Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2025 – 12:11 PM EST

PDB ID	:	9AVN
Title	:	Crystal Structure of CARD9 coiled-coil K156-K214 bound to Compound 1
Authors	:	Raymond, D.D.; Lemke, C.T.
Deposited on	:	2024-03-04
Resolution	:	2.73 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:

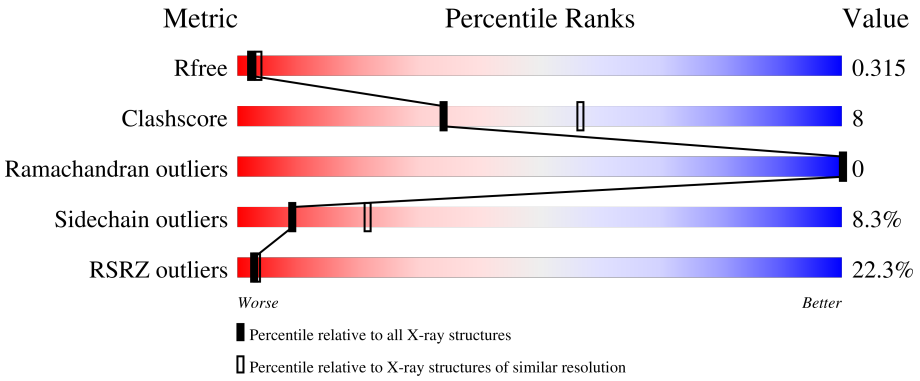
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.73 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}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	60	13% 72% 22% • 5%
1	B	60	25% 70% 23% • 5%
1	C	60	13% 72% 20% • 5%
1	D	60	22% 75% 17% • 5%
1	E	60	18% 68% 17% • 12%

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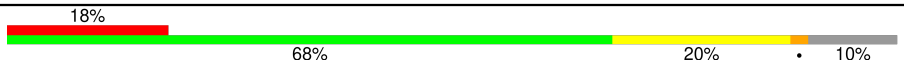
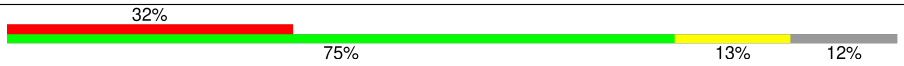
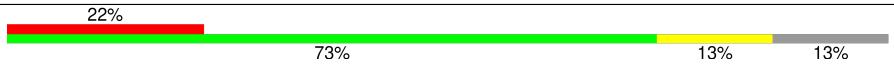
Mol	Chain	Length	Quality of chain
1	F	60	
1	G	60	
1	H	60	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3713 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.

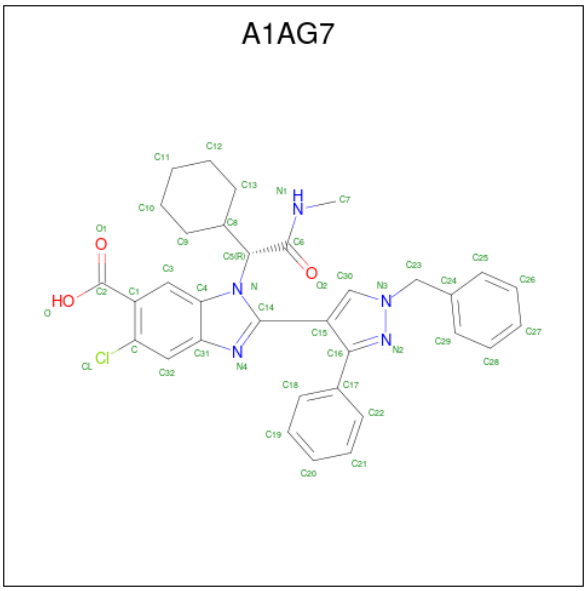
- Molecule 1 is a protein called Caspase recruitment domain-containing protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	0	0
			471	282	92	93	4			
1	B	57	Total	C	N	O	S	0	0	0
			471	282	92	93	4			
1	C	57	Total	C	N	O	S	0	0	0
			471	282	92	93	4			
1	D	57	Total	C	N	O	S	0	0	0
			471	282	92	93	4			
1	E	53	Total	C	N	O	S	0	0	0
			435	261	84	86	4			
1	F	54	Total	C	N	O	S	0	0	0
			444	266	87	87	4			
1	G	53	Total	C	N	O	S	0	0	0
			433	260	83	86	4			
1	H	52	Total	C	N	O	S	0	0	0
			426	255	82	85	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	ALA	-	expression tag	UNP Q9H257
B	155	ALA	-	expression tag	UNP Q9H257
C	155	ALA	-	expression tag	UNP Q9H257
D	155	ALA	-	expression tag	UNP Q9H257
E	155	ALA	-	expression tag	UNP Q9H257
F	155	ALA	-	expression tag	UNP Q9H257
G	155	ALA	-	expression tag	UNP Q9H257
H	155	ALA	-	expression tag	UNP Q9H257

- Molecule 2 is (2P)-2-(1-benzyl-3-phenyl-1H-pyrazol-4-yl)-5-chloro-1-[(1R)-1-cyclohexyl-2-(methylamino)-2-oxoethyl]-1H-1,3-benzimidazole-6-carboxylic acid (three-letter code: A1AG7) (formula: $C_{33}H_{32}ClN_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			42	33	1	5	3		
2	D	1	Total	C	Cl	N	O	0	0
			42	33	1	5	3		

- Molecule 3 is water.

