



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:04 AM UTC

PDB ID : 9F9M / pdb_00009f9m
Title : Crystal structure of MUS81-EME1 bound by compound 21.
Authors : Collie, G.W.
Deposited on : 2024-05-08
Resolution : 2.47 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

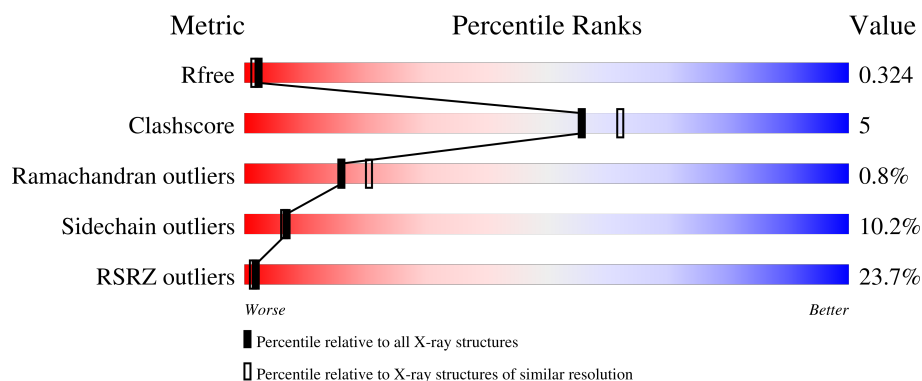
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	308	17% 47% 10% • 42%
1	C	308	16% 44% 14% •• 41%
2	B	326	8% 36% 6% • 57%
2	D	326	7% 35% 6% • 58%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4941 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1407	892	251	260	4			
1	C	183	Total	C	N	O	S	0	0	0
			1428	906	256	262	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP Q96NY9
A	245	SER	-	expression tag	UNP Q96NY9
C	244	GLY	-	expression tag	UNP Q96NY9
C	245	SER	-	expression tag	UNP Q96NY9

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1034	658	169	199	8			
2	D	137	Total	C	N	O	S	0	0	0
			1022	650	168	197	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	245	GLY	-	expression tag	UNP Q96AY2
D	245	GLY	-	expression tag	UNP Q96AY2

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

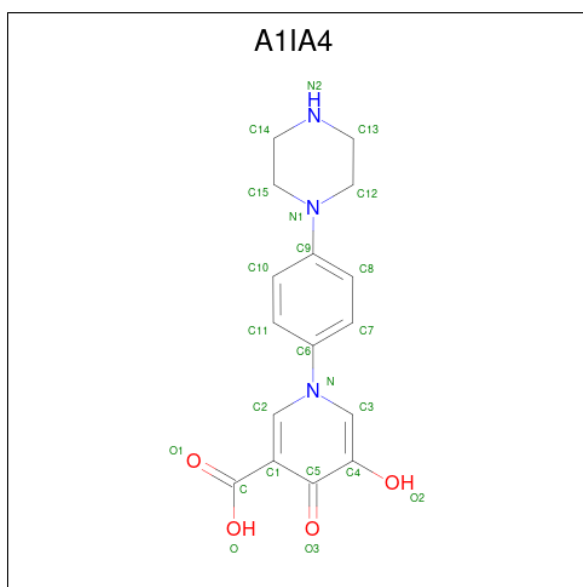
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is 5-oxidanyl-4-oxidanylidene-1-(4-piperazin-1-ylphenyl)pyridine-3-carboxylic acid (CCD ID: A1IA4) (formula: C₁₆H₁₇N₃O₄) (labeled as "Ligand of Interest" by depositor).

