wwPDB X-ray Structure Validation Summary Report (i)

Nov 10, 2026 – 06:09 PM EST

PDB ID	:	11QH / pdb_000011qh
Title	:	Crystal structure of Serine/threonine-protein kinase 33 (STK33) Kinase Domain in complex with inhibitor CDD-3094
Authors	:	Ta, H.M.; Ku, A.F.; Kim, C.; Matzuk, M.M.
Deposited on	:	2026-03-10
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

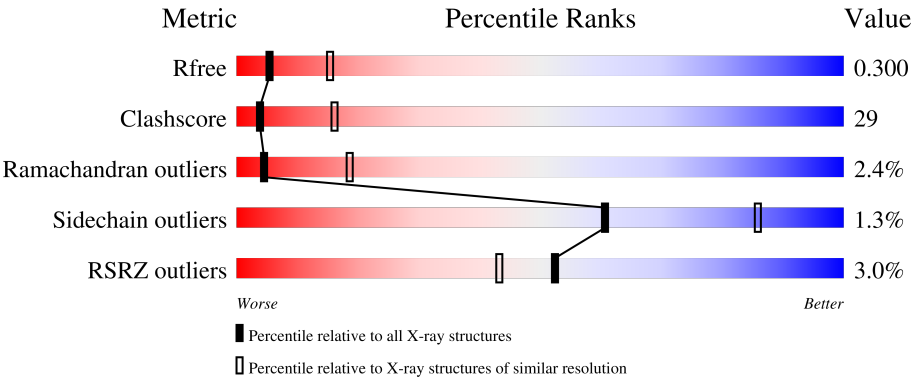
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	291	% 47% 43% • 7%
1	B	291	4% 51% 40% • 7%
1	C	291	3% 57% 37% • •
1	D	291	4% 54% 37% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17506 atoms, of which 8719 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 Serine/threonine-protein kinase 33.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	H	N	O	S	0	0	0
			4341	1382	2176	366	406	11			
1	B	271	Total	C	H	N	O	S	0	0	0
			4259	1362	2121	367	400	9			
1	C	280	Total	C	H	N	O	S	0	0	0
			4387	1395	2197	377	407	11			
1	D	274	Total	C	H	N	O	S	1	1	0
			4255	1363	2117	366	399	10			

There are 44 discrepancies between the modelled and reference sequences:

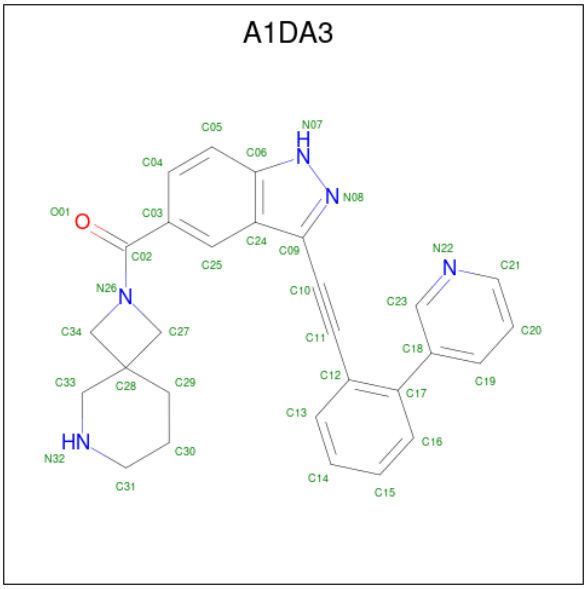
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ILE	MET	conflict	UNP A0A2R9BDV8
A	150	GLU	VAL	conflict	UNP A0A2R9BDV8
A	273	GLN	GLU	conflict	UNP A0A2R9BDV8
A	312	VAL	ILE	conflict	UNP A0A2R9BDV8
A	345	ALA	PRO	conflict	UNP A0A2R9BDV8
A	384	GLU	-	expression tag	UNP A0A2R9BDV8
A	385	ASN	-	expression tag	UNP A0A2R9BDV8
A	386	LEU	-	expression tag	UNP A0A2R9BDV8
A	387	TYR	-	expression tag	UNP A0A2R9BDV8
A	388	PHE	-	expression tag	UNP A0A2R9BDV8
A	389	GLN	-	expression tag	UNP A0A2R9BDV8
B	129	ILE	MET	conflict	UNP A0A2R9BDV8
B	150	GLU	VAL	conflict	UNP A0A2R9BDV8
B	273	GLN	GLU	conflict	UNP A0A2R9BDV8
B	312	VAL	ILE	conflict	UNP A0A2R9BDV8
B	345	ALA	PRO	conflict	UNP A0A2R9BDV8
B	384	GLU	-	expression tag	UNP A0A2R9BDV8
B	385	ASN	-	expression tag	UNP A0A2R9BDV8
B	386	LEU	-	expression tag	UNP A0A2R9BDV8
B	387	TYR	-	expression tag	UNP A0A2R9BDV8
B	388	PHE	-	expression tag	UNP A0A2R9BDV8