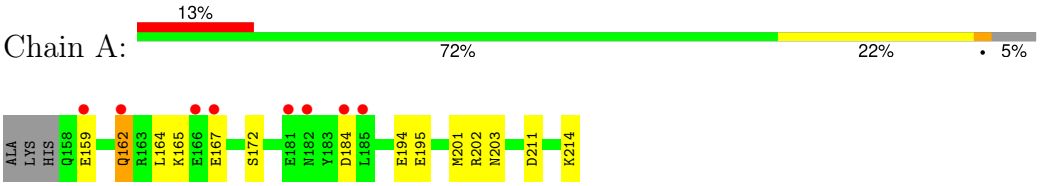
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	1	Total	O	0	0
			1	1		
3	D	2	Total	O	0	0
			2	2		
3	G	1	Total	O	0	0
			1	1		

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.

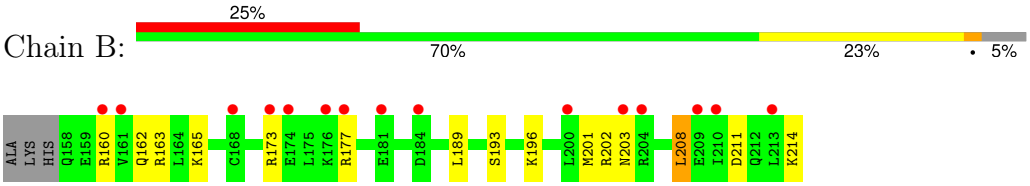
• Molecule 1: Caspase recruitment domain-containing protein 9

Chain A:



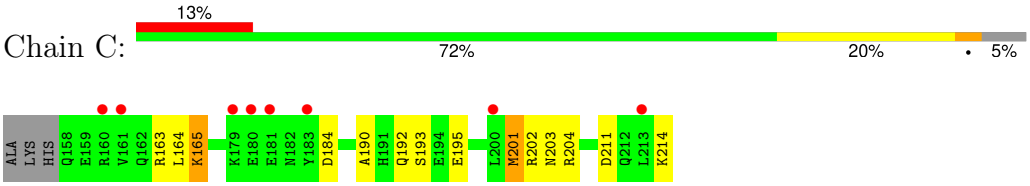
• Molecule 1: Caspase recruitment domain-containing protein 9

Chain B:



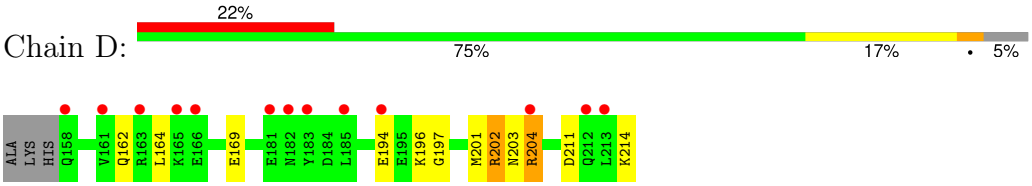
• Molecule 1: Caspase recruitment domain-containing protein 9

Chain C:



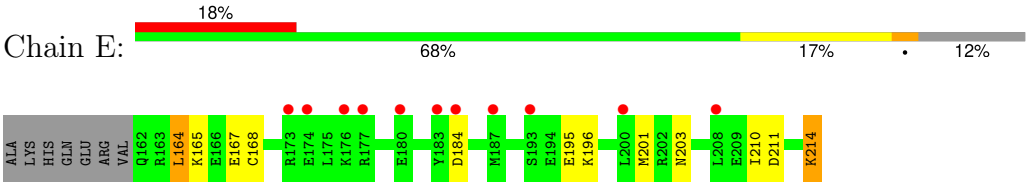
• Molecule 1: Caspase recruitment domain-containing protein 9

Chain D:



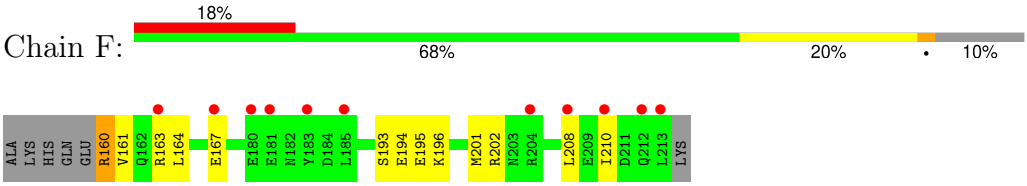
• Molecule 1: Caspase recruitment domain-containing protein 9

