



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2024 – 08:04 PM EST

PDB ID : 9AX3
Title : Structure of full-length amyloidogenic immunoglobulin light chain H9 in complex with 4-(3-ethyl-3-phenylpyrrolidin-1-yl)-1,6-dimethylpyridin-2(1H)-one
Authors : Lederberg, O.L.; Yan, N.L.; Stanfield, R.L.; Wilson, I.A.; Kelly, J.W.
Deposited on : 2024-03-05
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 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) : 2.40

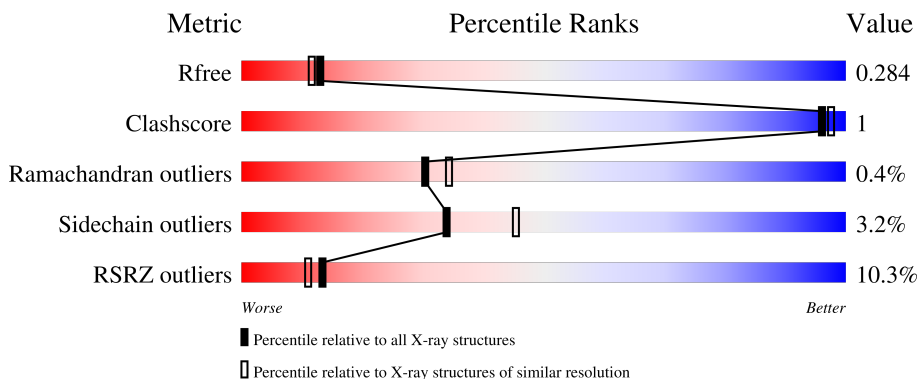
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	216	 10% 92% 8%
1	B	216	 10% 95% .
1	C	216	 11% 96% .
1	D	216	 11% 94% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12728 atoms, of which 6072 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 H9 Immunoglobulin Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	215	3087	978	1509	264	331	5	0	0	0
1	B	215	3087	978	1509	264	331	5	0	0	0
1	C	216	3098	981	1514	265	333	5	0	0	0
1	D	216	3098	981	1514	265	333	5	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



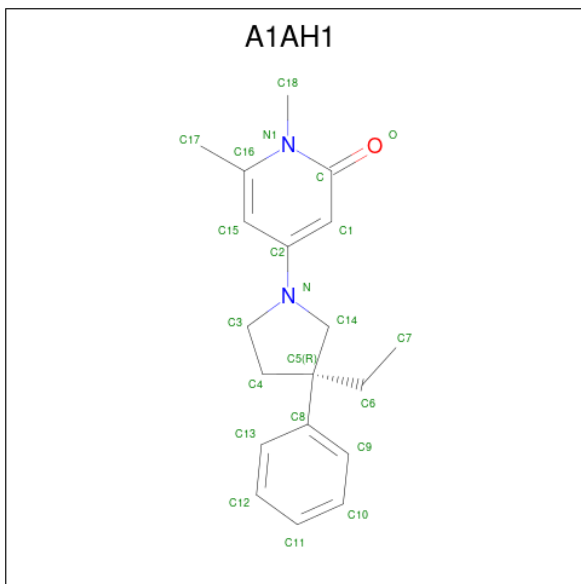
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			O	P		
2	A	1	Total 5	4 1	0	0
2	B	1	Total 5	4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0

- Molecule 3 is 4-[(3R)-3-ethyl-3-phenylpyrrolidin-1-yl]-1,6-dimethylpyridin-2(1H)-one (three-letter code: A1AH1) (formula: C₁₉H₂₄N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	B	1	35	19	13	2	1	0	0
3	D	1	35	19	13	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	72	72	72	0	0