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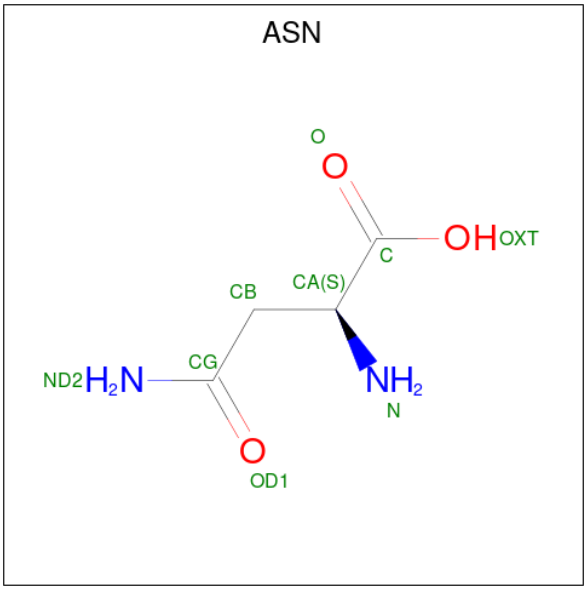
Chain	Residue	Modelled	Actual	Comment	Reference
B	389	GLN	-	expression tag	UNP A0A2R9BDV8
C	129	ILE	MET	conflict	UNP A0A2R9BDV8
C	150	GLU	VAL	conflict	UNP A0A2R9BDV8
C	273	GLN	GLU	conflict	UNP A0A2R9BDV8
C	312	VAL	ILE	conflict	UNP A0A2R9BDV8
C	345	ALA	PRO	conflict	UNP A0A2R9BDV8
C	384	GLU	-	expression tag	UNP A0A2R9BDV8
C	385	ASN	-	expression tag	UNP A0A2R9BDV8
C	386	LEU	-	expression tag	UNP A0A2R9BDV8
C	387	TYR	-	expression tag	UNP A0A2R9BDV8
C	388	PHE	-	expression tag	UNP A0A2R9BDV8
C	389	GLN	-	expression tag	UNP A0A2R9BDV8
D	129	ILE	MET	conflict	UNP A0A2R9BDV8
D	150	GLU	VAL	conflict	UNP A0A2R9BDV8
D	273	GLN	GLU	conflict	UNP A0A2R9BDV8
D	312	VAL	ILE	conflict	UNP A0A2R9BDV8
D	345	ALA	PRO	conflict	UNP A0A2R9BDV8
D	384	GLU	-	expression tag	UNP A0A2R9BDV8
D	385	ASN	-	expression tag	UNP A0A2R9BDV8
D	386	LEU	-	expression tag	UNP A0A2R9BDV8
D	387	TYR	-	expression tag	UNP A0A2R9BDV8
D	388	PHE	-	expression tag	UNP A0A2R9BDV8
D	389	GLN	-	expression tag	UNP A0A2R9BDV8

- Molecule 2 is (2,6-diazaspiro[3.5]nonan-2-yl)(3-{[(2M)-2-(pyridin-3-yl)phenyl]ethynyl}-1H-indazol-5-yl)methanone (CCD ID: A1DA3) (formula: $C_{28}H_{25}N_5O$) (labeled as "Ligand of Interest" by depositor).



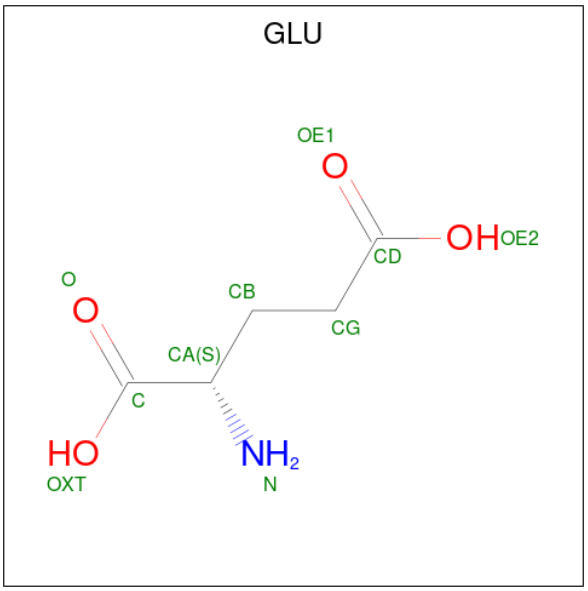
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			59	28	25	5	1		
2	B	1	Total	C	H	N	O	0	0
			59	28	25	5	1		
2	C	1	Total	C	H	N	O	0	0
			59	28	25	5	1		
2	D	1	Total	C	H	N	O	0	0
			59	28	25	5	1		

- Molecule 3 is ASPARAGINE (CCD ID: ASN) (formula: $C_4H_8N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			7	3	2	1	1		
3	B	1	Total	C	H	N	O	0	0
			7	3	2	1	1		

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



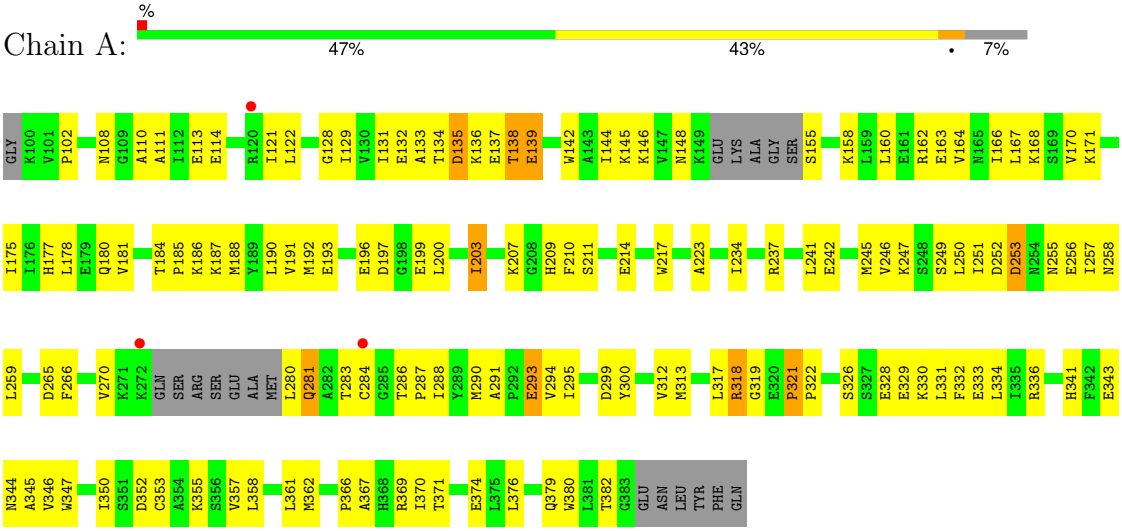
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			7	3	2	1	1		
4	C	1	Total	C	H	N	O	0	0
			7	3	2	1	1		

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.

