



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:43 PM UTC

PDB ID : 9GBH / pdb_00009gbh
Title : CRYSTAL STRUCTURE OF HUMAN CHYMASE IN COMPLEX WITH COMPOUND1
Authors : Schaefer, M.; Fuerstner, C.; Ackerstaff, J.; Meier, H.; Straub, A.; Mittendorf, J.; Schamberger, J.; Boerngen, K.; Joerissen, H.; Zubow, D.; Zimmermann, K.; Tersteegen, A.; Geiss, V.; Hartmann, E.; Albrecht-Kuepper, B.; Dorleans-Juste, P.; Lapointe, C.; Vincent, L.; Heitmeier, S.; Tinel, H.
Deposited on : 2024-07-31
Resolution : 2.38 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)

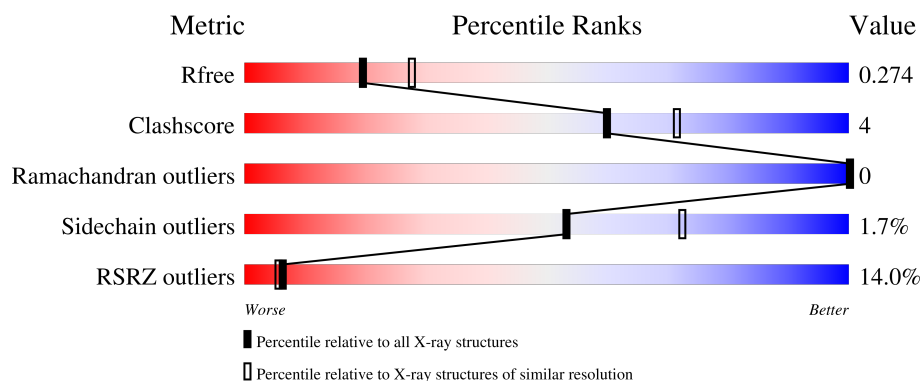
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	AAA	226	13% 84% 11% 5%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1878 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.

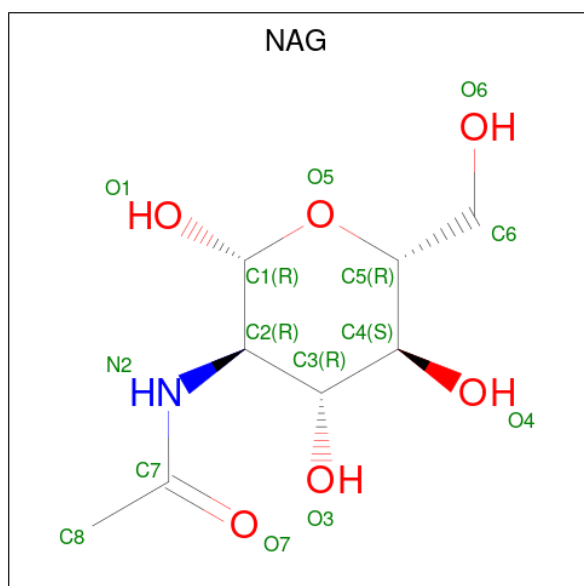
- Molecule 1 is a protein called Chymase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	215	1677	1061	307	298	11	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	127	ARG	PHE	engineered mutation	UNP P23946
AAA	208	ALA	VAL	engineered mutation	UNP P23946
AAA	235	GLN	ARG	engineered mutation	UNP P23946