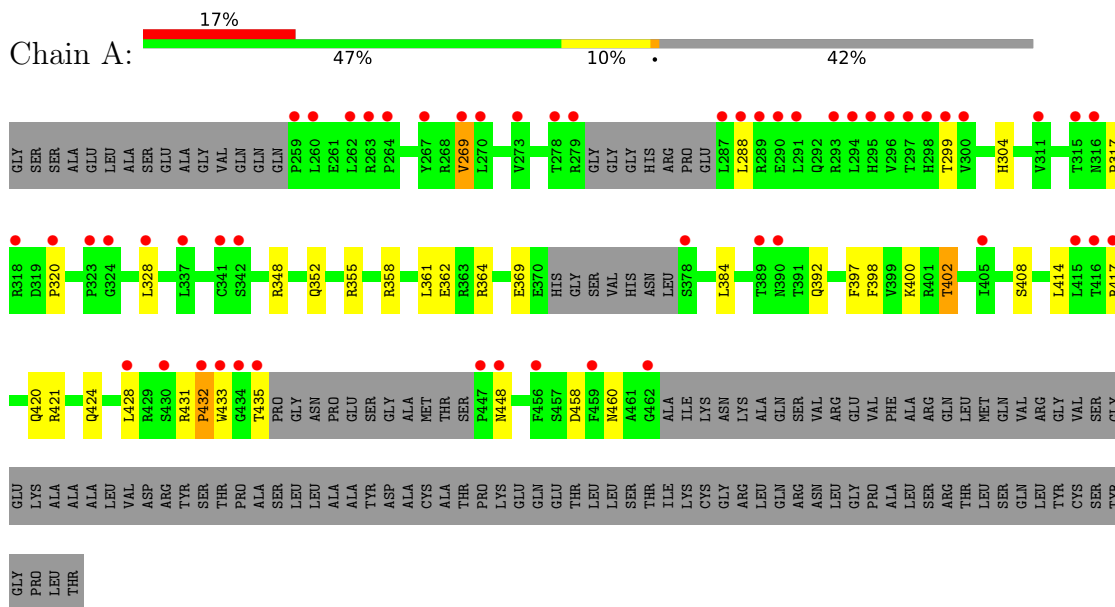


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	16	3	4		
4	C	1	Total	C	N	O	0	0
			23	16	3	4		

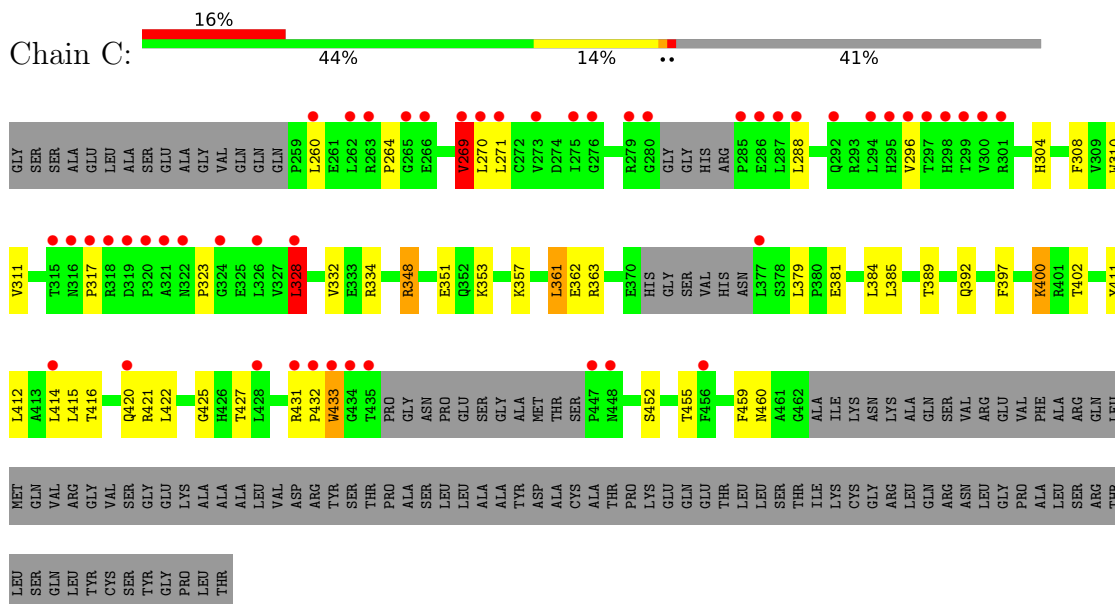
3 Residue-property plots

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: Crossover junction endonuclease MUS81



- Molecule 1: Crossover junction endonuclease MUS81



[illegible]

Chain D:

Amino Acid	Percentage
ARG	7%
VAL	35%
ILE	6%
THR	58%
MET	1%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.90Å 83.56Å 91.53Å 90.00° 92.18° 90.00°	Depositor
Resolution (Å)	50.23 – 2.47 50.23 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.23-2.47) 99.8 (50.23-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.306 , 0.326 0.298 , 0.324	Depositor DCC
R_{free} test set	1685 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4941	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3079e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1IA4, MG

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	0.65	0/1432	1.07	4/1941 (0.2%)
1	C	0.69	0/1454	1.20	9/1971 (0.5%)
2	B	0.65	0/1045	1.02	0/1423
2	D	0.70	0/1032	1.10	0/1404
All	All	0.67	0/4963	1.11	13/6739 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LEU	N-CA-C	9.26	123.30	112.93
1	C	328	LEU	N-CA-C	7.24	121.76	113.15
1	A	269	VAL	N-CA-CB	6.35	118.64	111.21
1	C	420	GLN	CA-C-N	6.23	128.63	120.28
1	C	420	GLN	C-N-CA	6.23	128.63	120.28
1	C	348	ARG	CA-C-N	5.57	129.17	120.82
1	C	348	ARG	C-N-CA	5.57	129.17	120.82
1	C	269	VAL	N-CA-CB	5.37	116.57	110.72
1	C	362	GLU	N-CA-C	5.35	117.86	111.71
1	A	362	GLU	N-CA-C	5.28	118.98	112.54
1	A	397	PHE	CA-CB-CG	5.17	118.97	113.80
1	C	363	ARG	CA-C-N	5.16	128.20	120.87
1	C	363	ARG	C-N-CA	5.16	128.20	120.87