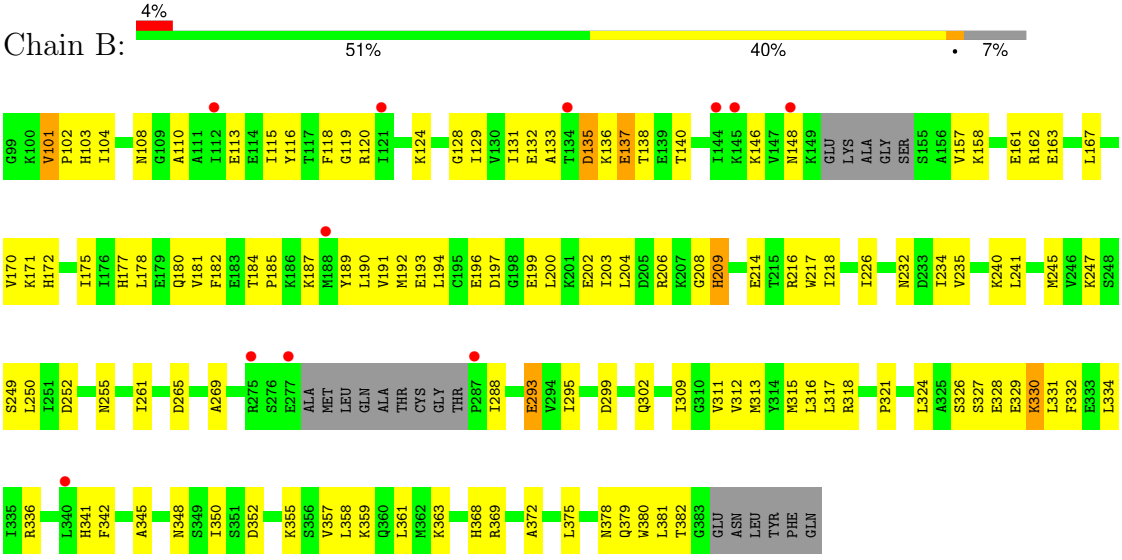
• Molecule 1: Serine/threonine-protein kinase 33

Chain A:



• Molecule 1: Serine/threonine-protein kinase 33

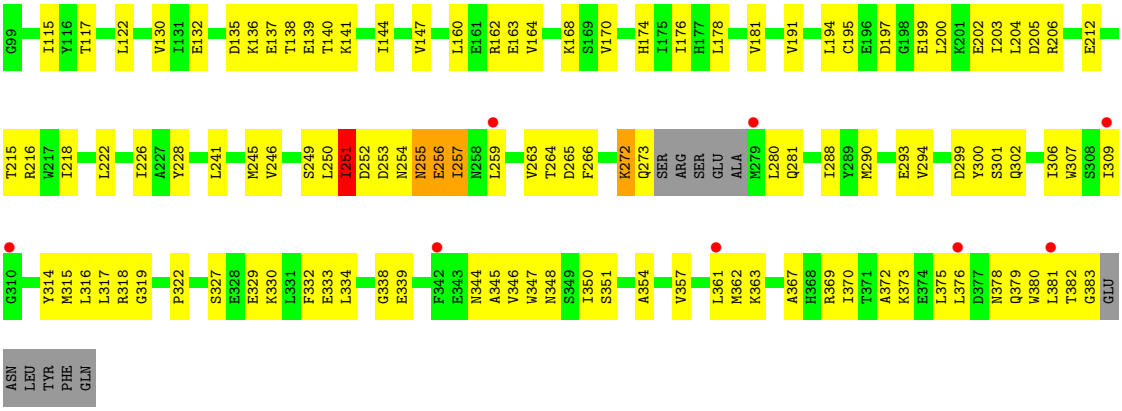
Chain B:



• Molecule 1: Serine/threonine-protein kinase 33

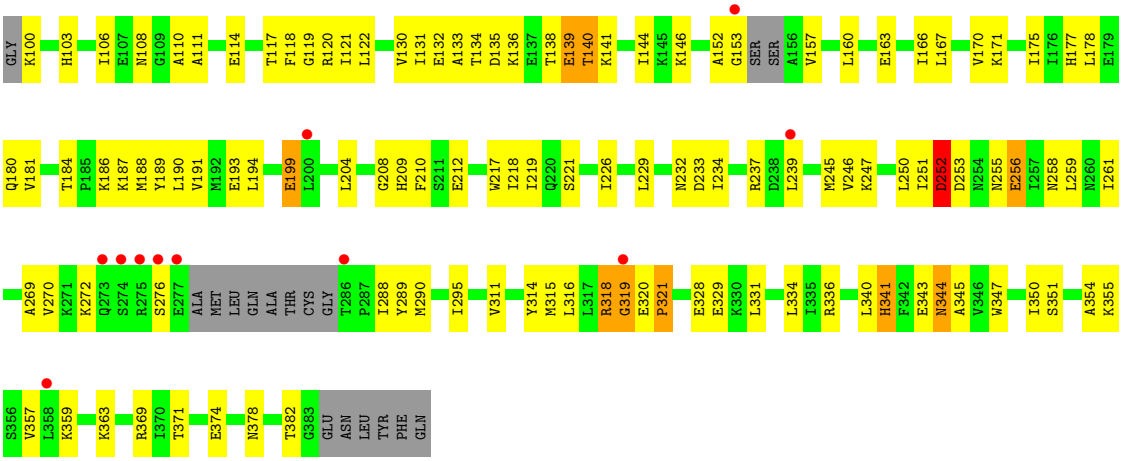
Chain C:





• Molecule 1: Serine/threonine-protein kinase 33





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.92Å 134.29Å 140.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 2.90 49.13 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.13-2.90) 99.9 (49.13-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.91Å)	Xtriage
Refinement program	PHENIX (2.0_5936: ???)	Depositor
R, R_{free}	0.253 , 0.300 0.253 , 0.300	Depositor DCC
R_{free} test set	1789 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	101.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 74.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17506	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: A1DA3

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	0.57	1/2203 (0.0%)	0.69	1/2975 (0.0%)
1	B	0.58	1/2176 (0.0%)	0.69	1/2934 (0.0%)
1	C	0.58	1/2228 (0.0%)	0.71	2/3008 (0.1%)
1	D	0.60	1/2179 (0.0%)	0.73	1/2943 (0.0%)
All	All	0.58	4/8786 (0.0%)	0.70	5/11860 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	PRO	CA-C	10.46	1.57	1.51
1	D	321	PRO	CA-C	-8.56	1.47	1.51
1	A	321	PRO	CA-C	8.16	1.56	1.51
1	C	257	ILE	CG1-CD1	-5.52	1.30	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	PRO	O-C-N	8.67	125.30	121.31
1	C	257	ILE	CB-CG1-CD1	-8.22	96.53	113.80
1	D	321	PRO	O-C-N	-6.50	118.32	121.31
1	A	321	PRO	O-C-N	6.27	124.20	121.31
1	C	251	ILE	CB-CG1-CD1	-5.43	102.40	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	ARG	Mainchain

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	2165	2176	2175	151	0
1	B	2138	2121	2120	128	0
1	C	2190	2197	2196	122	0
1	D	2138	2117	2112	113	0
2	A	34	25	0	3	0
2	B	34	25	0	2	0
2	C	34	25	0	1	0
2	D	34	25	0	0	0
3	A	5	2	1	0	0
3	B	5	2	2	0	0
4	B	5	2	1	0	0
4	C	5	2	1	1	0
All	All	8787	8719	8608	496	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 29.

The worst 5 of 496 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:117:THR:OG1	1:D:136:LYS:NZ	1.85	1.09
1:C:327:SER:OG	1:C:329:GLU:OE1	1.82	0.95
1:C:241:LEU:HD11	1:C:315:MET:HE2	1.54	0.90
1:A:138:THR:HG23	1:A:139:GLU:H	1.38	0.88
1:D:318:ARG:O	1:D:320:GLU:N	2.08	0.86

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	266/291 (91%)	243 (91%)	15 (6%)	8 (3%)	3 14
1	B	265/291 (91%)	239 (90%)	21 (8%)	5 (2%)	6 23
1	C	276/291 (95%)	257 (93%)	14 (5%)	5 (2%)	6 25
1	D	269/291 (92%)	247 (92%)	14 (5%)	8 (3%)	3 14
All	All	1076/1164 (92%)	986 (92%)	64 (6%)	26 (2%)	4 18

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	139	GLU
1	A	253	ASP
1	A	256	GLU
1	B	341	HIS

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	238/257 (93%)	235 (99%)	3 (1%)	61 86
1	B	229/257 (89%)	227 (99%)	2 (1%)	70 90
1	C	235/257 (91%)	233 (99%)	2 (1%)	70 90
1	D	226/257 (88%)	221 (98%)	5 (2%)	45 77
All	All	928/1028 (90%)	916 (99%)	12 (1%)	61 86

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	140	THR
1	D	199	GLU
1	D	318	ARG
1	D	219	ILE
1	B	293	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	368	HIS
1	D	260	ASN
1	D	103	HIS
1	D	303	GLN
1	D	220	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\|>2$
4	GLU	B	401	3	3,4,9	1.00	0	2,4,11	1.03	0
4	GLU	C	401	3	3,4,9	0.81	0	2,4,11	0.98	0
2	A1DA3	A	401	-	37,39,39	3.66	18 (48%)	42,56,56	2.91	13 (30%)
2	A1DA3	B	403	-	37,39,39	3.64	19 (51%)	42,56,56	2.71	13 (30%)
3	ASN	B	402	4	3,4,8	0.68	0	2,4,10	0.64	0
3	ASN	A	402	4	3,4,8	0.79	0	2,4,10	0.67	0
2	A1DA3	D	401	-	37,39,39	3.78	20 (54%)	42,56,56	2.68	12 (28%)
2	A1DA3	C	402	-	37,39,39	3.51	19 (51%)	42,56,56	2.76	13 (30%)

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	GLU	B	401	3	-	0/1/2/9	-
4	GLU	C	401	3	-	0/1/2/9	-
2	A1DA3	A	401	-	-	6/15/37/37	0/6/6/6
2	A1DA3	B	403	-	-	4/15/37/37	0/6/6/6
3	ASN	B	402	4	-	0/1/2/8	-
3	ASN	A	402	4	-	0/1/2/8	-
2	A1DA3	D	401	-	-	4/15/37/37	0/6/6/6
2	A1DA3	C	402	-	-	4/15/37/37	0/6/6/6

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	A1DA3	C14-C13	8.70	1.53	1.38
2	C	402	A1DA3	C15-C16	8.67	1.53	1.38
2	D	401	A1DA3	C27-C28	-8.59	1.46	1.54
2	D	401	A1DA3	C15-C16	8.44	1.53	1.38
2	B	403	A1DA3	C15-C16	8.40	1.53	1.38

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	A1DA3	C06-N07-N08	12.52	121.19	111.90
2	B	403	A1DA3	C06-N07-N08	11.49	120.42	111.90
2	C	402	A1DA3	C06-N07-N08	11.13	120.16	111.90
2	D	401	A1DA3	C06-N07-N08	10.94	120.02	111.90

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	402	A1DA3	C24-C09-N08	6.69	114.17	110.36