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



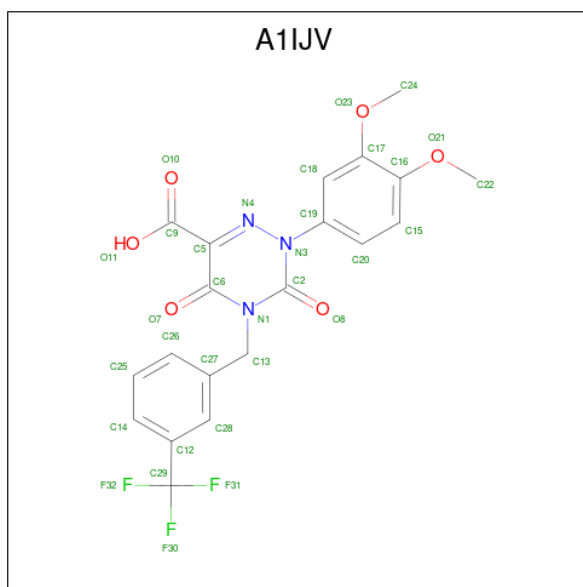
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	AAA	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
2	AAA	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-(3,4-dimethoxyphenyl)-3,5-bis(oxidanylidene)-4-[[3-(trifluoromethyl)phenyl]methyl]-1,2,4-triazine-6-carboxylic acid (CCD ID: A1IJV) (formula: $C_{20}H_{16}F_3N_3O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	F	N	O	0
			32	20	3	3	6	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Zn	0	0
			1	1		

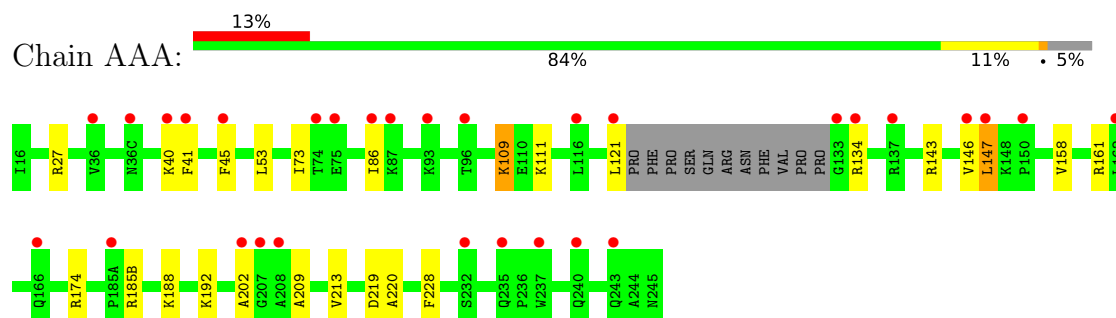
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	126	Total	O	0	0
			126	126		

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: Chymase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	74.09Å 74.09Å 49.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.04 – 2.38 37.04 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.04-2.38) 99.6 (37.04-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.274 0.202 , 0.274	Depositor DCC
R_{free} test set	528 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	1878	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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: ZN, A1IJV, NAG

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	AAA	0.62	0/1720	1.00	1/2321 (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	AAA	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	111	LYS	CB-CA-C	5.11	118.17	109.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	161	ARG	Sidechain
1	AAA	174	ARG	Sidechain

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	AAA	1677	0	1695	12	0
2	AAA	42	0	39	3	0
3	AAA	32	0	0	0	0
4	AAA	1	0	0	0	0
5	AAA	126	0	0	1	0
All	All	1878	0	1734	15	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 4.

All (15) 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)
2:AAA:302:NAG:O4	2:AAA:303:NAG:C1	2.14	0.95
2:AAA:302:NAG:C4	2:AAA:303:NAG:C1	2.69	0.70
1:AAA:146:VAL:HG12	1:AAA:147:LEU:HD22	1.83	0.59
1:AAA:86[A]:ILE:HG21	1:AAA:109[A]:LYS:HG2	1.91	0.53
1:AAA:158:VAL:HG21	1:AAA:188:LYS:HB3	1.91	0.53
2:AAA:302:NAG:H4	2:AAA:303:NAG:C1	2.38	0.52
1:AAA:27:ARG:NE	5:AAA:405:HOH:O	2.44	0.49
1:AAA:121:LEU:HD21	1:AAA:209:ALA:HB2	1.96	0.47
1:AAA:134:ARG:HH22	1:AAA:202:ALA:HB2	1.81	0.45
1:AAA:219:ASP:O	1:AAA:220:ALA:HB3	2.19	0.43
1:AAA:143:ARG:HD2	1:AAA:192:LYS:HB2	1.99	0.43
1:AAA:45:PHE:CZ	1:AAA:53:LEU:HD23	2.54	0.42
1:AAA:40:LYS:HG2	1:AAA:41:PHE:N	2.35	0.42
1:AAA:73:ILE:HD12	1:AAA:73:ILE:HA	1.93	0.41
1:AAA:213:VAL:HG22	1:AAA:228:PHE:CE2	2.55	0.41