Chain E:



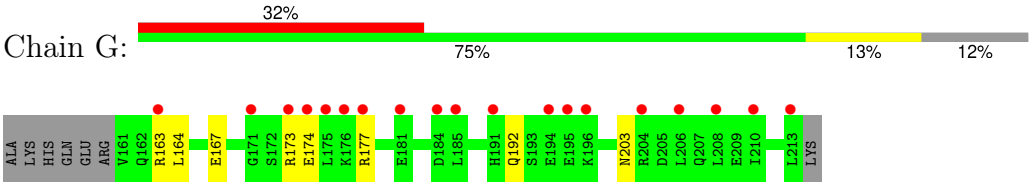
• Molecule 1: Caspase recruitment domain-containing protein 9

Chain F:



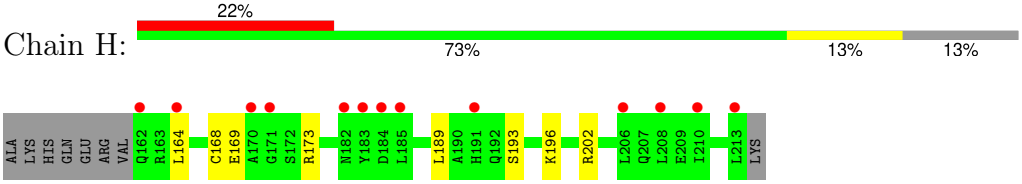
• Molecule 1: Caspase recruitment domain-containing protein 9

Chain G:



• Molecule 1: Caspase recruitment domain-containing protein 9

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.39Å 56.05Å 84.30Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	83.53 – 2.73 83.53 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (83.53-2.73) 98.8 (83.53-2.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.274 , 0.299 0.289 , 0.315	Depositor DCC
R_{free} test set	708 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.4	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	0.89	EDS
Total number of atoms	3713	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.37% 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: A1AG7

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	0.44	0/472	0.55	0/624
1	B	0.39	0/472	0.50	0/624
1	C	0.43	0/472	0.50	0/624
1	D	0.43	0/472	0.58	0/624
1	E	0.37	0/436	0.50	0/576
1	F	0.41	0/445	0.52	0/589
1	G	0.37	0/434	0.48	0/575
1	H	0.41	0/427	0.48	0/565
All	All	0.41	0/3630	0.52	0/4801

