



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:11 PM UTC

PDB ID : 8RX9 / pdb_00008rx9
Title : LTA4 hydrolase in complex with compound3
Authors : Srinivas, H.
Deposited on : 2024-02-06
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

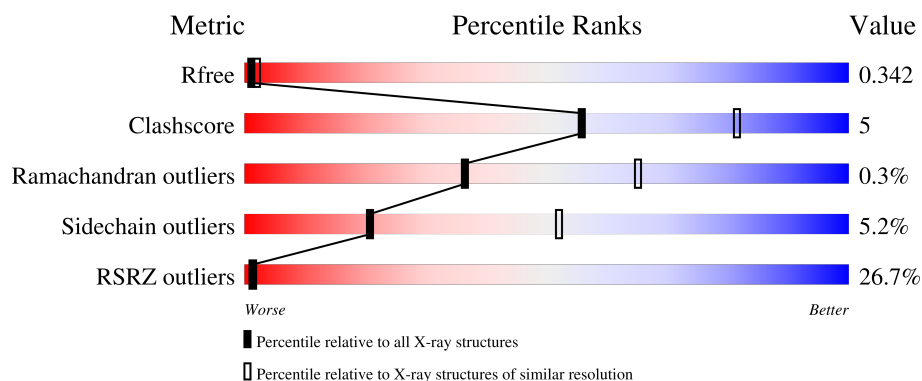
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	613	26% 82% 16% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5024 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 Leukotriene A-4 hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	2	0
			4852	3115	808	908	21			

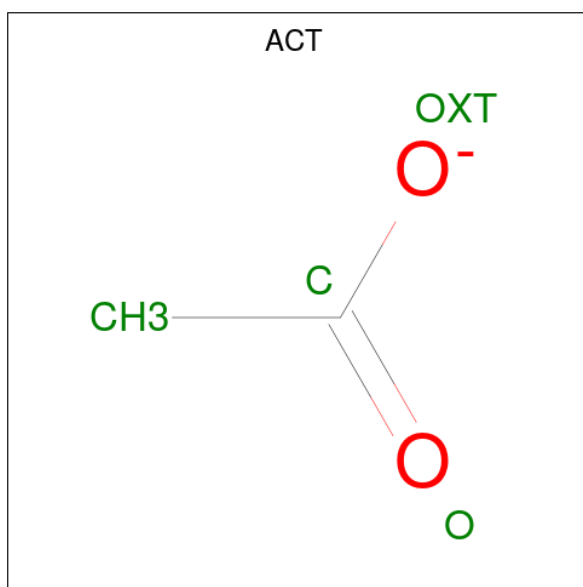
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P09960
A	-1	PRO	-	expression tag	UNP P09960
A	0	GLY	-	expression tag	UNP P09960

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

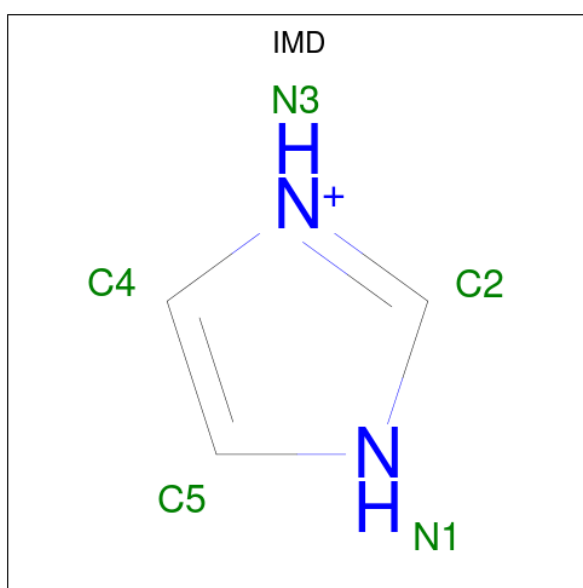


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is YTTERBIUM (III) ION (CCD ID: Yb) (formula: Yb).