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	AAA	213/226 (94%)	210 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	AAA	181/190 (95%)	177 (98%)	4 (2%)	45	65

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

Mol	Chain	Res	Type
1	AAA	109[A]	LYS
1	AAA	109[B]	LYS
1	AAA	147	LEU
1	AAA	185(B)	ARG

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

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
2	NAG	AAA	303	-	14,14,15	0.36	0	17,19,21	0.74	1 (5%)
2	NAG	AAA	302	1	14,14,15	0.43	0	17,19,21	1.31	2 (11%)
3	A1IJV	AAA	304	-	34,34,34	1.80	9 (26%)	48,50,50	2.04	14 (29%)
2	NAG	AAA	301	1	14,14,15	0.50	0	17,19,21	1.52	4 (23%)

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	NAG	AAA	303	-	-	2/6/23/26	0/1/1/1
2	NAG	AAA	302	1	-	2/6/23/26	0/1/1/1
3	A1IJV	AAA	304	-	-	1/21/22/22	0/3/3/3
2	NAG	AAA	301	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	304	A1IJV	N3-N4	-6.34	1.21	1.38
3	AAA	304	A1IJV	C5-C9	3.50	1.55	1.48
3	AAA	304	A1IJV	C19-N3	-3.39	1.36	1.43
3	AAA	304	A1IJV	C2-N3	2.99	1.42	1.39
3	AAA	304	A1IJV	C29-C12	2.61	1.55	1.49
3	AAA	304	A1IJV	O11-C9	-2.22	1.24	1.30
3	AAA	304	A1IJV	C26-C27	2.21	1.43	1.38
3	AAA	304	A1IJV	C5-C6	-2.09	1.40	1.45
3	AAA	304	A1IJV	C20-C15	2.03	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	304	A1IJV	C6-N1-C2	-6.28	117.89	125.62
3	AAA	304	A1IJV	C13-N1-C2	4.64	123.40	116.92
2	AAA	302	NAG	C2-N2-C7	3.87	128.08	122.90
3	AAA	304	A1IJV	C18-C19-N3	-3.84	113.70	119.27
3	AAA	304	A1IJV	C26-C27-C28	3.38	123.21	118.55
3	AAA	304	A1IJV	N3-C2-N1	3.12	117.88	113.51
3	AAA	304	A1IJV	F30-C29-C12	-3.10	106.25	112.90
3	AAA	304	A1IJV	C15-C20-C19	-2.93	116.59	120.30
3	AAA	304	A1IJV	C19-N3-N4	2.88	118.48	113.58
2	AAA	301	NAG	C3-C4-C5	-2.85	105.06	110.23
2	AAA	301	NAG	O5-C1-C2	2.79	115.61	111.29
3	AAA	304	A1IJV	C20-C19-N3	2.61	123.65	119.72
2	AAA	301	NAG	C4-C3-C2	-2.53	107.31	111.02
3	AAA	304	A1IJV	O10-C9-C5	-2.44	114.73	120.92
3	AAA	304	A1IJV	C25-C26-C27	-2.36	117.29	120.61
2	AAA	301	NAG	O4-C4-C3	2.29	115.77	110.38
2	AAA	303	NAG	C1-C2-N2	2.26	113.99	110.43
2	AAA	302	NAG	O5-C1-C2	-2.15	107.97	111.29
3	AAA	304	A1IJV	F31-C29-C12	2.12	117.44	112.90
3	AAA	304	A1IJV	C13-C27-C28	-2.10	116.32	120.27
3	AAA	304	A1IJV	C5-N4-N3	2.08	123.26	118.85