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	471	0	471	9	0
1	B	471	0	471	14	0
1	C	471	0	471	14	0
1	D	471	0	471	16	0
1	E	435	0	435	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	444	0	444	15	0
1	G	433	0	431	11	0
1	H	426	0	422	5	0
2	A	42	0	0	1	0
2	D	42	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
3	G	1	0	0	0	0
All	All	3713	0	3616	55	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 8.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:GLU:HG2	1:F:193:SER:HB3	1.33	1.05
1:C:211:ASP:HA	1:C:214:LYS:HD2	1.42	1.01
1:E:211:ASP:HA	1:E:214:LYS:HE2	1.42	0.97
1:D:211:ASP:HA	1:D:214:LYS:HD2	1.47	0.94
1:B:211:ASP:HA	1:B:214:LYS:HD2	1.49	0.92
1:A:211:ASP:HA	1:A:214:LYS:HD2	1.53	0.90
1:B:173:ARG:HH11	1:G:173:ARG:NH1	1.77	0.82
1:E:211:ASP:HA	1:E:214:LYS:CE	2.12	0.78
1:D:194:GLU:HG2	1:F:193:SER:CB	2.14	0.78
1:G:203:ASN:HD21	1:H:202:ARG:HG2	1.51	0.76
1:C:192:GLN:HE22	1:D:196:LYS:NZ	1.91	0.67
1:B:177:ARG:HD3	1:G:177:ARG:NE	2.13	0.64
1:B:173:ARG:HD2	1:G:173:ARG:NH1	2.14	0.62
1:D:201:MET:HA	1:D:204:ARG:HD3	1.83	0.60
1:D:194:GLU:CG	1:F:193:SER:HB3	2.20	0.59
1:C:165:LYS:HG2	1:D:164:LEU:HD21	1.85	0.59
1:C:164:LEU:HD23	1:D:164:LEU:HB3	1.86	0.58
1:E:164:LEU:HB3	1:F:164:LEU:HD23	1.86	0.58
1:E:210:ILE:HG12	1:F:210:ILE:HG13	1.87	0.57
1:E:164:LEU:HD23	1:F:164:LEU:HB3	1.87	0.57
1:D:197:GLY:HA3	1:F:194:GLU:HG2	1.87	0.56
1:G:174:GLU:HG3	1:G:177:ARG:HH21	1.70	0.56
1:D:202:ARG:HD3	1:F:201:MET:HB3	1.87	0.56
1:B:173:ARG:HH11	1:G:173:ARG:CZ	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ARG:HD2	1:F:161:VAL:HG23	1.88	0.55
1:A:203:ASN:HD21	1:B:203:ASN:HB2	1.71	0.54
1:A:195:GLU:HB3	1:B:196:LYS:HD2	1.91	0.53
1:F:163:ARG:O	1:F:167:GLU:HG2	2.10	0.51
1:C:195:GLU:HB3	1:D:196:LYS:HD2	1.91	0.51
1:D:211:ASP:HA	1:D:214:LYS:CD	2.31	0.51
1:C:192:GLN:HE22	1:D:196:LYS:HZ2	1.58	0.50
1:B:193:SER:HB2	1:C:193:SER:HB3	1.93	0.49
1:C:203:ASN:HD21	1:D:202:ARG:HG2	1.78	0.48
1:B:173:ARG:NH1	1:G:173:ARG:CZ	2.78	0.47
1:B:211:ASP:HA	1:B:214:LYS:CD	2.31	0.47
1:B:189:LEU:HD23	1:C:190:ALA:HB1	1.97	0.47
1:B:173:ARG:NH1	1:G:173:ARG:NH1	2.57	0.46
1:G:192:GLN:HE22	1:H:196:LYS:NZ	2.13	0.46
1:C:192:GLN:HE22	1:D:196:LYS:HZ3	1.61	0.46
1:B:177:ARG:HD3	1:G:177:ARG:CZ	2.46	0.46
1:E:195:GLU:HB3	1:F:196:LYS:HD2	1.98	0.45
1:A:195:GLU:OE1	1:C:201:MET:SD	2.75	0.45
1:G:164:LEU:HD23	1:H:164:LEU:HD23	1.99	0.44
1:A:202:ARG:NH1	1:C:204:ARG:NH1	2.65	0.44
1:A:211:ASP:HA	1:A:214:LYS:CD	2.35	0.44
1:C:163:ARG:HG3	1:C:164:LEU:N	2.32	0.44
1:E:196:LYS:HD2	1:F:195:GLU:HB3	2.01	0.43
1:A:194:GLU:HG2	1:H:193:SER:O	2.18	0.42
1:C:202:ARG:HB3	1:D:203:ASN:HD21	1.85	0.42
1:A:159:GLU:OE1	1:A:162:GLN:NE2	2.53	0.42
1:F:160:ARG:HA	1:F:163:ARG:HG2	2.01	0.42
1:E:203:ASN:HD21	1:F:202:ARG:HG2	1.84	0.41
1:A:172:SER:OG	2:A:301:A1AG7:N4	2.53	0.41
1:B:208:LEU:HG	1:F:208:LEU:HD21	2.03	0.41
1:H:169:GLU:HG2	1:H:173:ARG:HH12	1.87	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	55/60 (92%)	54 (98%)	1 (2%)	0	100	100
1	B	55/60 (92%)	54 (98%)	1 (2%)	0	100	100
1	C	55/60 (92%)	53 (96%)	2 (4%)	0	100	100
1	D	55/60 (92%)	54 (98%)	1 (2%)	0	100	100
1	E	51/60 (85%)	50 (98%)	1 (2%)	0	100	100
1	F	52/60 (87%)	52 (100%)	0	0	100	100
1	G	51/60 (85%)	51 (100%)	0	0	100	100
1	H	50/60 (83%)	50 (100%)	0	0	100	100
All	All	424/480 (88%)	418 (99%)	6 (1%)	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	50/52 (96%)	44 (88%)	6 (12%)	4	9
1	B	50/52 (96%)	43 (86%)	7 (14%)	3	6
1	C	50/52 (96%)	47 (94%)	3 (6%)	16	36
1	D	50/52 (96%)	46 (92%)	4 (8%)	10	23
1	E	46/52 (88%)	39 (85%)	7 (15%)	2	5
1	F	47/52 (90%)	46 (98%)	1 (2%)	48	75
1	G	46/52 (88%)	44 (96%)	2 (4%)	25	50
1	H	45/52 (86%)	43 (96%)	2 (4%)	24	49
All	All	384/416 (92%)	352 (92%)	32 (8%)	9	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	164	LEU
1	A	165	LYS
1	A	167	GLU
1	A	184	ASP
1	A	201	MET
1	B	160	ARG
1	B	162	GLN
1	B	163	ARG
1	B	165	LYS
1	B	201	MET
1	B	202	ARG
1	B	208	LEU
1	C	165	LYS
1	C	184	ASP
1	C	201	MET
1	D	162	GLN
1	D	169	GLU
1	D	202	ARG
1	D	204	ARG
1	E	164	LEU
1	E	165	LYS
1	E	167	GLU
1	E	168	CYS
1	E	184	ASP
1	E	201	MET
1	E	214	LYS
1	F	160	ARG
1	G	163	ARG
1	G	167	GLU
1	H	168	CYS
1	H	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	182	ASN
1	A	191	HIS
1	A	192	GLN
1	A	203	ASN
1	A	212	GLN
1	B	162	GLN