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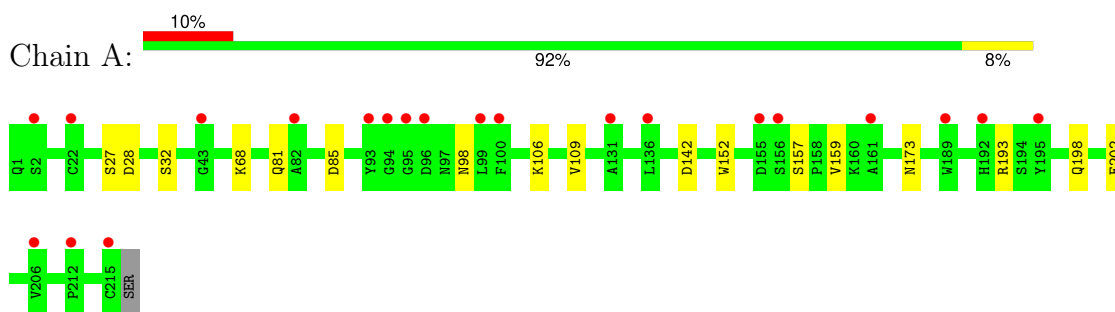
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	67	Total O 67 67	0	0
4	C	55	Total O 55 55	0	0
4	D	59	Total O 59 59	0	0

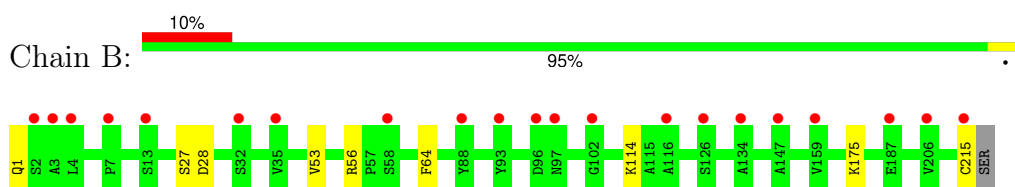
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

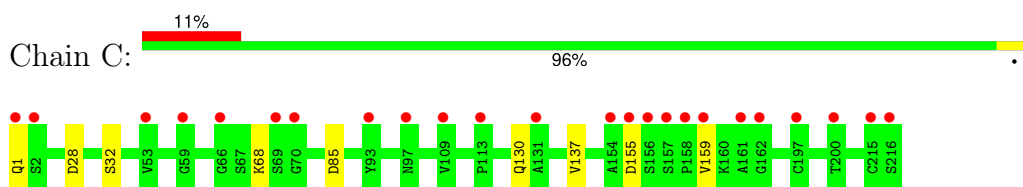
- Molecule 1: H9 Immunoglobulin Light Chain



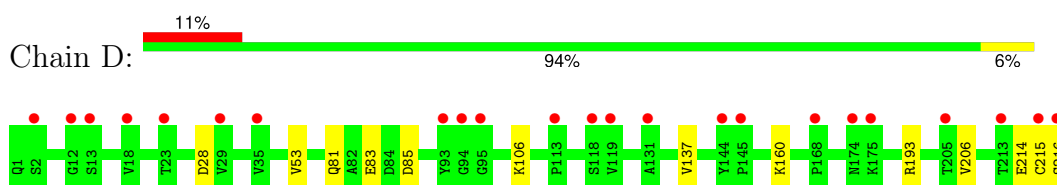
- Molecule 1: H9 Immunoglobulin Light Chain



- Molecule 1: H9 Immunoglobulin Light Chain



- Molecule 1: H9 Immunoglobulin Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.97Å 63.71Å 86.26Å 84.41° 86.91° 80.63°	Depositor
Resolution (Å)	48.53 – 2.20 48.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.3 (48.53-2.20) 91.5 (48.53-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, R_{free}	0.232 , 0.284 0.233 , 0.284	Depositor DCC
R_{free} test set	2434 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtrriage
Anisotropy	0.557	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12728	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% 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: PO4, A1AH1

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	0.29	0/1616	0.46	0/2206
1	B	0.29	0/1616	0.48	0/2206
1	C	0.29	0/1622	0.46	0/2214
1	D	0.29	0/1622	0.48	0/2214
All	All	0.29	0/6476	0.47	0/8840

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 [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	1578	1509	1509	6	0
1	B	1578	1509	1509	2	0
1	C	1584	1514	1514	2	0
1	D	1584	1514	1514	3	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
3	B	22	13	0	0	0
3	D	22	13	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	72	0	0	1	0
4	B	67	0	0	1	0
4	C	55	0	0	0	0
4	D	59	0	0	0	0
All	All	6656	6072	6046	12	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 1.