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	A1DA3	N26-C02-C03-C25
2	C	402	A1DA3	N26-C02-C03-C25
2	D	401	A1DA3	N26-C02-C03-C04
2	A	401	A1DA3	C10-C11-C12-C13
2	A	401	A1DA3	N26-C02-C03-C25

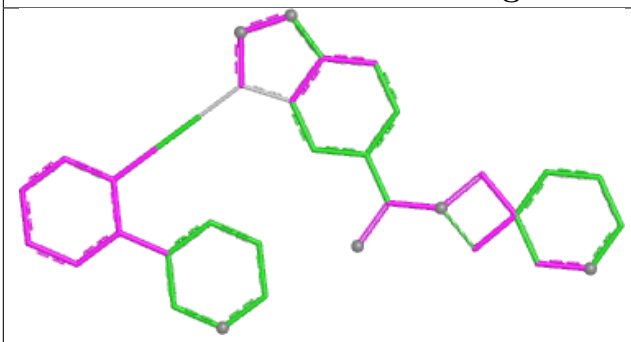
There are no ring outliers.

4 monomers are involved in 7 short contacts:

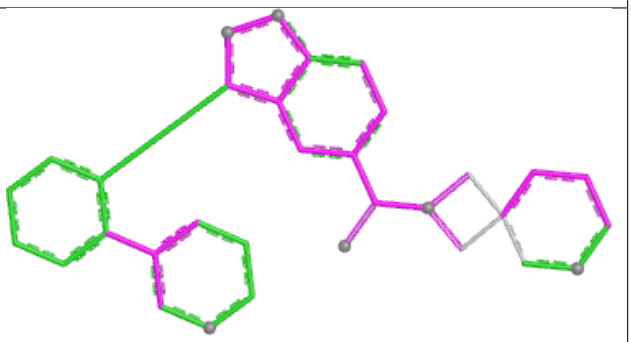
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	GLU	1	0
2	A	401	A1DA3	3	0
2	B	403	A1DA3	2	0
2	C	402	A1DA3	1	0

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.