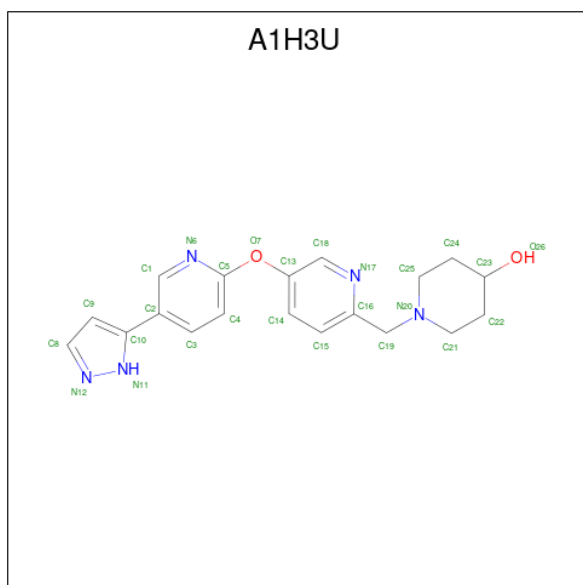
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Yb	0	0
			3	3		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is 1-[[5-[5-(1 {H}-pyrazol-5-yl)pyridin-2-yl]oxy]pyridin-2-yl]methyl]piperidin-4-ol (CCD ID: A1H3U) (formula: C₁₉H₂₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			26	19	5	2		

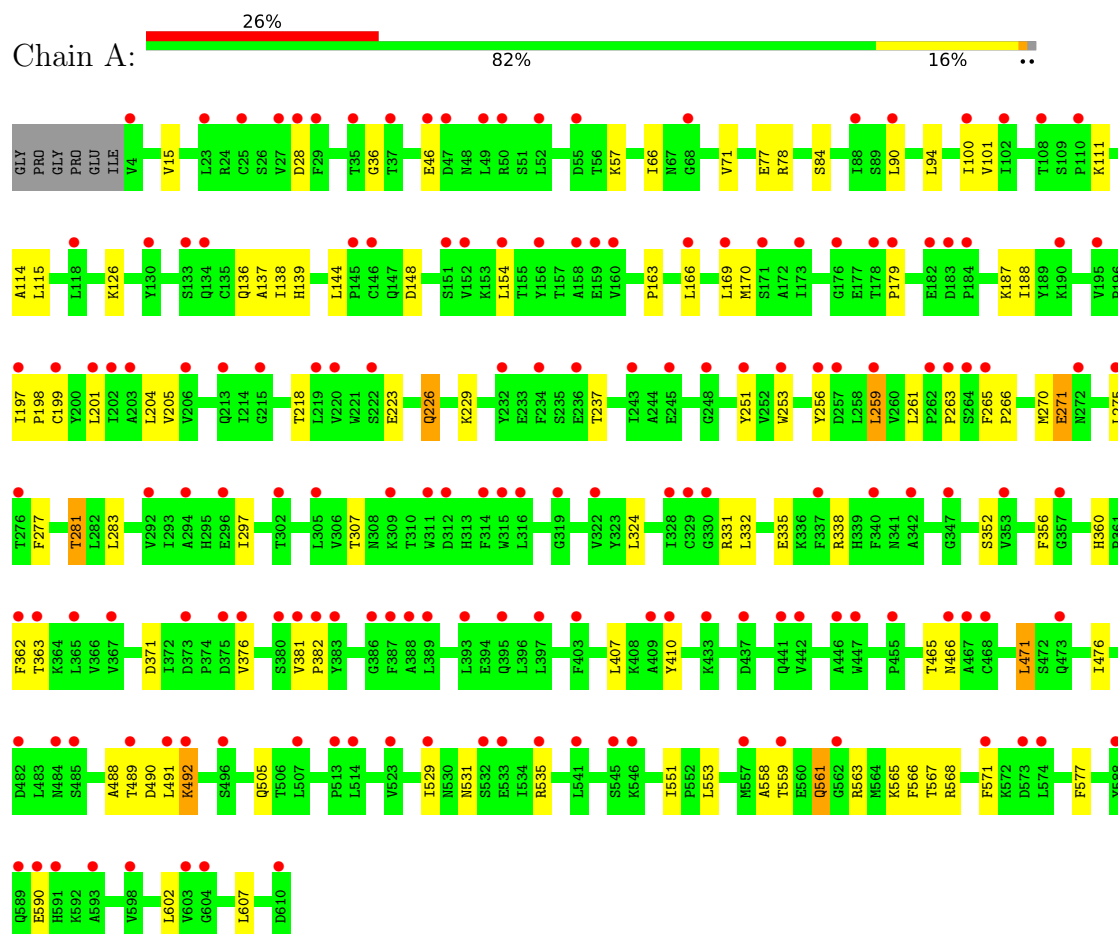
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	128	Total	O	0	0
			128	128		