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:142:ASP:OD1	1:A:173:ASN:ND2	2.30	0.63
1:A:85:ASP:OD1	1:A:106:LYS:NZ	2.26	0.61
1:D:81:GLN:NE2	1:D:83:GLU:OE2	2.33	0.60
1:A:202:GLU:OE1	4:A:401:HOH:O	2.20	0.49
1:A:81:GLN:O	1:A:109:VAL:HG21	2.13	0.49
1:C:32:SER:O	1:C:68:LYS:NZ	2.47	0.48
1:A:32:SER:O	1:A:68:LYS:NZ	2.47	0.47
1:C:137:VAL:HG11	1:D:137:VAL:HG11	1.95	0.47
1:B:56:ARG:HD3	1:B:64:PHE:O	2.18	0.44
1:B:175:LYS:NZ	4:B:404:HOH:O	2.53	0.42
1:A:152:TRP:HB2	1:A:159:VAL:HG22	2.01	0.42
1:D:85:ASP:OD1	1:D:106:LYS:NZ	2.49	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	A	213/216 (99%)	203 (95%)	10 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/216 (99%)	199 (93%)	13 (6%)	1 (0%)	25	28
1	C	214/216 (99%)	202 (94%)	11 (5%)	1 (0%)	25	28
1	D	214/216 (99%)	201 (94%)	12 (6%)	1 (0%)	25	28
All	All	854/864 (99%)	805 (94%)	46 (5%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	155	ASP
1	D	53	VAL
1	B	53	VAL

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	179/180 (99%)	173 (97%)	6 (3%)	32	42
1	B	179/180 (99%)	174 (97%)	5 (3%)	38	51
1	C	180/180 (100%)	175 (97%)	5 (3%)	38	51
1	D	180/180 (100%)	173 (96%)	7 (4%)	27	37
All	All	718/720 (100%)	695 (97%)	23 (3%)	34	45

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	28	ASP
1	A	98	ASN
1	A	157	SER
1	A	193	ARG
1	A	198	GLN
1	B	1	GLN
1	B	27	SER

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Mol	Chain	Res	Type
1	B	28	ASP
1	B	114	LYS
1	B	215	CYS
1	C	1	GLN
1	C	28	ASP
1	C	85	ASP
1	C	130	GLN
1	C	159	VAL
1	D	28	ASP
1	D	160	LYS
1	D	193	ARG
1	D	206	VAL
1	D	214	GLU
1	D	215	CYS
1	D	216	SER

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

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](#)

9 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	PO4	B	303	-	4,4,4	1.68	1 (25%)	6,6,6	0.53	0
3	A1AH1	B	304	-	24,24,24	0.29	0	25,35,35	0.41	0
2	PO4	B	301	-	4,4,4	1.70	1 (25%)	6,6,6	0.42	0
2	PO4	A	301	-	4,4,4	1.56	1 (25%)	6,6,6	0.51	0
2	PO4	C	302	-	4,4,4	1.70	1 (25%)	6,6,6	0.52	0
3	A1AH1	D	401	-	24,24,24	0.30	0	25,35,35	0.36	0
2	PO4	C	301	-	4,4,4	1.59	1 (25%)	6,6,6	0.49	0
2	PO4	B	302	-	4,4,4	1.59	1 (25%)	6,6,6	0.47	0
2	PO4	C	303	-	4,4,4	1.66	1 (25%)	6,6,6	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1AH1	B	304	-	-	2/13/24/24	0/3/3/3
3	A1AH1	D	401	-	-	5/13/24/24	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	PO4	P-O1	2.95	1.57	1.50
2	C	302	PO4	P-O1	2.93	1.57	1.50
2	C	303	PO4	P-O1	2.89	1.57	1.50
2	B	303	PO4	P-O1	2.82	1.57	1.50
2	B	302	PO4	P-O1	2.76	1.57	1.50
2	C	301	PO4	P-O1	2.65	1.56	1.50
2	A	301	PO4	P-O1	2.64	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	A1AH1	C4-C5-C8-C13

