



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:42 AM UTC

PDB ID : 1QJE / pdb_00001qje
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

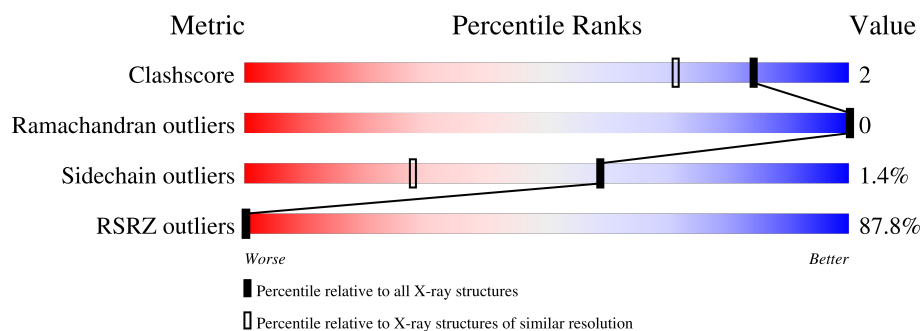
1 Overall quality at a glance

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	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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 $\leq 5\%$. 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	331	

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.

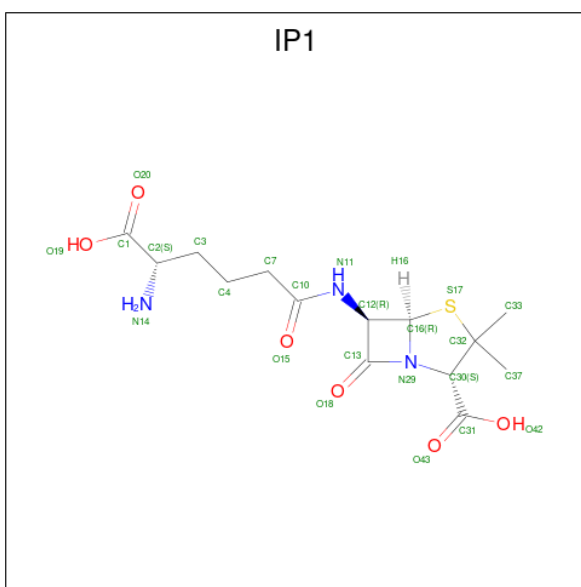
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2635	1684	444	502	5	0	1	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



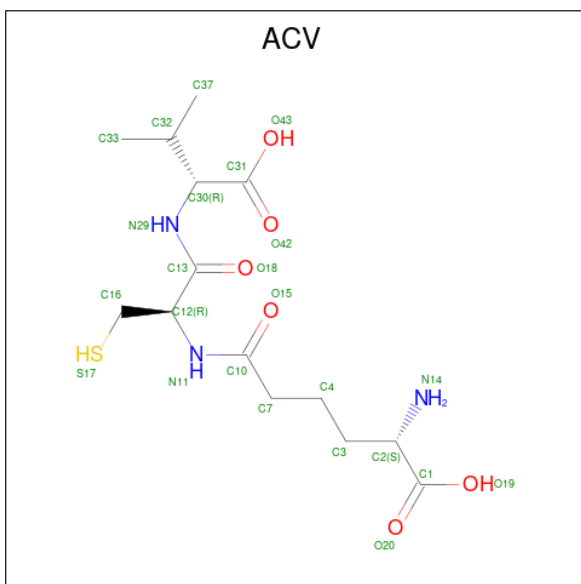
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is ISOPENICILLIN N (CCD ID: IP1) (formula: C₁₄H₂₁N₃O₆S).



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 (CCD ID: 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 (CCD ID: FE2) (formula: Fe).