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: Leukotriene A-4 hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.19Å 86.94Å 99.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.98 – 2.90 28.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.98-2.90) 99.6 (28.98-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.263 , 0.335 0.284 , 0.342	Depositor DCC
R_{free} test set	776 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.845	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5024	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1H3U, YB, ACT, ZN, IMD

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	0.76	1/4982 (0.0%)	1.30	11/6771 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	551	ILE	CA-CB	5.81	1.57	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	577	PHE	CA-C-N	5.88	128.48	120.54
1	A	577	PHE	C-N-CA	5.88	128.48	120.54
1	A	331	ARG	N-CA-C	-5.67	107.36	114.56
1	A	559	THR	CA-C-N	5.51	128.22	120.28
1	A	559	THR	C-N-CA	5.51	128.22	120.28
1	A	488	ALA	CA-C-N	5.33	127.96	120.28
1	A	488	ALA	C-N-CA	5.33	127.96	120.28
1	A	36	GLY	N-CA-C	5.13	118.96	110.55
1	A	226	GLN	CA-C-N	5.10	126.99	120.56
1	A	226	GLN	C-N-CA	5.10	126.99	120.56

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	4852	0	4814	46	0
2	A	1	0	0	0	0
3	A	4	0	3	0	0
4	A	3	0	0	0	0
5	A	10	0	10	1	0
6	A	26	0	0	1	0
7	A	128	0	0	0	0
All	All	5024	0	4827	46	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 5.

All (46) 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:363:THR:HA	1:A:381:VAL:HG11	1.76	0.68
1:A:505:GLN:HE21	5:A:706:IMD:H2	1.63	0.63
1:A:563:ARG:HH21	1:A:565:LYS:HD2	1.68	0.58
1:A:561:GLN:NE2	1:A:566:PHE:HB2	2.22	0.54
1:A:561:GLN:HE21	1:A:563:ARG:HB3	1.73	0.54
1:A:529:ILE:HG22	1:A:531:ASN:H	1.72	0.54
1:A:561:GLN:HE22	1:A:566:PHE:HB2	1.73	0.53
1:A:489:THR:HA	1:A:492:LYS:HG3	1.91	0.53
1:A:198:PRO:HG2	1:A:307:THR:HG21	1.89	0.52
1:A:561:GLN:HG2	1:A:563:ARG:H	1.74	0.52
1:A:15:VAL:HA	1:A:46:GLU:HG2	1.92	0.51
1:A:471:LEU:HD11	1:A:490:ASP:HB3	1.93	0.51
1:A:94:LEU:HD21	1:A:100:ILE:HG12	1.94	0.50
1:A:229:LYS:HG3	1:A:283:LEU:HD22	1.93	0.50
1:A:136:GLN:HE21	1:A:270:MET:HE1	1.77	0.50
1:A:259:LEU:HD13	1:A:275:LEU:HD21	1.93	0.49
1:A:263:PRO:HB3	1:A:561:GLN:HA	1.92	0.49
1:A:205:VAL:HG21	1:A:259:LEU:HD21	1.95	0.48
1:A:376:VAL:HA	1:A:602:LEU:HD21	1.95	0.48
1:A:136:GLN:HG2	6:A:708:A1H3U:N17	2.30	0.47
1:A:229:LYS:HE2	1:A:283:LEU:HB3	1.97	0.46
1:A:281:THR:HG21	1:A:561:GLN:HG3	1.97	0.46
1:A:381:VAL:HG23	1:A:382:PRO:HD3	1.98	0.45
1:A:571:PHE:HB3	1:A:607:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HD23	1:A:261:LEU:HD22	1.98	0.45
1:A:218:THR:HA	1:A:256:TYR:O	2.17	0.45
1:A:265:PHE:HA	1:A:266:PRO:HD3	1.91	0.45
1:A:163:PRO:HD2	1:A:166:LEU:HD12	1.99	0.45
1:A:136:GLN:HA	1:A:137:ALA:HA	1.81	0.44
1:A:170:MET:HE3	1:A:204:LEU:HB2	2.00	0.43
1:A:179:PRO:HA	1:A:187:LYS:HA	2.00	0.43
1:A:251:TYR:CZ	1:A:253:TRP:HB2	2.54	0.43
1:A:223:GLU:HB2	1:A:226:GLN:HE21	1.84	0.43
1:A:270:MET:HB3	1:A:277:PHE:HB2	1.99	0.43
1:A:148:ASP:HA	1:A:199:CYS:SG	2.59	0.43
1:A:114:ALA:HB2	1:A:139:HIS:HB3	2.01	0.42
1:A:535:ARG:HH12	1:A:553:LEU:HD22	1.84	0.42
1:A:66:ILE:HD12	1:A:71:VAL:HG21	2.02	0.42
1:A:360:HIS:HE1	1:A:362:PHE:CD2	2.38	0.42
1:A:201:LEU:HD21	1:A:271:GLU:HG3	2.02	0.41
1:A:237:THR:HG23	1:A:297:ILE:HD11	2.02	0.41
1:A:407:LEU:HA	1:A:410:TYR:HB3	2.03	0.41
1:A:568:ARG:HD2	1:A:602:LEU:HB3	2.02	0.41
1:A:335:GLU:CD	1:A:338:ARG:HE	2.29	0.41
1:A:197:ILE:HD13	1:A:253:TRP:HH2	1.86	0.40
1:A:558:ALA:HA	1:A:567:THR:HG22	2.03	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	607/613 (99%)	563 (93%)	42 (7%)	2 (0%)	36 65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	GLU
1	A	126	LYS