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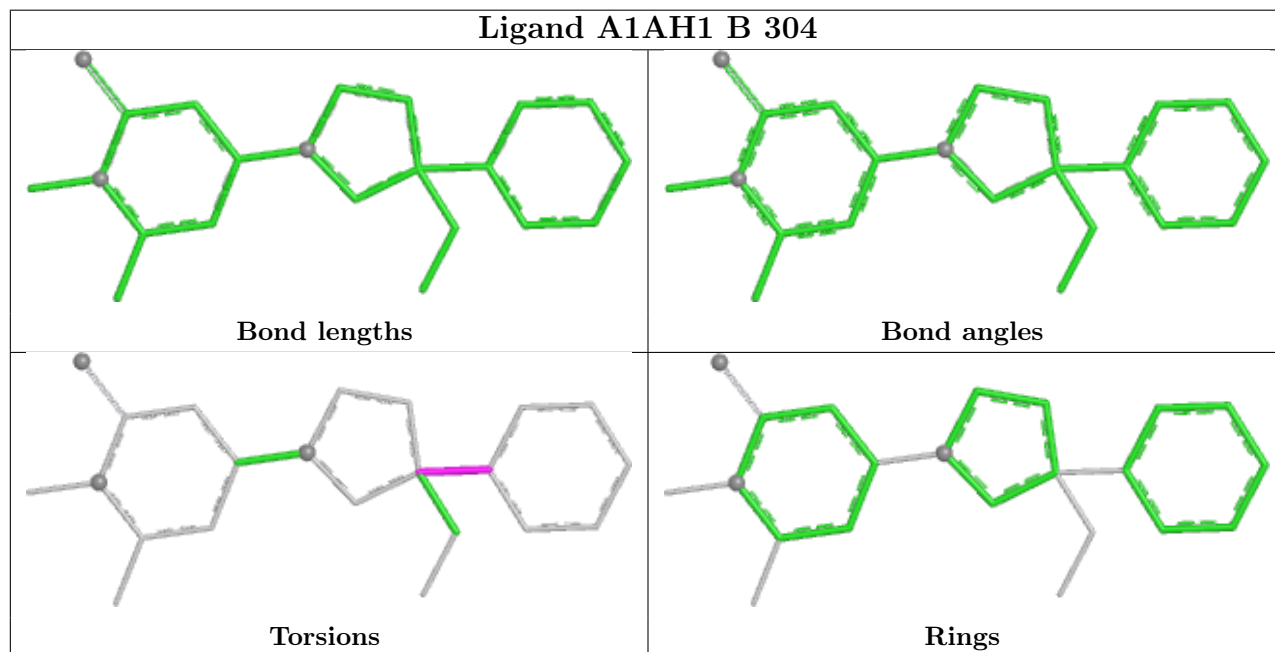
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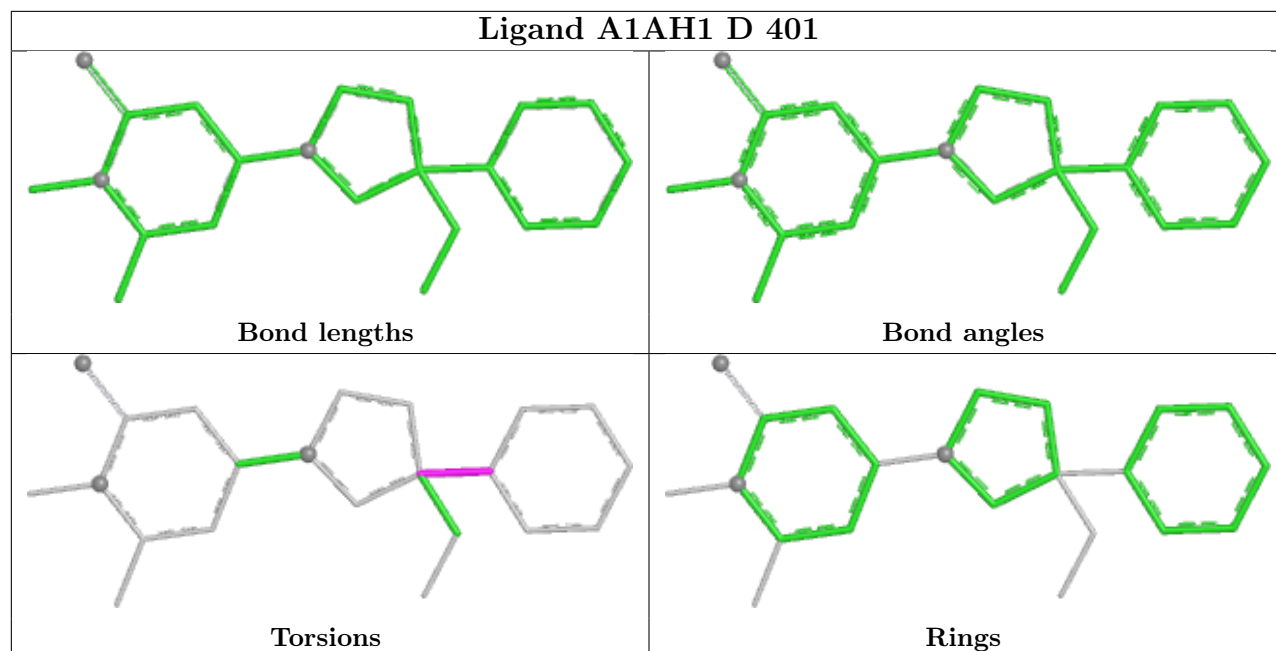
Mol	Chain	Res	Type	Atoms
3	D	401	A1AH1	C4-C5-C8-C9
3	D	401	A1AH1	C14-C5-C8-C13
3	B	304	A1AH1	C4-C5-C8-C13
3	D	401	A1AH1	C6-C5-C8-C13
3	B	304	A1AH1	C14-C5-C8-C13
3	D	401	A1AH1	C14-C5-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