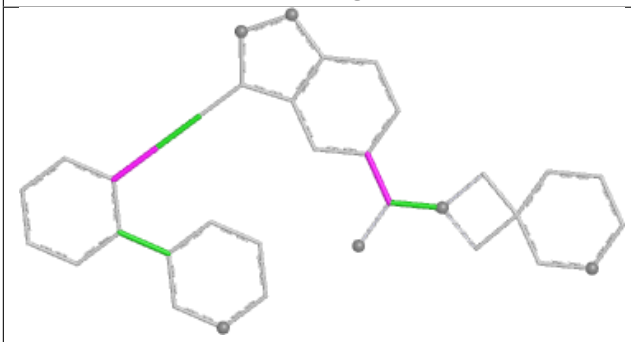
Ligand A1DA3 A 401



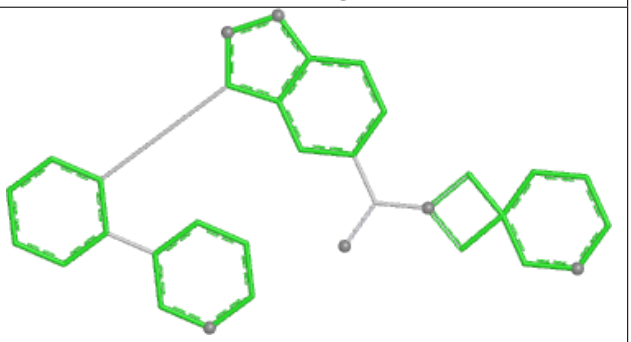
Bond lengths



Bond angles

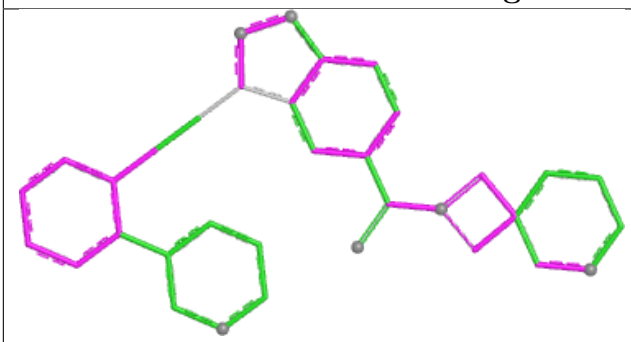


Torsions

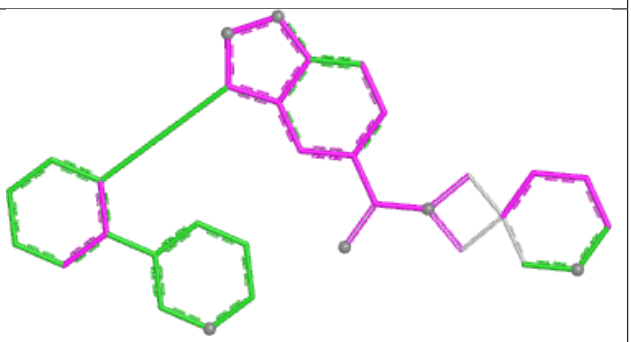


Rings

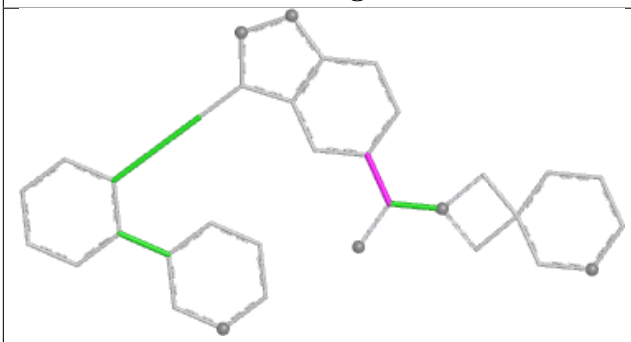
Ligand A1DA3 B 403



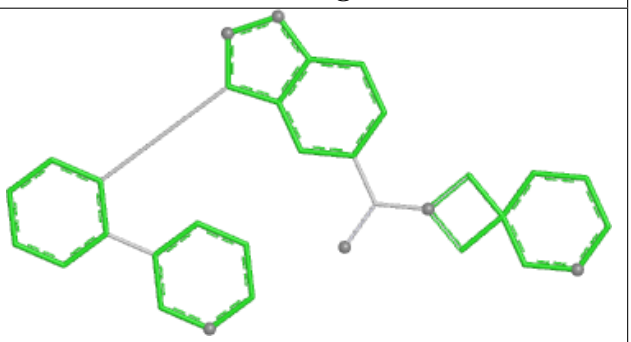
Bond lengths



Bond angles

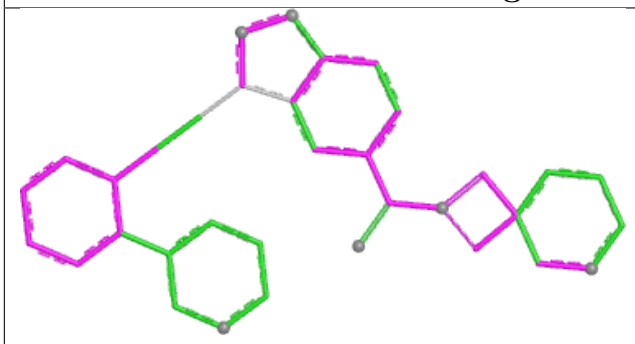


Torsions

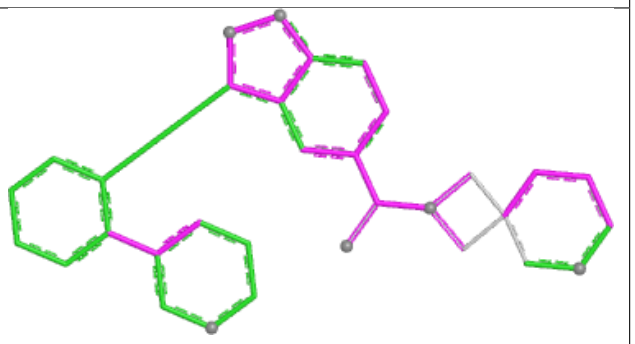


Rings

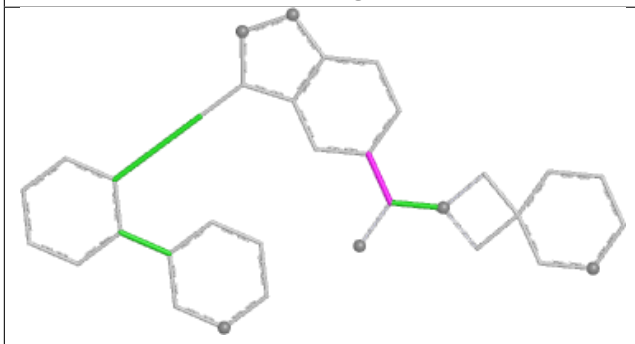
Ligand A1DA3 D 401



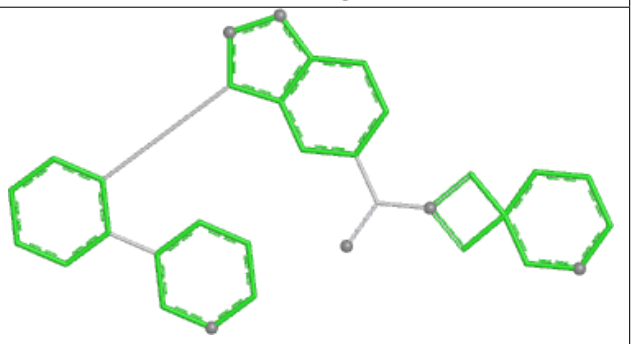
Bond lengths



Bond angles

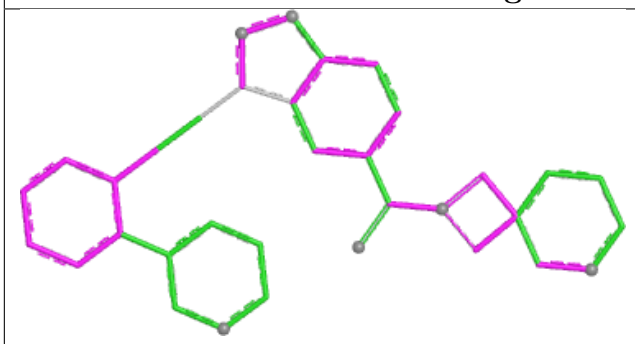


Torsions

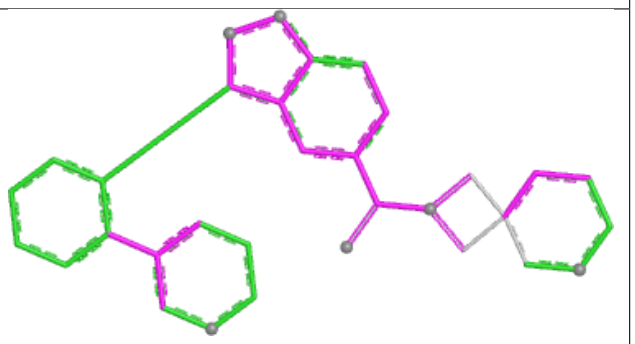


Rings

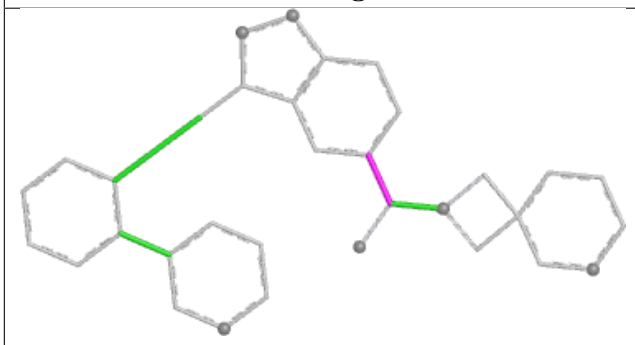
Ligand A1DA3 C 402



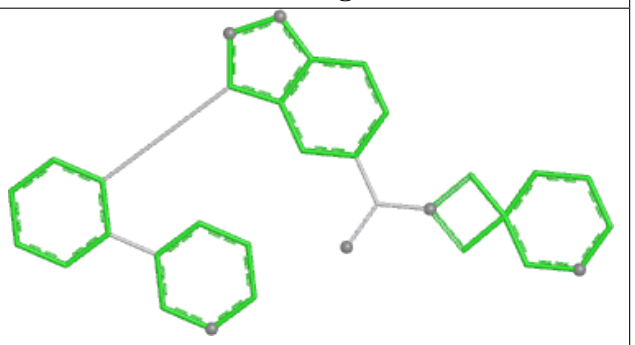
Bond lengths



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

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	272/291 (93%)	0.13	3 (1%)	78	71	74, 109, 164, 298	0
1	B	271/291 (93%)	0.14	11 (4%)	41	33	69, 118, 171, 195	0
1	C	280/291 (96%)	0.16	8 (2%)	53	45	71, 110, 177, 226	0
1	D	274/291 (94%)	0.25	11 (4%)	42	34	73, 120, 181, 443	0