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Mol	Chain	Res	Type
1	B	212	GLN
1	C	191	HIS
1	C	192	GLN
1	C	203	ASN
1	D	158	GLN
1	D	192	GLN
1	D	203	ASN
1	D	212	GLN
1	E	203	ASN
1	E	212	GLN
1	F	212	GLN
1	G	162	GLN
1	G	192	GLN
1	G	203	ASN
1	G	212	GLN
1	H	191	HIS
1	H	192	GLN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1AG7	A	301	-	41,47,47	0.90	3 (7%)	53,67,67	1.07	6 (11%)
2	A1AG7	D	301	-	41,47,47	0.94	3 (7%)	53,67,67	1.25	9 (16%)

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
2	A1AG7	A	301	-	-	2/22/38/38	0/6/6/6
2	A1AG7	D	301	-	-	2/22/38/38	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	A1AG7	O1-C2	2.97	1.31	1.22
2	A	301	A1AG7	O1-C2	2.91	1.31	1.22
2	D	301	A1AG7	O-C2	-2.69	1.22	1.30
2	A	301	A1AG7	O-C2	-2.48	1.23	1.30
2	A	301	A1AG7	C16-N2	-2.33	1.33	1.35
2	D	301	A1AG7	C16-N2	-2.20	1.33	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	A1AG7	C13-C8-C9	4.22	116.65	109.43
2	D	301	A1AG7	O1-C2-C1	-2.95	114.92	121.97
2	A	301	A1AG7	C3-C1-C2	-2.76	115.11	120.21
2	A	301	A1AG7	O1-C2-C1	-2.72	115.48	121.97
2	D	301	A1AG7	C12-C13-C8	2.56	116.46	111.89
2	A	301	A1AG7	C32-C-CL	-2.44	116.75	119.19
2	D	301	A1AG7	O-C2-C1	2.33	121.90	115.28
2	D	301	A1AG7	C3-C1-C2	-2.22	116.10	120.21
2	D	301	A1AG7	C30-N3-N2	2.21	113.17	111.45
2	A	301	A1AG7	C15-C30-N3	-2.16	106.60	109.47
2	D	301	A1AG7	C15-C30-N3	-2.15	106.60	109.47
2	A	301	A1AG7	O-C2-C1	2.11	121.29	115.28
2	D	301	A1AG7	C10-C9-C8	2.06	115.57	111.89
2	A	301	A1AG7	C30-N3-N2	2.05	113.05	111.45
2	D	301	A1AG7	C3-C4-C31	2.04	122.56	120.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	A1AG7	C15-C16-C17-C22
2	A	301	A1AG7	C15-C16-C17-C22
2	D	301	A1AG7	C15-C16-C17-C18
2	A	301	A1AG7	C15-C16-C17-C18

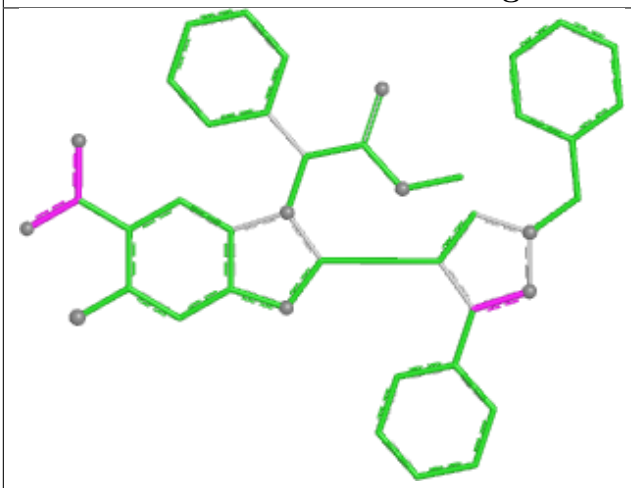
There are no ring outliers.

1 monomer is involved in 1 short contact:

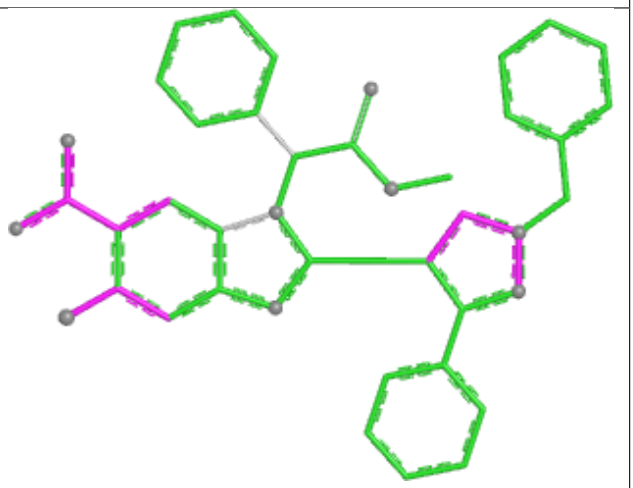
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	A1AG7	1	0

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.