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	A	539/543 (99%)	511 (95%)	28 (5%)	21 52

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	77	GLU
1	A	78	ARG
1	A	84	SER
1	A	90	LEU
1	A	101	VAL
1	A	111	LYS
1	A	115	LEU
1	A	138	ILE
1	A	144	LEU
1	A	154	LEU
1	A	169	LEU
1	A	188	ILE
1	A	259	LEU
1	A	281	THR
1	A	324	LEU
1	A	332	LEU
1	A	352	SER
1	A	356	PHE
1	A	371	ASP
1	A	465	THR
1	A	466	ASN
1	A	471	LEU
1	A	476	ILE
1	A	491	LEU

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Mol	Chain	Res	Type
1	A	492	LYS
1	A	561	GLN
1	A	590	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	97	ASN
1	A	128	HIS
1	A	134	GLN
1	A	136	GLN
1	A	193	GLN
1	A	226	GLN
1	A	272	ASN
1	A	341	ASN
1	A	440	ASN
1	A	500	ASN
1	A	505	GLN
1	A	561	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](#)

Of 8 ligands modelled in this entry, 4 are 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
5	IMD	A	706	-	5,5,5	0.33	0	5,5,5	0.52	0
6	A1H3U	A	708	-	29,29,29	1.54	5 (17%)	39,39,39	1.93	9 (23%)
3	ACT	A	702	4	3,3,3	1.06	0	3,3,3	1.00	0
5	IMD	A	707	-	5,5,5	0.33	0	5,5,5	0.55	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
5	IMD	A	706	-	-	-	0/1/1/1
6	A1H3U	A	708	-	-	1/12/22/22	0/4/4/4
5	IMD	A	707	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	708	A1H3U	C10-N11	-4.56	1.30	1.35
6	A	708	A1H3U	C9-C8	3.67	1.46	1.39
6	A	708	A1H3U	C9-C10	-2.98	1.33	1.38
6	A	708	A1H3U	C8-N12	-2.76	1.26	1.33
6	A	708	A1H3U	C2-C10	2.42	1.51	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	708	A1H3U	C1-N6-C5	6.03	122.20	116.72
6	A	708	A1H3U	C2-C10-N11	3.83	127.78	122.62
6	A	708	A1H3U	C2-C10-C9	-3.61	123.73	130.58
6	A	708	A1H3U	C9-C8-N12	-3.39	105.64	110.91
6	A	708	A1H3U	C4-C5-N6	-3.33	119.44	124.65
6	A	708	A1H3U	C18-N17-C16	3.24	122.12	118.00
6	A	708	A1H3U	C8-N12-N11	2.61	110.63	105.25
6	A	708	A1H3U	C13-O7-C5	2.21	124.96	119.06
6	A	708	A1H3U	O7-C5-C4	2.01	123.29	116.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