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	302	NAG	C8-C7-N2-C2
2	AAA	302	NAG	O7-C7-N2-C2
2	AAA	303	NAG	C8-C7-N2-C2
2	AAA	301	NAG	C8-C7-N2-C2
2	AAA	301	NAG	O7-C7-N2-C2
2	AAA	303	NAG	O7-C7-N2-C2
3	AAA	304	A1IJV	C6-C5-C9-O11

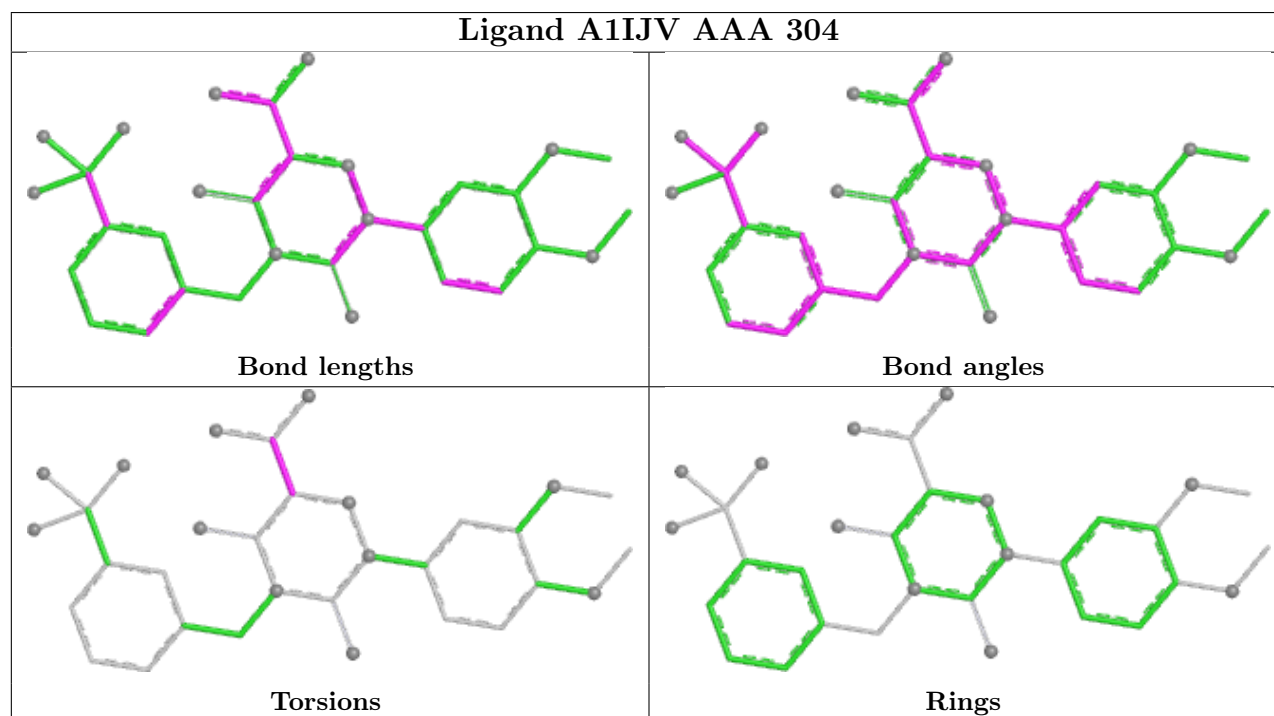
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	303	NAG	3	0
2	AAA	302	NAG	3	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	AAA	215/226 (95%)	1.18	30 (13%) 6 5	23, 39, 59, 84	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	202	ALA	4.5
1	AAA	133	GLY	4.2
1	AAA	137	ARG	4.0
1	AAA	235	GLN	3.8
1	AAA	40	LYS	3.6
1	AAA	134	ARG	3.5
1	AAA	207	GLY	3.5
1	AAA	147	LEU	3.4
1	AAA	146	VAL	3.4
1	AAA	41	PHE	3.3
1	AAA	36	VAL	3.1
1	AAA	150	PRO	2.8
1	AAA	162	LEU	2.7
1	AAA	87	LYS	2.5
1	AAA	116	LEU	2.5
1	AAA	75	GLU	2.5
1	AAA	185(A)	PRO	2.4
1	AAA	45	PHE	2.4
1	AAA	93	LYS	2.3
1	AAA	96	THR	2.3
1	AAA	166	GLN	2.3
1	AAA	36(C)	ASN	2.3
1	AAA	232	SER	2.3
1	AAA	208	ALA	2.3
1	AAA	121	LEU	2.2
1	AAA	74	THR	2.2
1	AAA	243	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	240	GLN	2.1
1	AAA	86[A]	ILE	2.1
1	AAA	237	TRP	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](#)