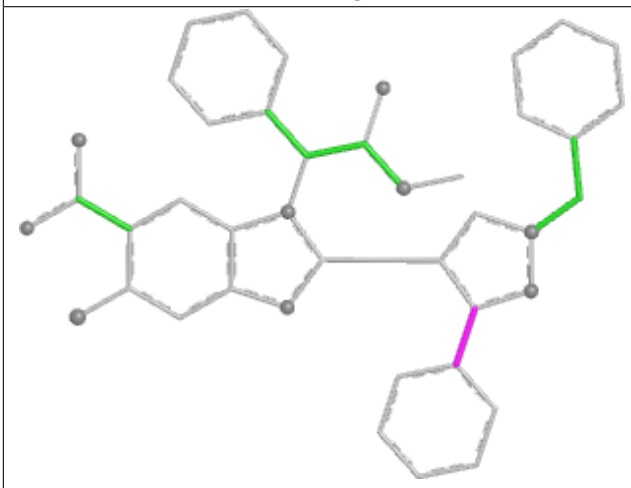
Ligand A1AG7 A 301



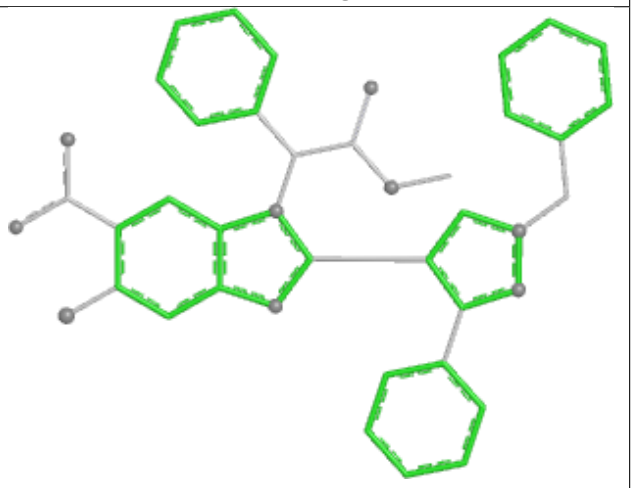
Bond lengths



Bond angles

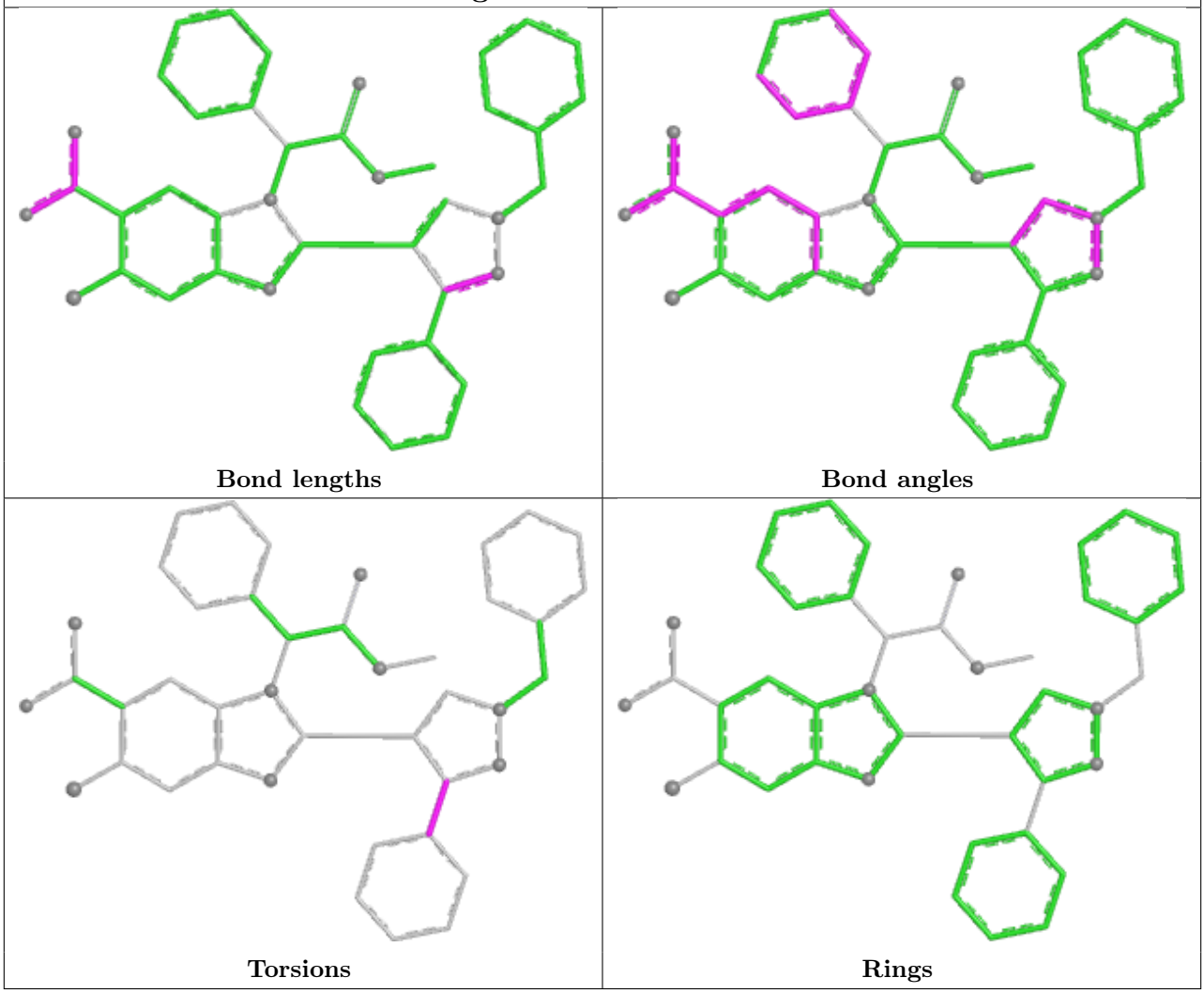


Torsions



Rings

Ligand A1AG7 D 301



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	57/60 (95%)	0.99	8 (14%)	7	7	37, 55, 84, 92	0
1	B	57/60 (95%)	1.31	15 (26%)	2	2	37, 63, 98, 105	0
1	C	57/60 (95%)	1.07	8 (14%)	7	7	41, 56, 97, 101	0
1	D	57/60 (95%)	1.21	13 (22%)	2	3	38, 56, 78, 94	0
1	E	53/60 (88%)	1.46	11 (20%)	3	4	55, 71, 109, 115	0
1	F	54/60 (90%)	1.49	11 (20%)	3	4	41, 66, 102, 105	0
1	G	53/60 (88%)	1.80	19 (35%)	1	1	39, 77, 127, 133	0
1	H	52/60 (86%)	1.55	13 (25%)	2	2	51, 78, 109, 115	0
All	All	440/480 (91%)	1.35	98 (22%)	3	3	37, 64, 104, 133	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	163	ARG	6.1
1	G	213	LEU	4.9
1	E	173	ARG	4.9
1	H	162	GLN	4.7
1	H	182	ASN	4.6
1	F	183	TYR	4.4
1	G	191	HIS	4.4
1	C	180	GLU	4.4
1	E	176	LYS	4.3
1	B	177	ARG	4.2
1	F	204	ARG	4.0
1	F	213	LEU	4.0
1	H	184	ASP	3.7
1	B	184	ASP	3.7
1	D	158	GLN	3.5
1	A	184	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	176	LYS	3.4
1	D	182	ASN	3.4
1	G	177	ARG	3.4
1	G	196	LYS	3.4
1	A	162	GLN	3.3
1	A	185	LEU	3.3
1	D	161	VAL	3.2
1	E	174	GLU	3.2
1	F	181	GLU	3.1
1	D	185	LEU	3.1