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

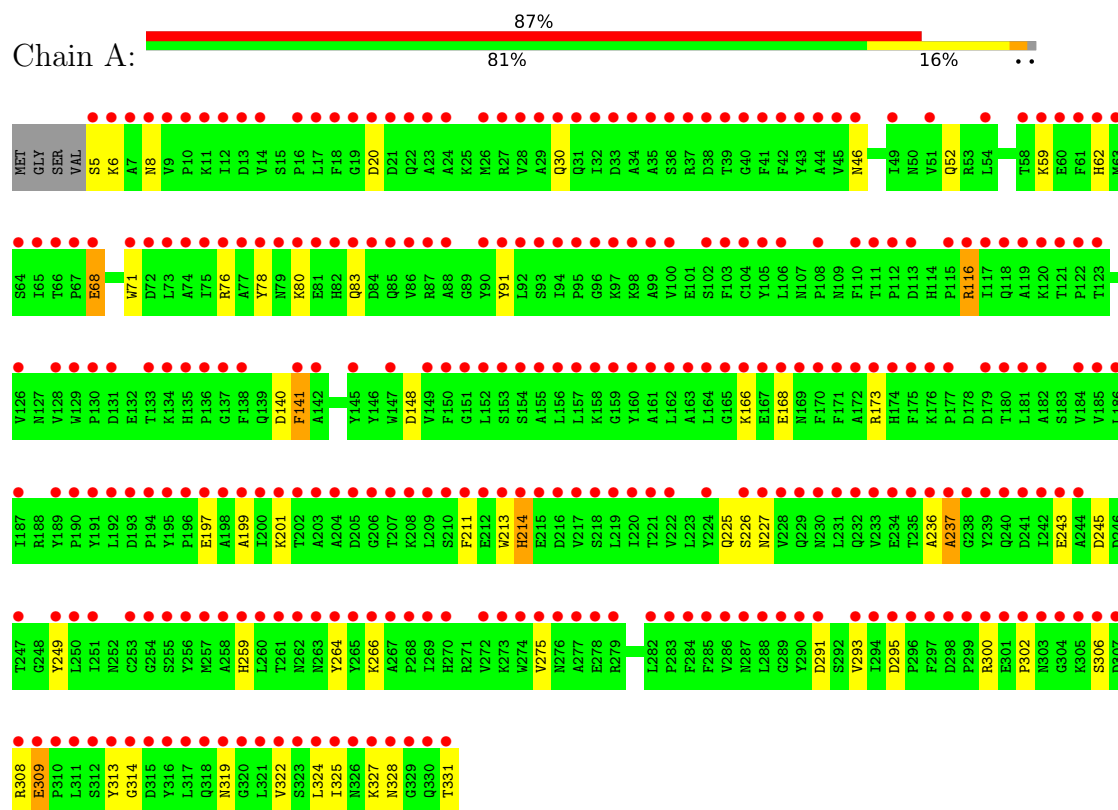
- Molecule 6 is water.

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

3 Residue-property plots

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: ISOPENICILLIN N SYNTHASE



4 Data and refinement statistics

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 25.00 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.2 (25.00-1.35) 91.2 (25.00-1.35)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.35Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.131 , 0.187 (Not available) , (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)	0.49 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: IP1, FE2, ACV, SO4

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	1.26	3/2715 (0.1%)	1.98	70/3694 (1.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	THR	C-OXT	6.80	1.37	1.23
1	A	76	ARG	CD-NE	-5.23	1.39	1.46
1	A	259	HIS	CE1-NE2	5.10	1.37	1.32