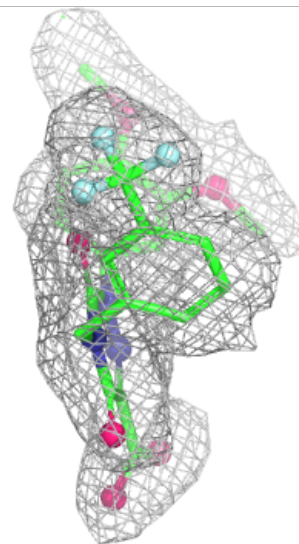
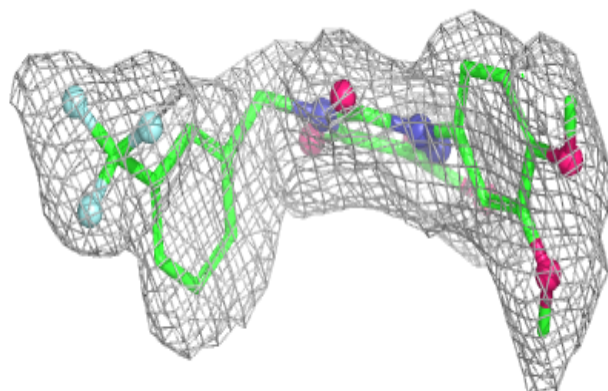
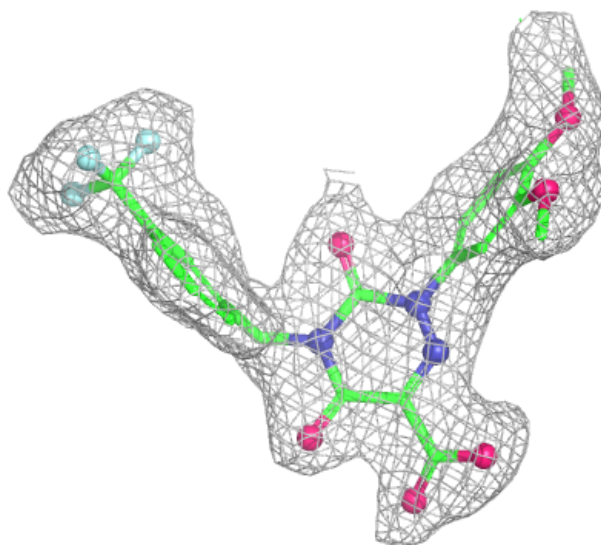
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	AAA	303	14/15	0.49	0.24	65,87,102,122	0
2	NAG	AAA	301	14/15	0.74	0.18	48,59,72,74	0
2	NAG	AAA	302	14/15	0.75	0.17	57,63,69,71	0
3	A1IJV	AAA	304	32/32	0.90	0.12	35,42,47,48	0
4	ZN	AAA	305	1/1	0.99	0.03	38,38,38,38	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 A1IJV AAA 304:

$2mF_o-DF_c$ (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.