1	D	212	GLN	3.1
1	G	184	ASP	3.1
1	H	213	LEU	3.1
1	C	213	LEU	3.1
1	B	161	VAL	3.1
1	H	183	TYR	3.1
1	B	210	ILE	3.0
1	C	181	GLU	3.0
1	D	204	ARG	3.0
1	D	213	LEU	2.9
1	A	182	ASN	2.9
1	F	185	LEU	2.9
1	H	191	HIS	2.8
1	B	160	ARG	2.8
1	F	163	ARG	2.8
1	D	163	ARG	2.8
1	A	166	GLU	2.8
1	C	183	TYR	2.8
1	G	185	LEU	2.8
1	C	179	LYS	2.8
1	G	195	GLU	2.8
1	C	160	ARG	2.8
1	G	181	GLU	2.7
1	B	168	CYS	2.7
1	G	206	LEU	2.7
1	E	183	TYR	2.7
1	B	213	LEU	2.7
1	G	194	GLU	2.6
1	C	200	LEU	2.6
1	E	200	LEU	2.6
1	E	177	ARG	2.6
1	B	174	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	2.6
1	E	208	LEU	2.6
1	G	210	ILE	2.6
1	E	180	GLU	2.5
1	E	187	MET	2.5
1	H	210	ILE	2.5
1	D	181	GLU	2.4
1	D	166	GLU	2.4
1	F	212	GLN	2.4
1	G	208	LEU	2.4
1	G	173	ARG	2.4
1	A	181	GLU	2.3
1	B	181	GLU	2.3
1	C	161	VAL	2.3
1	B	204	ARG	2.3
1	G	174	GLU	2.3
1	G	171	GLY	2.3
1	F	180	GLU	2.3
1	H	171	GLY	2.3
1	D	165	LYS	2.2
1	H	185	LEU	2.3
1	B	176	LYS	2.2
1	G	175	LEU	2.2
1	A	159	GLU	2.1
1	B	203	ASN	2.1
1	H	206	LEU	2.1
1	H	208	LEU	2.1
1	A	167	GLU	2.1
1	E	193	SER	2.1
1	H	164	LEU	2.1
1	H	170	ALA	2.1
1	F	167	GLU	2.0
1	F	210	ILE	2.0
1	F	208	LEU	2.0
1	B	173	ARG	2.0
1	G	204	ARG	2.0
1	D	183	TYR	2.0
1	B	209	GLU	2.0
1	D	194	GLU	2.0
1	E	184	ASP	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)