All	All	1097/1164 (94%)	0.17	33 (3%)	52	43	69, 115, 175, 443	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	6.1
1	D	277	GLU	4.9
1	D	273	GLN	4.1
1	B	275	ARG	3.4
1	D	275[A]	ARG	3.3

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

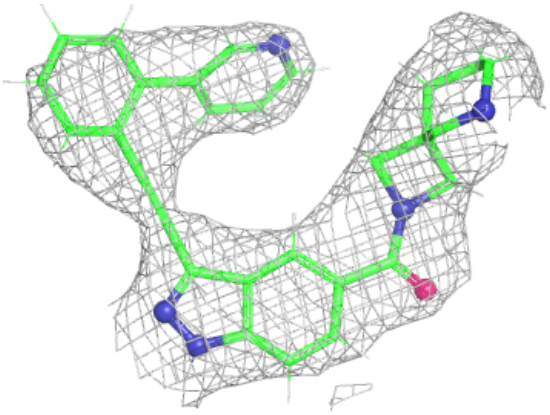
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

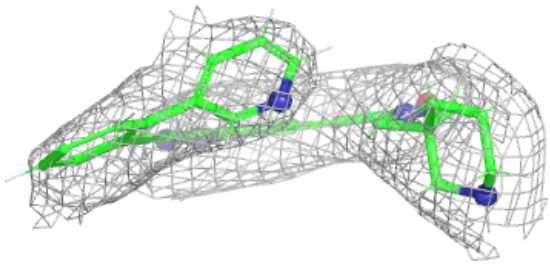
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ASN	A	402	5/9	0.27	0.26	98,105,132,149	0
4	GLU	C	401	5/10	0.64	0.16	114,123,149,157	0
3	ASN	B	402	5/9	0.68	0.20	131,132,160,160	0
4	GLU	B	401	5/10	0.72	0.17	116,123,143,149	0
2	A1DA3	C	402	34/34	0.93	0.10	72,87,109,115	0
2	A1DA3	D	401	34/34	0.93	0.13	94,114,139,142	0
2	A1DA3	A	401	34/34	0.93	0.09	83,91,109,115	0
2	A1DA3	B	403	34/34	0.94	0.12	88,106,129,131	0

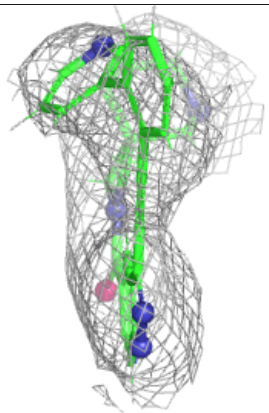
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1DA3 C 402:

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

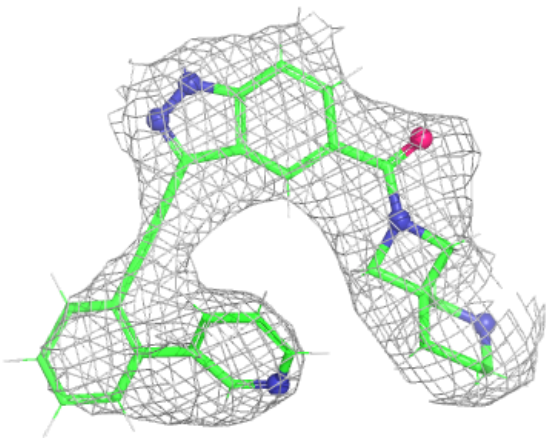


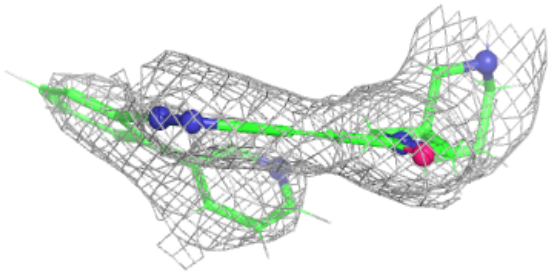


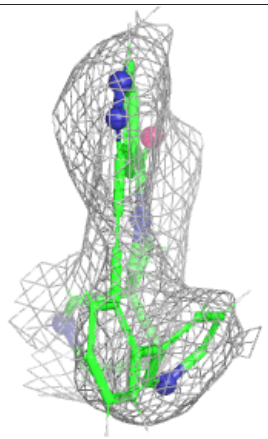


Electron density around A1DA3 D 401:

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

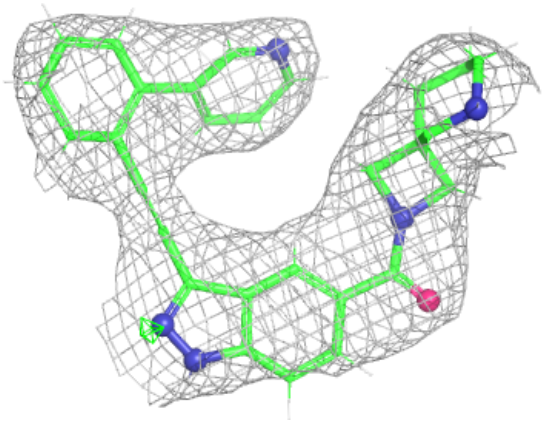


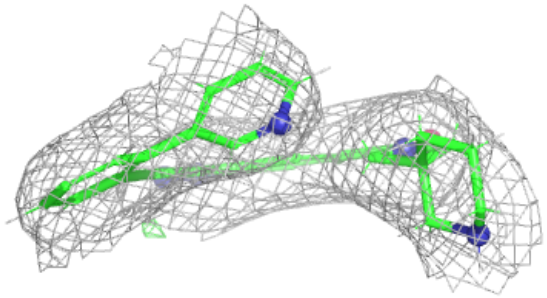


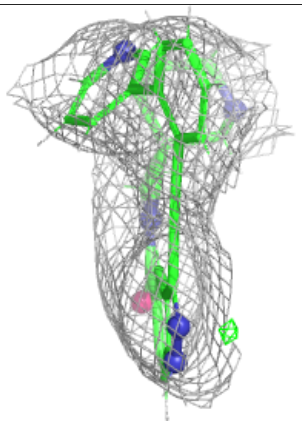


Electron density around A1DA3 A 401:

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

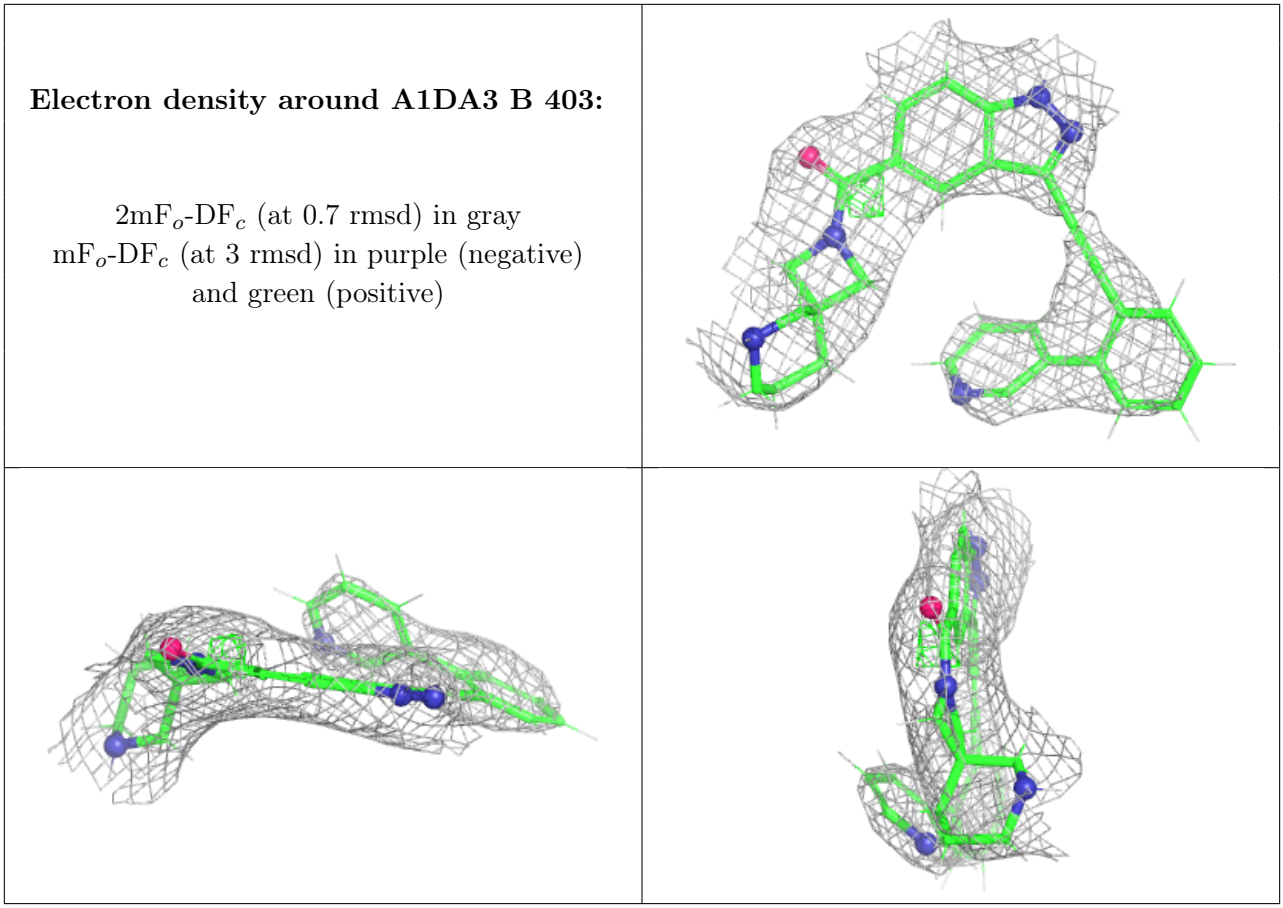






Electron density around A1DA3 B 403:

$2mF_o$-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

There are no such residues in this entry.