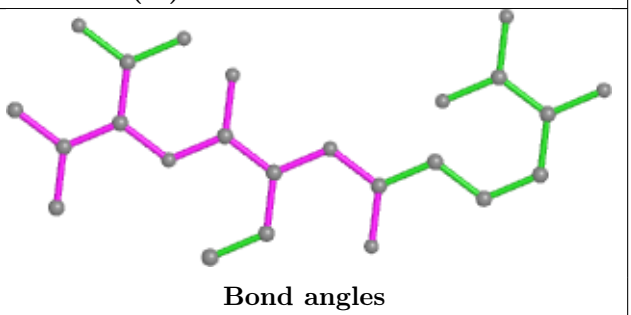


Rings

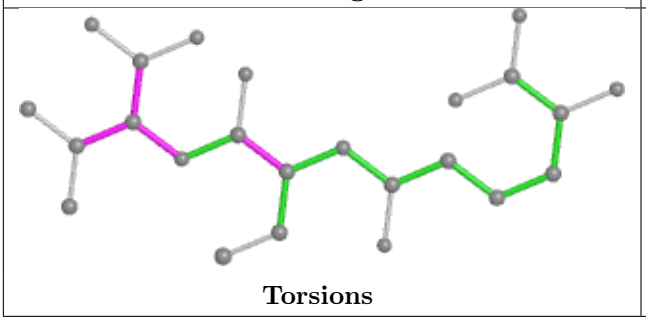
Ligand ACV A 1334 (B)



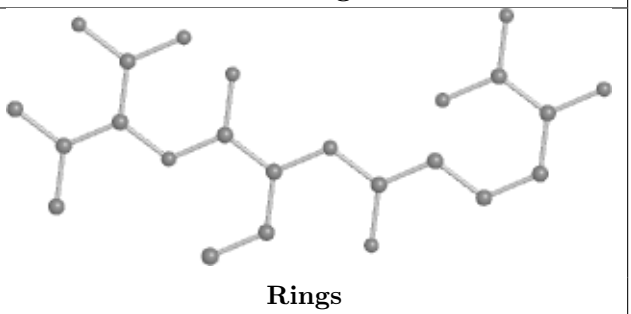
Bond lengths



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

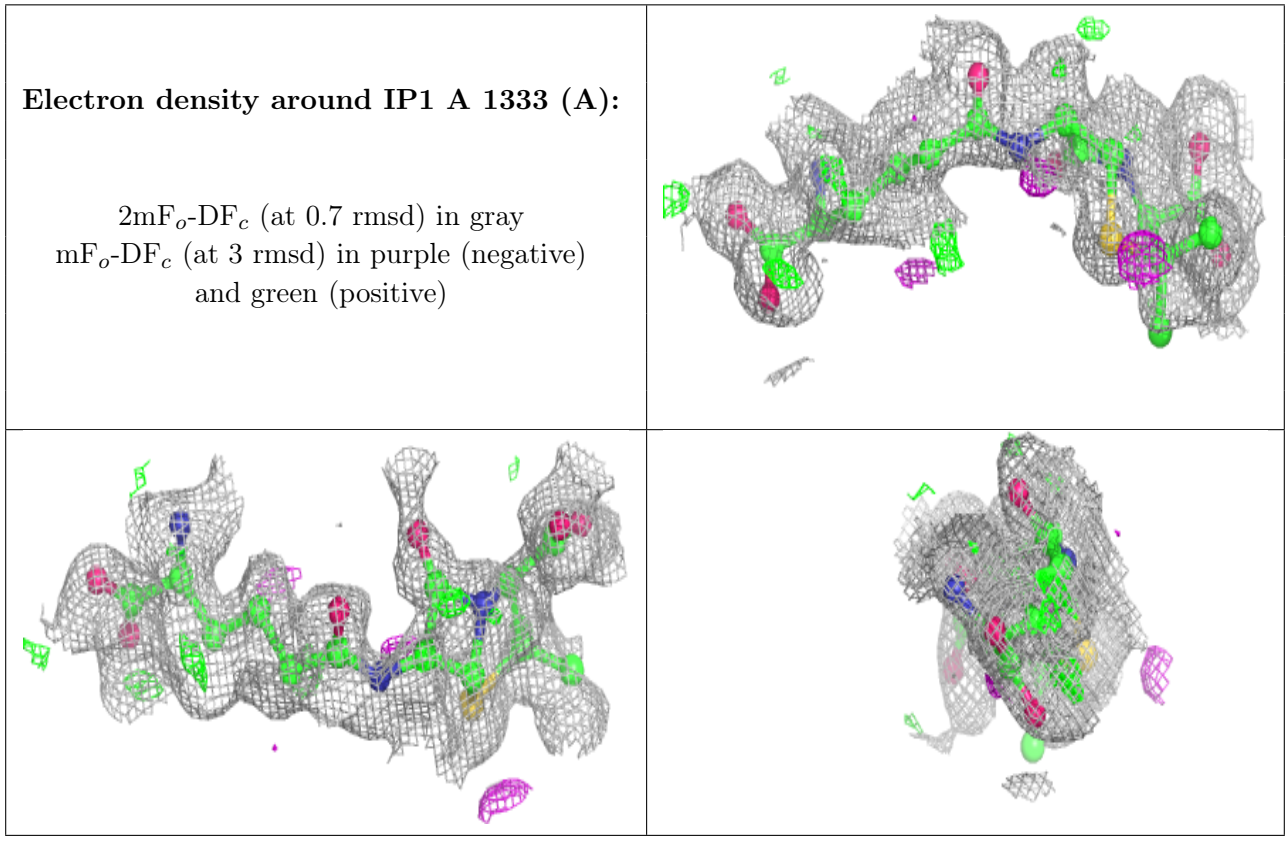
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