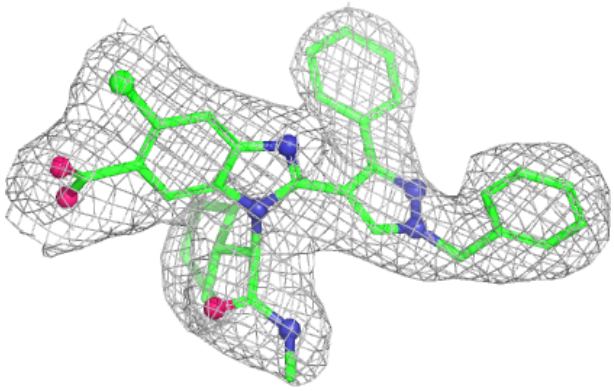
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

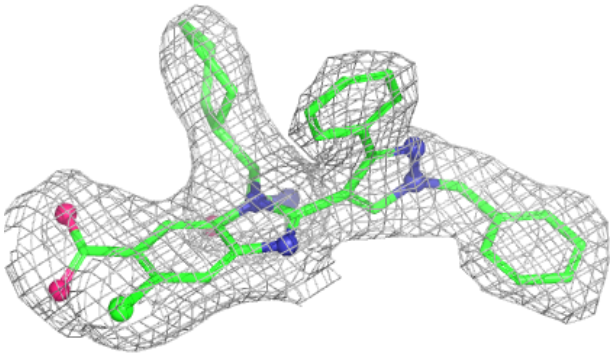
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1AG7	A	301	42/42	0.90	0.10	34,43,46,47	0
2	A1AG7	D	301	42/42	0.91	0.09	41,44,45,46	0

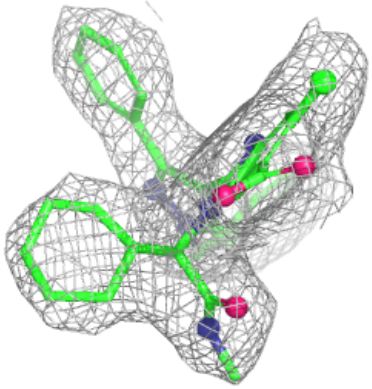
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AG7 A 301:

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

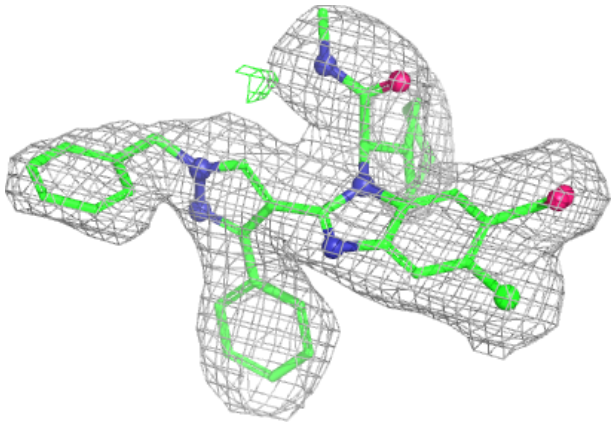


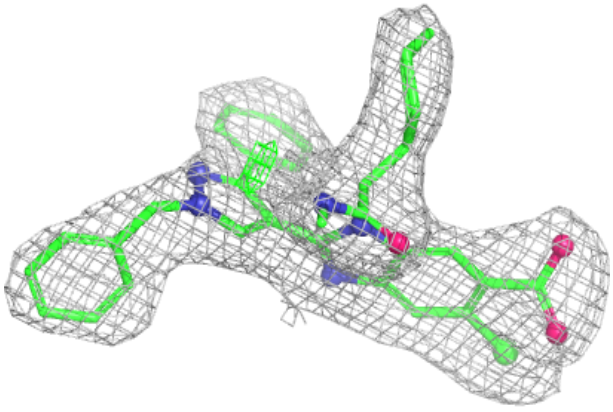


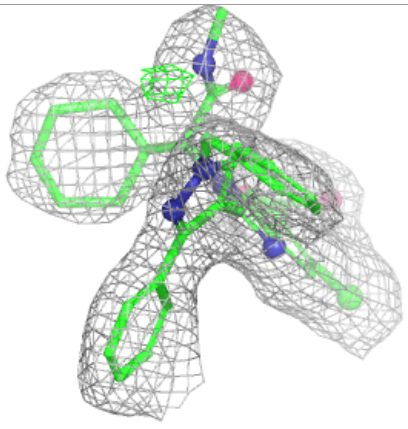


Electron density around A1AG7 D 301:

$2mF_o$-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.