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	CD-NE-CZ	26.22	161.10	124.40
1	A	300	ARG	CD-NE-CZ	18.95	150.93	124.40
1	A	243	GLU	CB-CG-CD	11.94	132.89	112.60
1	A	6	LYS	CG-CD-CE	10.94	136.47	111.30
1	A	249	TYR	OH-CZ-CE2	10.93	152.70	119.90
1	A	309	GLU	CB-CG-CD	10.85	131.05	112.60
1	A	20	ASP	CA-CB-CG	-9.22	103.38	112.60
1	A	295	ASP	CA-CB-CG	-8.89	103.71	112.60
1	A	116	ARG	NE-CZ-NH2	-7.65	112.32	119.20
1	A	83	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	A	328	ASN	O-C-N	7.56	131.25	122.25
1	A	68	GLU	CA-C-O	7.52	128.53	120.55
1	A	302	PRO	O-C-N	7.50	130.86	122.24
1	A	116	ARG	CD-NE-CZ	-7.46	113.95	124.40
1	A	249	TYR	CE1-CZ-OH	-7.43	97.62	119.90
1	A	46	ASN	OD1-CG-ND2	7.36	129.96	122.60
1	A	225	GLN	OE1-CD-NE2	7.29	129.90	122.60
1	A	6	LYS	CB-CG-CD	7.26	128.01	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ASN	CA-CB-CG	7.23	119.83	112.60
1	A	293	VAL	CA-C-O	7.19	127.36	120.25
1	A	201	LYS	O-C-N	-7.13	114.97	123.03
1	A	20	ASP	CA-C-O	-7.01	111.21	119.48
1	A	8	ASN	CA-CB-CG	-6.99	105.61	112.60
1	A	30	GLN	OE1-CD-NE2	6.93	129.53	122.60
1	A	314	GLY	O-C-N	6.69	128.68	122.19
1	A	309	GLU	CB-CA-C	6.68	118.48	108.86
1	A	20	ASP	O-C-N	6.60	130.17	122.19
1	A	227	ASN	OD1-CG-ND2	-6.51	116.08	122.60
1	A	30	GLN	CA-C-O	-6.43	114.07	120.82
1	A	322	VAL	CA-C-O	6.42	127.65	120.85
1	A	227	ASN	CB-CG-ND2	6.40	126.00	116.40
1	A	322	VAL	N-CA-C	6.38	117.17	110.72
1	A	52	GLN	OE1-CD-NE2	6.36	128.96	122.60
1	A	275	VAL	CA-CB-CG1	-6.30	99.69	110.40
1	A	328	ASN	CA-C-O	-6.26	112.21	119.59
1	A	199	ALA	CA-C-O	6.17	126.74	119.28
1	A	295	ASP	O-C-N	6.14	126.89	121.18
1	A	148	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	78	TYR	O-C-N	-5.98	115.25	122.48
1	A	264	TYR	N-CA-C	-5.84	105.00	111.36
1	A	52	GLN	CB-CG-CD	5.79	122.44	112.60
1	A	322	VAL	N-CA-CB	-5.70	102.03	110.58
1	A	308	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	A	168	GLU	CA-C-N	-5.64	113.66	122.73
1	A	168	GLU	C-N-CA	-5.64	113.66	122.73
1	A	214	HIS	O-C-N	5.64	129.04	123.46
1	A	226	SER	CB-CA-C	-5.63	97.06	110.02
1	A	214	HIS	ND1-CE1-NE2	5.62	114.02	108.40
1	A	302	PRO	CA-C-N	-5.46	112.49	122.38
1	A	302	PRO	C-N-CA	-5.46	112.49	122.38
1	A	141	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	168	GLU	CA-C-O	-5.37	112.78	119.38
1	A	197	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	325	ILE	CA-C-O	5.36	126.52	120.95
1	A	236	ALA	CA-C-O	5.35	125.96	119.49
1	A	249	TYR	CE1-CZ-CE2	-5.34	109.62	120.30
1	A	308	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	8	ASN	OD1-CG-ND2	5.31	127.91	122.60
1	A	62	HIS	CA-C-O	5.31	126.10	120.10
1	A	71	TRP	O-C-N	5.22	127.66	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	266	LYS	CB-CG-CD	5.19	123.23	111.30
1	A	313	TYR	CA-CB-CG	-5.15	104.63	113.90
1	A	227	ASN	CB-CA-C	-5.15	104.62	111.88
1	A	236	ALA	CA-C-N	5.14	132.23	121.94
1	A	236	ALA	C-N-CA	5.14	132.23	121.94
1	A	243	GLU	CA-CB-CG	-5.08	103.94	114.10
1	A	237	ALA	CB-CA-C	-5.05	100.51	110.11
1	A	324	LEU	CB-CA-C	5.02	119.38	110.85
1	A	249	TYR	CZ-CE2-CD2	5.00	128.60	119.60

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	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	291/331 (88%)	283 (97%)	8 (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%)	278 (99%)	4 (1%)	59 28