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	215/216 (99%)	1.21	21 (9%) 14 12	44, 60, 98, 158	0
1	B	215/216 (99%)	1.10	21 (9%) 14 12	44, 59, 93, 228	0
1	C	216/216 (100%)	1.17	24 (11%) 12 9	46, 65, 90, 138	0
1	D	216/216 (100%)	1.16	23 (10%) 13 10	44, 62, 92, 155	0
All	All	862/864 (99%)	1.16	89 (10%) 13 11	44, 62, 94, 228	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	TRP	4.5
1	B	215	CYS	4.2
1	A	2	SER	4.2
1	B	2	SER	3.7
1	C	2	SER	3.6
1	C	155	ASP	3.5
1	A	93	TYR	3.5
1	B	3	ALA	3.3
1	D	216	SER	3.3
1	C	1	GLN	3.2
1	A	43	GLY	3.2
1	B	126	SER	3.2
1	D	213	THR	3.2
1	C	157	SER	3.2
1	B	159	VAL	3.1
1	D	215	CYS	3.1
1	B	134	ALA	3.0
1	A	161	ALA	3.0
1	D	13	SER	3.0
1	C	161	ALA	2.9
1	A	156	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	159	VAL	2.8
1	A	195	TYR	2.8
1	B	7	PRO	2.8
1	A	95	GLY	2.8
1	D	174	ASN	2.8
1	B	4	LEU	2.7
1	D	118	SER	2.7
1	B	32	SER	2.7
1	C	158	PRO	2.7
1	C	131	ALA	2.7
1	D	144	TYR	2.7
1	D	2	SER	2.6
1	D	12	GLY	2.6
1	C	216	SER	2.6
1	A	192	HIS	2.6
1	C	197	CYS	2.6
1	D	145	PRO	2.5
1	C	215	CYS	2.5
1	D	29	VAL	2.5
1	D	94	GLY	2.4
1	C	53	VAL	2.4
1	D	168	PRO	2.4
1	B	58	SER	2.4
1	C	156	SER	2.4
1	D	93	TYR	2.4
1	C	162	GLY	2.4
1	A	100	PHE	2.4
1	C	200	THR	2.4
1	C	69	SER	2.4
1	A	82	ALA	2.4
1	B	147	ALA	2.4
1	A	155	ASP	2.3
1	A	131	ALA	2.3
1	B	116	ALA	2.3
1	C	70	GLY	2.3
1	A	212	PRO	2.3
1	D	119	VAL	2.3
1	A	94	GLY	2.3
1	A	99	LEU	2.2
1	C	154	ALA	2.2
1	B	102	GLY	2.2
1	B	187	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	93	TYR	2.2
1	C	113	PRO	2.2
1	D	113	PRO	2.2
1	A	215	CYS	2.2
1	D	23	THR	2.2
1	A	206	VAL	2.2
1	B	206	VAL	2.2
1	B	13	SER	2.1
1	B	93	TYR	2.1
1	D	205	THR	2.1
1	D	18	VAL	2.1
1	B	88	TYR	2.1
1	B	96	ASP	2.1
1	B	97	ASN	2.1
1	D	131	ALA	2.1
1	B	35	VAL	2.0
1	D	35	VAL	2.0
1	A	96	ASP	2.0
1	C	109	VAL	2.0
1	C	59	GLY	2.0
1	C	66	GLY	2.0
1	D	95	GLY	2.0
1	D	175	LYS	2.0
1	A	136	LEU	2.0
1	C	97	ASN	2.0
1	A	22	CYS	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 [\(i\)](#)