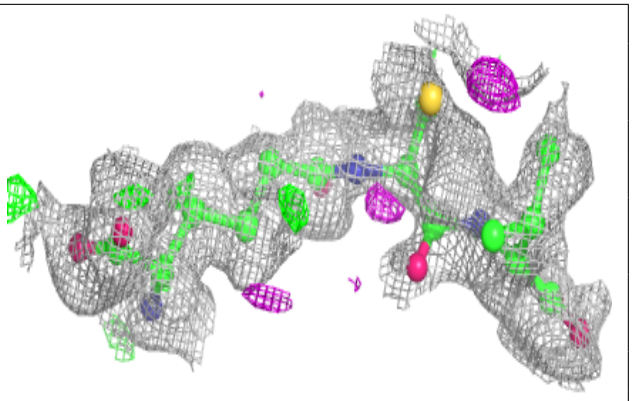
Electron density around IP1 A 1333 (A):

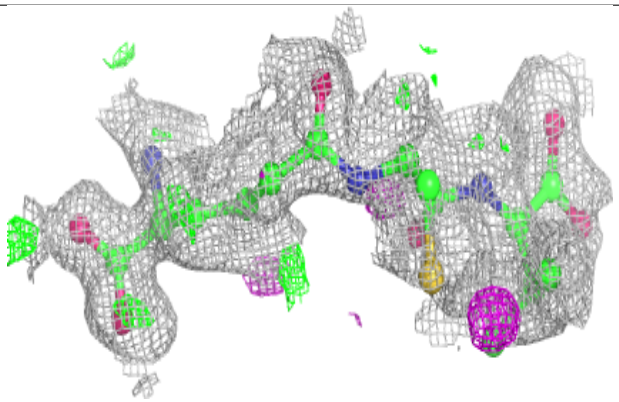
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

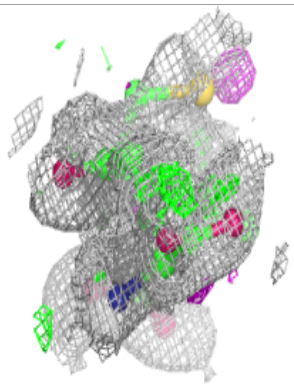


Electron density around ACV A 1334 (B):

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.