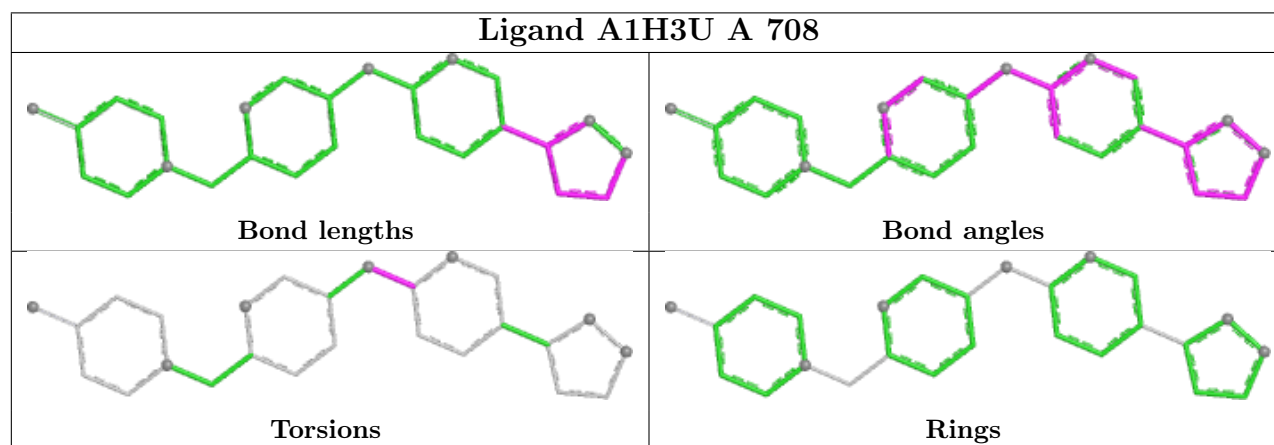
Mol	Chain	Res	Type	Atoms
6	A	708	A1H3U	N6-C5-O7-C13

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	706	IMD	1	0
6	A	708	A1H3U	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 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 ⓘ

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	607/613 (99%)	1.59	162 (26%) 1 1	33, 55, 73, 85	2 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	SER	5.1
1	A	302	THR	4.3
1	A	375	ASP	4.0
1	A	387	PHE	4.0
1	A	47	ASP	3.9
1	A	383	TYR	3.9
1	A	27	VAL	3.9
1	A	532	SER	3.8
1	A	145	PRO	3.8
1	A	588	TYR	3.7
1	A	248	GLY	3.6
1	A	276	THR	3.6
1	A	393	LEU	3.5
1	A	484	ASN	3.5
1	A	513	PRO	3.5
1	A	257	ASP	3.5
1	A	446	ALA	3.4
1	A	557	MET	3.4
1	A	173	ILE	3.3
1	A	206	VAL	3.3
1	A	382	PRO	3.3
1	A	46	GLU	3.3
1	A	171	SER	3.3
1	A	380	SER	3.2
1	A	533	GLU	3.2
1	A	234	PHE	3.2
1	A	590	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	545	SER	3.1
1	A	222[A]	SER	3.1
1	A	347	GLY	3.1
1	A	373	ASP	3.1
1	A	160	VAL	3.0
1	A	197	ILE	3.0
1	A	49	LEU	3.0
1	A	201	LEU	3.0
1	A	529	ILE	3.0
1	A	589	GLN	3.0
1	A	55	ASP	3.0
1	A	314	PHE	3.0
1	A	315	TRP	2.9
1	A	37	THR	2.9
1	A	604	GLY	2.9
1	A	213	GLN	2.9
1	A	496	SER	2.9
1	A	546	LYS	2.9
1	A	253	TRP	2.9
1	A	190	LYS	2.9
1	A	4	VAL	2.9
1	A	184	PRO	2.8
1	A	603	VAL	2.8
1	A	573	ASP	2.8
1	A	102	ILE	2.8
1	A	397	LEU	2.8
1	A	389	LEU	2.8
1	A	272	ASN	2.8
1	A	610	ASP	2.8
1	A	262	PRO	2.8
1	A	473	GLN	2.7
1	A	130	TYR	2.7
1	A	395	GLN	2.7
1	A	316	LEU	2.7
1	A	296	GLU	2.7
1	A	328	ILE	2.7
1	A	319	GLY	2.7
1	A	195	VAL	2.7
1	A	367	VAL	2.7
1	A	275	LEU	2.7
1	A	110	PRO	2.6
1	A	489	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	2.6
1	A	381	VAL	2.6
1	A	118	LEU	2.6
1	A	133	SER	2.6
1	A	410	TYR	2.6
1	A	562	GLY	2.6
1	A	169	LEU	2.6
1	A	362	PHE	2.6
1	A	312	ASP	2.6
1	A	158	ALA	2.6
1	A	28	ASP	2.6
1	A	514	LEU	2.5
1	A	468	CYS	2.5
1	A	482	ASP	2.5
1	A	219	LEU	2.5
1	A	159	GLU	2.5
1	A	100	ILE	2.5
1	A	152	VAL	2.5
1	A	50	ARG	2.5
1	A	182	GLU	2.4
1	A	571	PHE	2.4
1	A	35	THR	2.4
1	A	68	GLY	2.4
1	A	330	GLY	2.4
1	A	535	ARG	2.4
1	A	593	ALA	2.4
1	A	25	CYS	2.4
1	A	403	PHE	2.4
1	A	178	THR	2.4
1	A	90	LEU	2.4
1	A	442	VAL	2.4
1	A	598	VAL	2.4
1	A	492	LYS	2.4
1	A	337	PHE	2.4
1	A	251	TYR	2.4
1	A	220	VAL	2.3
1	A	386	GLY	2.3
1	A	342	ALA	2.3
1	A	467	ALA	2.3
1	A	166	LEU	2.3
1	A	340	PHE	2.3
1	A	305	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	507	LEU	2.3
1	A	108	THR	2.3
1	A	156	TYR	2.3
1	A	176	GLY	2.3
1	A	29	PHE	2.3
1	A	491	LEU	2.3
1	A	202	ILE	2.3
1	A	376	VAL	2.3
1	A	322	VAL	2.3
1	A	203	ALA	2.2
1	A	365	LEU	2.2
1	A	541	LEU	2.2
1	A	329	CYS	2.2
1	A	265	PHE	2.2
1	A	236	GLU	2.2
1	A	409	ALA	2.2
1	A	309	LYS	2.2
1	A	466	ASN	2.2
1	A	574	LEU	2.2
1	A	357	GLY	2.2
1	A	134	GLN	2.2
1	A	183	ASP	2.2
1	A	523	VAL	2.2
1	A	151	SER	2.2
1	A	433	LYS	2.2
1	A	447	TRP	2.2
1	A	232	TYR	2.2
1	A	294	ALA	2.1
1	A	154	LEU	2.1
1	A	256	TYR	2.1
1	A	388	ALA	2.1
1	A	88	ILE	2.1
1	A	311	TRP	2.1
1	A	243	ILE	2.1
1	A	245	GLU	2.1
1	A	179	PRO	2.1
1	A	455	PRO	2.1
1	A	485	SER	2.0
1	A	199	CYS	2.0
1	A	263	PRO	2.0
1	A	559	THR	2.0
1	A	353	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	441	GLN	2.0
1	A	591	HIS	2.0
1	A	146	CYS	2.0
1	A	52	LEU	2.0
1	A	259	LEU	2.0
1	A	215	GLY	2.0
1	A	363	THR	2.0
1	A	437	ASP	2.0
1	A	292	VAL	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](#)