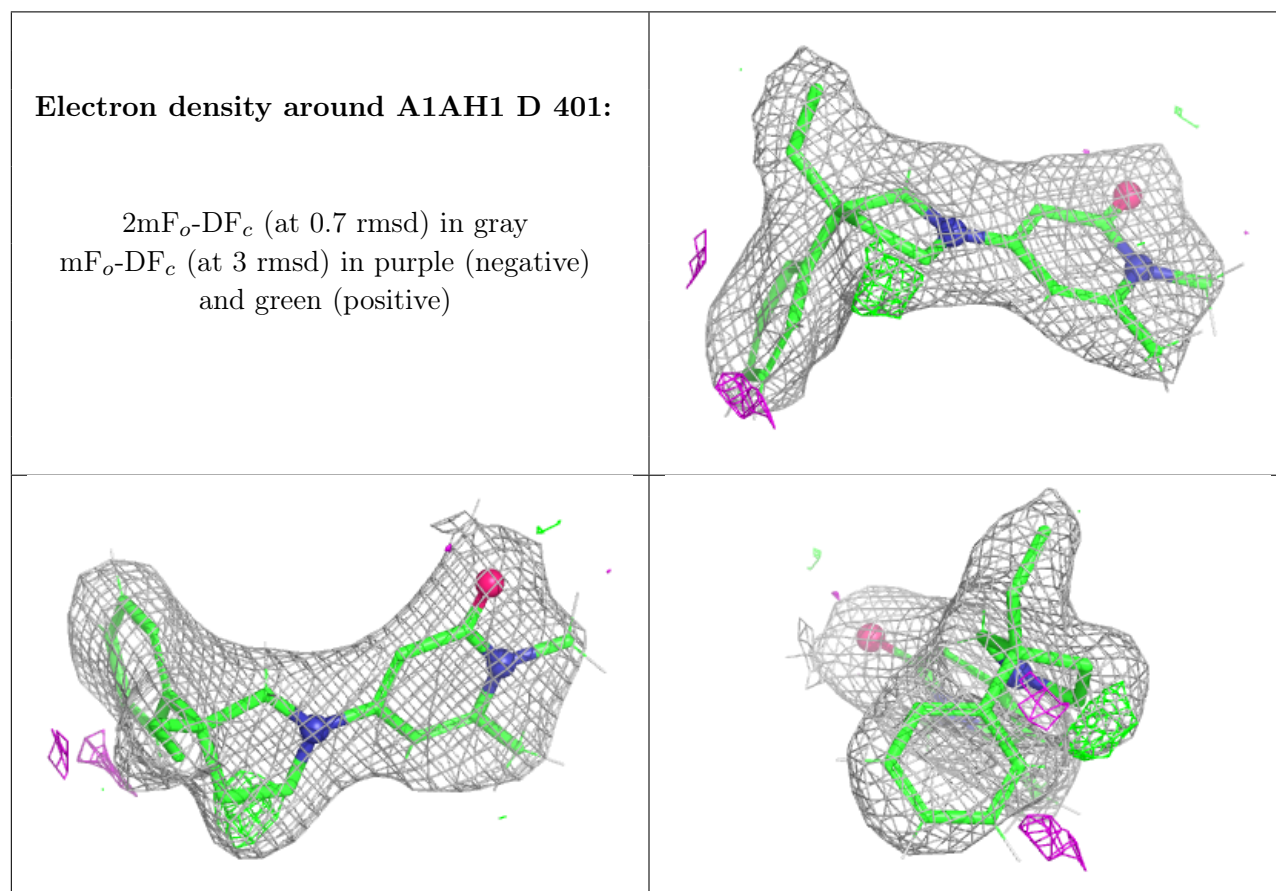
There are no monosaccharides in this entry.