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

Mol	Chain	Res	Type
1	A	5	SER
1	A	59	LYS
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	83	GLN
1	A	319	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.98	1 (4%)	35,38,38	1.91	11 (31%)
2	SO4	A	1332	-	4,4,4	0.49	0	6,6,6	1.12	1 (16%)
4	ACV	A	1334[B]	5	22,23,23	1.40	1 (4%)	27,30,30	2.17	11 (40%)

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	-5.34	1.43	1.52
3	A	1333[A]	IP1	C30-C31	2.92	1.56	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1334[B]	ACV	C16-C12-N11	-5.25	103.80	111.28
4	A	1334[B]	ACV	C32-C30-C31	4.29	120.46	111.04
3	A	1333[A]	IP1	C16-N29-C30	4.13	122.15	117.30
3	A	1333[A]	IP1	S17-C16-N29	-3.61	100.05	104.93
4	A	1334[B]	ACV	C31-C30-N29	3.29	117.41	110.17
4	A	1334[B]	ACV	O18-C13-C12	3.28	127.35	120.48
3	A	1333[A]	IP1	C13-C12-N11	-3.10	106.51	115.29
3	A	1333[A]	IP1	C37-C32-S17	3.07	114.12	109.18
3	A	1333[A]	IP1	O18-C13-N29	-3.03	127.58	131.75
4	A	1334[B]	ACV	C37-C32-C33	2.95	118.70	110.58
4	A	1334[B]	ACV	C12-N11-C10	2.87	128.88	121.68
3	A	1333[A]	IP1	C37-C32-C33	2.65	115.02	110.70
3	A	1333[A]	IP1	O43-C31-C30	-2.58	114.93	122.89
3	A	1333[A]	IP1	C32-C30-N29	-2.53	102.77	106.43
3	A	1333[A]	IP1	O18-C13-C12	2.47	142.41	136.11
3	A	1333[A]	IP1	C7-C10-N11	2.45	120.19	115.86
4	A	1334[B]	ACV	O15-C10-N11	-2.36	118.95	122.95
4	A	1334[B]	ACV	O18-C13-N29	-2.33	118.79	122.96
4	A	1334[B]	ACV	C16-C12-C13	-2.28	104.54	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1334[B]	ACV	C33-C32-C30	-2.18	105.19	111.16
3	A	1333[A]	IP1	C33-C32-C30	-2.11	107.06	111.61
4	A	1334[B]	ACV	C30-N29-C13	2.10	127.10	121.90
2	A	1332	SO4	O4-S-O2	-2.04	98.89	109.56

There are no chirality outliers.

All (10) torsion outliers are listed below:

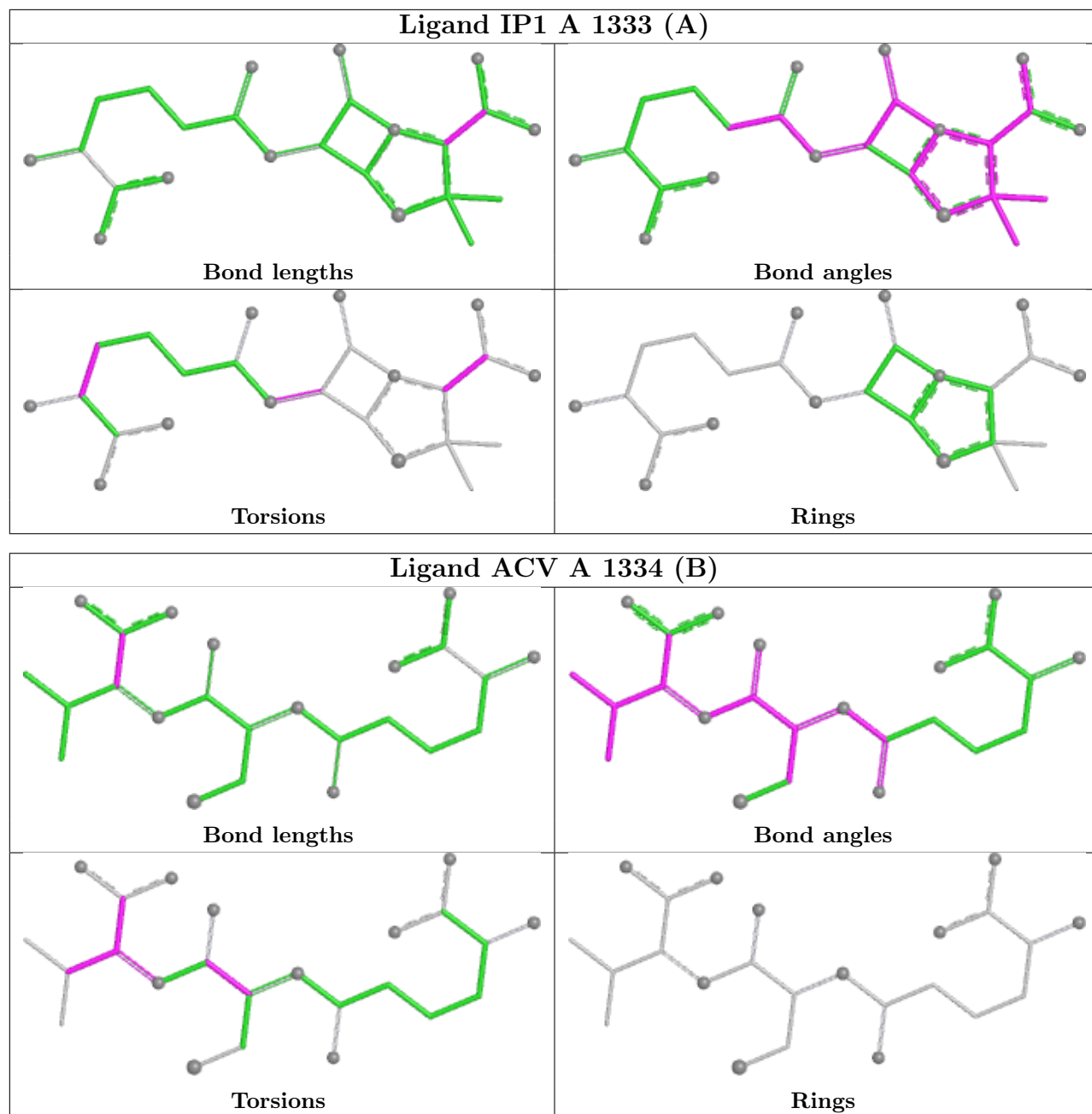
Mol	Chain	Res	Type	Atoms
4	A	1334[B]	ACV	C31-C30-C32-C33
4	A	1334[B]	ACV	C31-C30-C32-C37
3	A	1333[A]	IP1	C13-C12-N11-C10
3	A	1333[A]	IP1	N14-C2-C3-C4
4	A	1334[B]	ACV	N11-C12-C13-N29
4	A	1334[B]	ACV	N11-C12-C13-O18
4	A	1334[B]	ACV	C32-C30-N29-C13
3	A	1333[A]	IP1	C32-C30-C31-O42
3	A	1333[A]	IP1	C32-C30-C31-O43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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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



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, 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	327/331 (98%)	3.88	287 (87%) 0 0	7, 14, 28, 41	1 (0%)