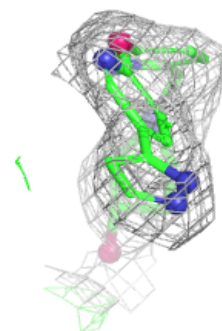
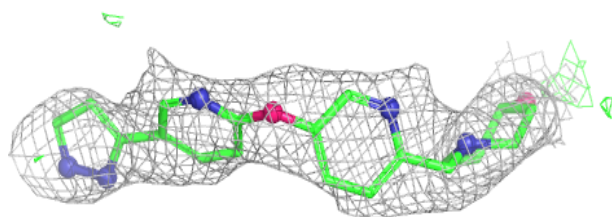
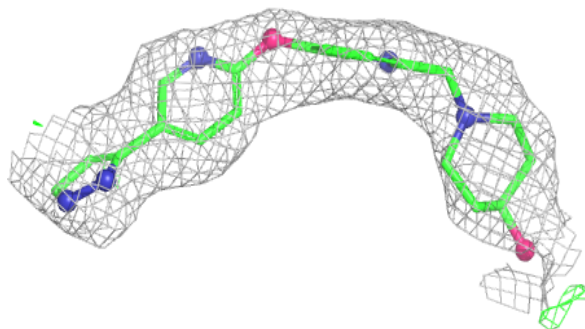
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	IMD	A	707	5/5	0.58	0.33	97,97,97,97	0
5	IMD	A	706	5/5	0.72	0.19	47,47,48,48	0
6	A1H3U	A	708	26/26	0.82	0.14	34,38,44,44	0
4	YB	A	704	1/1	0.89	0.09	85,85,85,85	1
3	ACT	A	702	4/4	0.90	0.14	40,41,41,42	0
2	ZN	A	701	1/1	0.95	0.08	60,60,60,60	0
4	YB	A	705	1/1	0.97	0.04	95,95,95,95	0
4	YB	A	703	1/1	0.97	0.06	61,61,61,61	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 A1H3U A 708:

$2mF_o-DF_c$ (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.