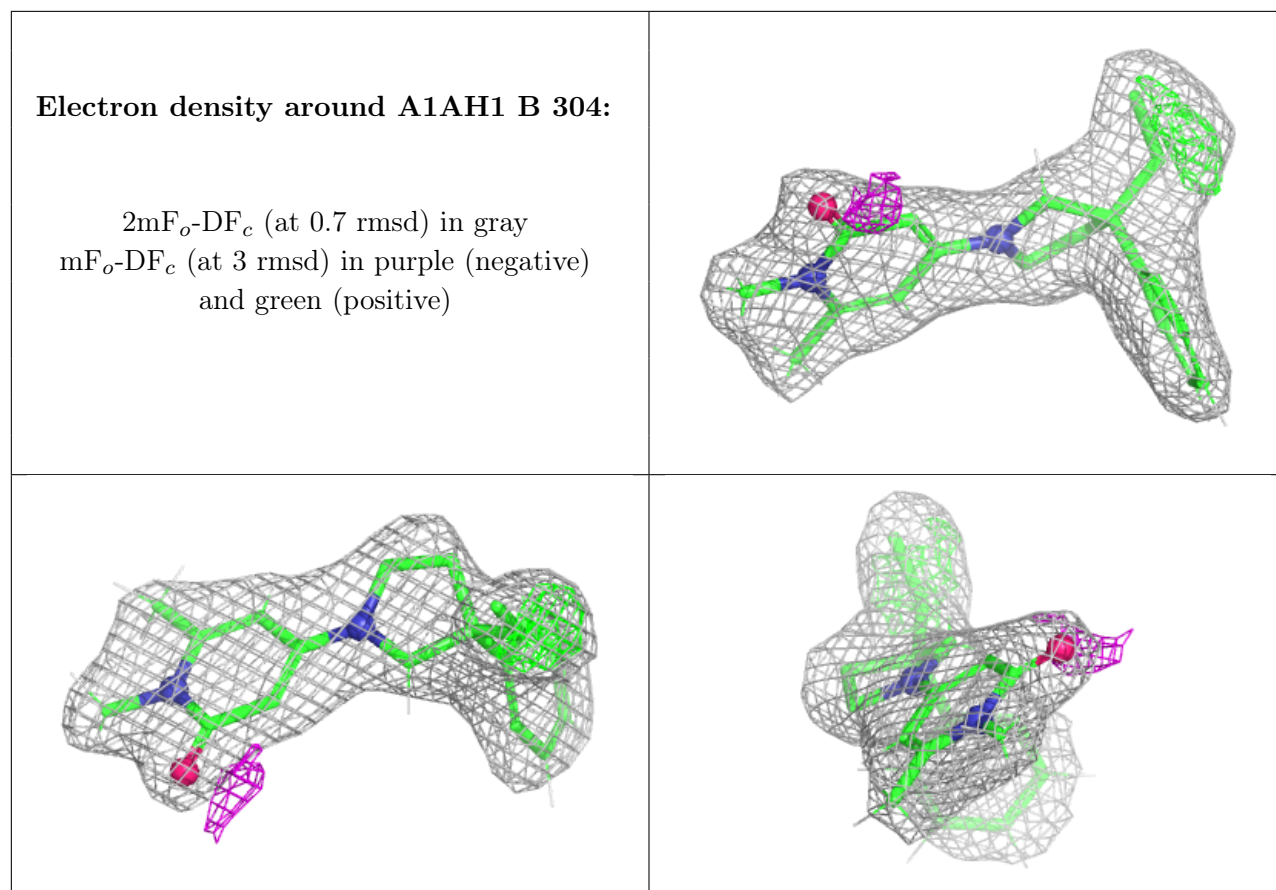
6.4 Ligands [\(i\)](#)

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, 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(\AA^2)	Q<0.9
2	PO4	A	301	5/5	0.74	0.14	59,66,73,74	0
2	PO4	B	301	5/5	0.80	0.13	63,64,78,81	0
2	PO4	C	301	5/5	0.80	0.11	65,69,82,86	0
2	PO4	C	302	5/5	0.80	0.13	64,64,75,83	0
2	PO4	C	303	5/5	0.82	0.13	71,72,85,86	0
2	PO4	B	302	5/5	0.84	0.13	62,66,71,76	0
2	PO4	B	303	5/5	0.85	0.10	63,72,73,79	0
3	A1AH1	D	401	22/22	0.89	0.15	38,46,59,59	0
3	A1AH1	B	304	22/22	0.90	0.13	33,42,51,53	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.