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	ILE	10.8
1	A	198	ALA	10.5
1	A	236	ALA	10.3
1	A	237	ALA	10.0
1	A	239	TYR	9.2
1	A	302	PRO	8.5
1	A	238	GLY	8.0
1	A	295	ASP	7.9
1	A	213	TRP	7.9
1	A	326	ASN	7.7
1	A	293	VAL	7.6
1	A	305	LYS	7.5
1	A	322	VAL	7.4
1	A	319	ASN	7.1
1	A	327	LYS	7.0
1	A	324	LEU	6.9
1	A	23	ALA	6.9
1	A	296	PRO	6.9
1	A	94	ILE	6.8
1	A	329	GLY	6.7
1	A	86	VAL	6.7
1	A	96	GLY	6.7
1	A	202	THR	6.6
1	A	304	GLY	6.6
1	A	5	SER	6.4
1	A	294	ILE	6.4
1	A	199	ALA	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	261	THR	6.3
1	A	201	LYS	6.3
1	A	263	ASN	6.2
1	A	205	ASP	6.2
1	A	161	ALA	6.2
1	A	264	TYR	6.2
1	A	211	PHE	6.1
1	A	206	GLY	6.1
1	A	311	LEU	5.9
1	A	29	ALA	5.9
1	A	328	ASN	5.9
1	A	297	PHE	5.9
1	A	320	GLY	5.9
1	A	235	THR	5.8
1	A	59	LYS	5.8
1	A	299	PRO	5.8
1	A	207	THR	5.7
1	A	196	PRO	5.7
1	A	323	SER	5.7
1	A	307	ASP	5.6
1	A	288	LEU	5.6
1	A	193	ASP	5.6
1	A	197	GLU	5.5
1	A	256	TYR	5.5
1	A	313	TYR	5.5
1	A	233	VAL	5.5
1	A	203	ALA	5.4
1	A	309	GLU	5.4
1	A	20	ASP	5.3
1	A	162	LEU	5.3
1	A	200	ILE	5.3
1	A	170	PHE	5.2
1	A	318	GLN	5.2
1	A	316	TYR	5.2
1	A	300	ARG	5.2
1	A	254	GLY	5.2
1	A	18	PHE	5.2
1	A	310[A]	PRO	5.2
1	A	40	GLY	5.1
1	A	231	LEU	5.1
1	A	189	TYR	5.1
1	A	9	VAL	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	228	VAL	5.1
1	A	92	LEU	5.1
1	A	290	TYR	5.0
1	A	71	TRP	5.0
1	A	260	LEU	5.0
1	A	321	LEU	5.0
1	A	65	ILE	4.9
1	A	77	ALA	4.9
1	A	269	ILE	4.9
1	A	262	ASN	4.9
1	A	176	LYS	4.9
1	A	314	GLY	4.9
1	A	308	ARG	4.8
1	A	80	LYS	4.8
1	A	195	TYR	4.8
1	A	331	THR	4.8
1	A	303	ASN	4.8
1	A	91	TYR	4.7
1	A	141	PHE	4.7
1	A	224	TYR	4.7
1	A	8	ASN	4.7
1	A	39	THR	4.7
1	A	83	GLN	4.7
1	A	244	ALA	4.7
1	A	38	ASP	4.7
1	A	274	TRP	4.6
1	A	204	ALA	4.6
1	A	192	LEU	4.6
1	A	17	LEU	4.6
1	A	275	VAL	4.6
1	A	306	SER	4.6
1	A	19	GLY	4.6
1	A	78	TYR	4.5
1	A	191	TYR	4.5
1	A	258	ALA	4.5
1	A	164	LEU	4.5
1	A	250	LEU	4.5
1	A	330	GLN	4.5
1	A	209	LEU	4.5
1	A	43	TYR	4.5
1	A	117	ILE	4.4
1	A	272	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	171	PHE	4.4
1	A	16	PRO	4.4
1	A	265	TYR	4.4
1	A	49	ILE	4.4
1	A	277	ALA	4.3
1	A	167	GLU	4.3
1	A	243	GLU	4.3
1	A	6	LYS	4.3
1	A	95	PRO	4.3
1	A	75	ILE	4.3
1	A	21	ASP	4.3
1	A	175	PHE	4.3
1	A	34	ALA	4.2
1	A	208	LYS	4.2
1	A	63	MET	4.2
1	A	123	THR	4.2
1	A	181	LEU	4.2
1	A	220	ILE	4.2
1	A	253	CYS	4.2
1	A	28	VAL	4.2
1	A	138	PHE	4.2
1	A	163	ALA	4.1
1	A	73	LEU	4.1
1	A	129	TRP	4.1
1	A	22	GLN	4.1
1	A	315	ASP	4.1
1	A	317	LEU	4.1
1	A	227	ASN	4.0
1	A	218	SER	4.0
1	A	217	VAL	4.0
1	A	312	SER	4.0
1	A	88	ALA	4.0
1	A	150	PHE	4.0
1	A	42	PHE	3.9
1	A	285	PHE	3.9
1	A	24	ALA	3.9
1	A	97	LYS	3.9
1	A	185	VAL	3.9
1	A	61	PHE	3.9
1	A	67	PRO	3.9
1	A	76	ARG	3.9
1	A	131	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	291	ASP	3.8
1	A	12	ILE	3.8
1	A	100	VAL	3.8
1	A	82	HIS	3.8
1	A	298	ASP	3.7
1	A	249	TYR	3.7
1	A	84	ASP	3.7
1	A	45	VAL	3.7
1	A	37	ARG	3.6
1	A	103	PHE	3.6
1	A	7	ALA	3.6
1	A	126	VAL	3.6
1	A	301	GLU	3.6
1	A	169	ASN	3.6
1	A	242	ILE	3.6
1	A	120	LYS	3.6
1	A	121	THR	3.6
1	A	85	GLN	3.6
1	A	156	LEU	3.5
1	A	166	LYS	3.5
1	A	41	PHE	3.5
1	A	157	LEU	3.5
1	A	160	TYR	3.5
1	A	151	GLY	3.5
1	A	222	VAL	3.5
1	A	187	ILE	3.5
1	A	247	THR	3.4
1	A	74	ALA	3.4
1	A	133	THR	3.4
1	A	99	ALA	3.4
1	A	110	PHE	3.4
1	A	90	TYR	3.4
1	A	44	ALA	3.4
1	A	11	LYS	3.4
1	A	273	LYS	3.4
1	A	270	HIS	3.3
1	A	152	LEU	3.3
1	A	173	ARG	3.3
1	A	119	ALA	3.3
1	A	142	ALA	3.3
1	A	186	LEU	3.3
1	A	194	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	134	LYS	3.3
1	A	10	PRO	3.2
1	A	283	PRO	3.2
1	A	159	GLY	3.2
1	A	35	ALA	3.2
1	A	112	PRO	3.2
1	A	221	THR	3.1
1	A	51	VAL	3.1
1	A	215	GLU	3.1
1	A	98	LYS	3.1
1	A	165	GLY	3.1
1	A	230	ASN	3.1
1	A	219	LEU	3.1
1	A	33	ASP	3.0
1	A	145	TYR	3.0
1	A	289	GLY	3.0
1	A	136	PRO	3.0
1	A	14	VAL	3.0
1	A	214	HIS	3.0
1	A	266	LYS	3.0
1	A	72	ASP	2.9
1	A	128	VAL	2.9
1	A	155	ALA	2.9
1	A	172	ALA	2.9
1	A	267	ALA	2.9
1	A	81	GLU	2.9
1	A	179	ASP	2.9
1	A	106	LEU	2.9
1	A	226	SER	2.9
1	A	102	SER	2.8
1	A	26	MET	2.8
1	A	64	SER	2.8
1	A	240	GLN	2.8
1	A	255	SER	2.8
1	A	31	GLN	2.7
1	A	268	PRO	2.7
1	A	284	PHE	2.7
1	A	79	ASN	2.7
1	A	212	GLU	2.7
1	A	105	TYR	2.7
1	A	286	VAL	2.7
1	A	232	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	36	SER	2.7
1	A	241	ASP	2.7
1	A	62	HIS	2.7
1	A	259	HIS	2.7
1	A	122	PRO	2.7
1	A	182	ALA	2.6
1	A	137	GLY	2.6
1	A	147	TRP	2.6
1	A	184	VAL	2.6
1	A	111	THR	2.6
1	A	116	ARG	2.6
1	A	93	SER	2.6
1	A	32	ILE	2.6
1	A	130	PRO	2.6
1	A	135	HIS	2.6
1	A	13	ASP	2.6
1	A	66	THR	2.5
1	A	68	GLU	2.5
1	A	168	GLU	2.5
1	A	46	ASN	2.5
1	A	276	ASN	2.5
1	A	30	GLN	2.5
1	A	251	ILE	2.5
1	A	154	SER	2.5
1	A	108	PRO	2.5
1	A	113	ASP	2.5
1	A	216	ASP	2.5
1	A	54	LEU	2.5
1	A	210	SER	2.4
1	A	190	PRO	2.4
1	A	177	PRO	2.4
1	A	287	ASN	2.4
1	A	27	ARG	2.4
1	A	149	VAL	2.4
1	A	104	CYS	2.4
1	A	158	LYS	2.3
1	A	58	THR	2.3
1	A	180	THR	2.3
1	A	282	LEU	2.3
1	A	87	ARG	2.3
1	A	234	GLU	2.2
1	A	279	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	115	PRO	2.2
1	A	174	HIS	2.1
1	A	118	GLN	2.1
1	A	229	GLN	2.1
1	A	153	SER	2.1
1	A	60	GLU	2.1
1	A	278	GLU	2.1
1	A	257	MET	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

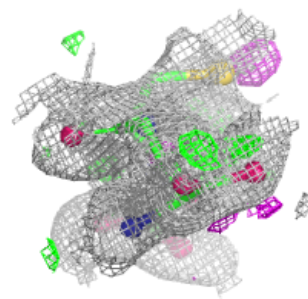
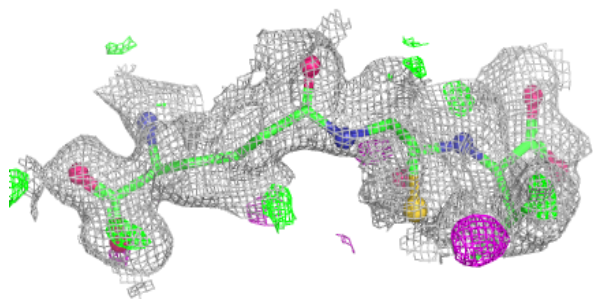
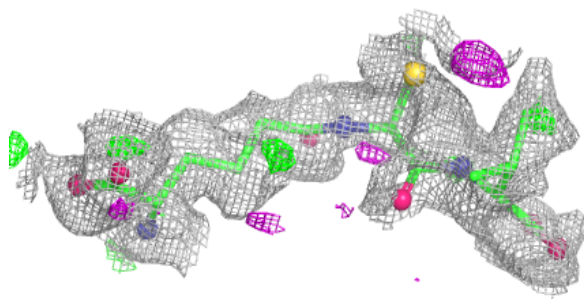
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACV	A	1334[B]	24/24	0.38	0.29	11,17,19,19	24
3	IP1	A	1333[A]	24/24	0.66	0.20	11,18,21,27	24
2	SO4	A	1332	5/5	0.69	0.20	39,44,47,61	0
5	FE2	A	1335	1/1	0.90	0.14	24,24,24,24	0

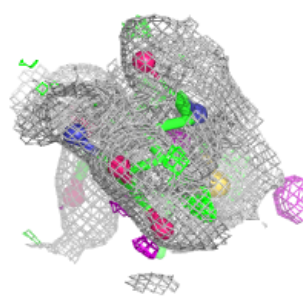
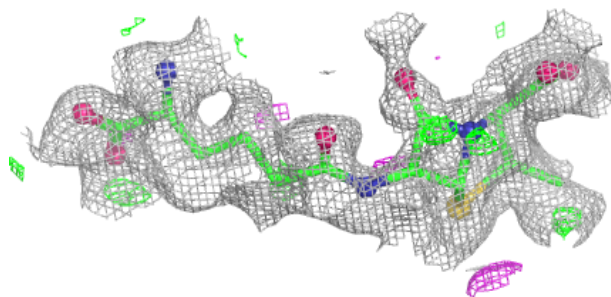
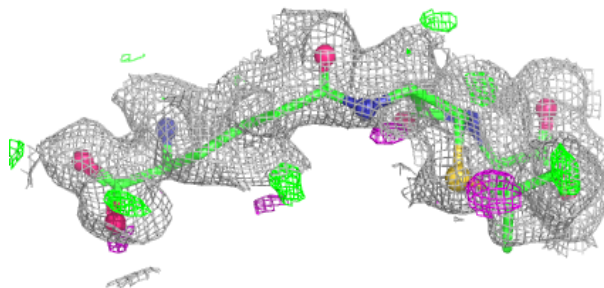
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.