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	1407	0	1386	14	0
1	C	1428	0	1407	16	0
2	B	1034	0	1029	10	0
2	D	1022	0	1021	10	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	23	0	0	0	0
4	C	23	0	0	1	0
All	All	4941	0	4843	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:417:ARG:NH1	1:A:421:ARG:HH12	1.76	0.84
2:B:291:VAL:HG13	2:B:313:LEU:HB3	1.67	0.76
1:A:402:THR:HG21	1:A:408:SER:OG	1.87	0.73
1:A:421:ARG:O	1:A:424:GLN:HG2	1.92	0.70
2:D:310:PRO:HA	2:D:357:LYS:HG2	1.75	0.69
2:D:291:VAL:HG13	2:D:313:LEU:HB3	1.76	0.66
2:B:347:VAL:HG21	2:B:415:LEU:HD11	1.81	0.63
2:B:360:SER:HA	2:B:422:GLN:HB3	1.82	0.62
1:A:317:PRO:HG2	1:A:320:PRO:HA	1.84	0.59
2:D:360:SER:HA	2:D:422:GLN:HB3	1.83	0.59
2:D:260:LEU:HB2	2:D:289:CYS:HA	1.84	0.59
1:C:264:PRO:HB3	1:C:425:GLY:HA2	1.85	0.57
1:C:271:LEU:HD11	1:C:308:PHE:HB3	1.87	0.57
1:A:417:ARG:NH1	1:A:421:ARG:NH1	2.50	0.56
1:C:304:HIS:HD2	1:C:460:ASN:HA	1.71	0.56
1:C:317:PRO:HG3	1:C:323:PRO:HB3	1.89	0.55
1:A:348:ARG:O	1:A:352:GLN:HG3	2.09	0.53
1:A:369:GLU:HG3	1:A:402:THR:HG22	1.91	0.53
1:A:304:HIS:HD2	1:A:460:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:LEU:HB2	2:B:289:CYS:HA	1.91	0.51
2:B:263:MET:SD	2:B:315:LEU:HD23	2.50	0.50
1:A:432:PRO:O	1:A:458:ASP:OD2	2.30	0.50
2:D:258:PRO:O	2:D:262:GLN:HG3	2.11	0.50
1:A:431:ARG:HD3	1:A:435:THR:C	2.37	0.50
2:B:252:ILE:HD11	2:B:443:VAL:HG12	1.94	0.49
1:A:448:ASN:OD1	2:B:417:LEU:O	2.29	0.49
1:C:385:LEU:O	1:C:389:THR:HG23	2.11	0.49
1:C:304:HIS:CD2	1:C:460:ASN:HA	2.46	0.49
1:C:348:ARG:NH2	4:C:603:A1IA4:C8	2.78	0.47
1:A:392:GLN:NE2	2:B:422:GLN:HG2	2.30	0.46
1:C:308:PHE:HB2	1:C:332:VAL:HB	1.98	0.46
2:D:263:MET:HE2	2:D:429:TRP:HH2	1.78	0.46
1:C:412:LEU:O	1:C:416:THR:OG1	2.27	0.45
1:C:392:GLN:NE2	2:D:422:GLN:HG2	2.32	0.44
1:C:353:LYS:O	1:C:357:LYS:HD3	2.17	0.44
2:D:351:THR:HA	2:D:354:THR:HG22	1.98	0.44
2:D:264:GLU:HG2	2:D:429:TRP:CZ2	2.52	0.44
1:C:269:VAL:HA	1:C:311:VAL:O	2.18	0.43
2:D:315:LEU:HD11	2:D:364:VAL:HG23	2.00	0.43
1:C:310:TRP:HB3	1:C:328:LEU:HD22	2.01	0.43
1:C:361:LEU:HD22	1:C:459:PHE:CE1	2.55	0.42
1:C:357:LYS:HD2	1:C:397:PHE:HE1	1.85	0.41
2:B:315:LEU:HD11	2:B:364:VAL:HG23	2.03	0.40
1:A:369:GLU:HG3	1:A:402:THR:CG2	2.51	0.40
1:C:400:LYS:HG3	1:C:411:TYR:CZ	2.57	0.40
1:A:398:PHE:HA	2:B:422:GLN:OE1	2.21	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	171/308 (56%)	168 (98%)	1 (1%)	2 (1%)	10	11
1	C	175/308 (57%)	166 (95%)	7 (4%)	2 (1%)	11	12
2	B	131/326 (40%)	127 (97%)	3 (2%)	1 (1%)	16	20
2	D	129/326 (40%)	126 (98%)	3 (2%)	0	100	100
All	All	606/1268 (48%)	587 (97%)	14 (2%)	5 (1%)	16	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	PRO
1	C	432	PRO
1	A	433	TRP
2	B	355	ALA
1	C	433	TRP

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	151/260 (58%)	138 (91%)	13 (9%)	10	11
1	C	152/260 (58%)	129 (85%)	23 (15%)	3	2
2	B	110/275 (40%)	102 (93%)	8 (7%)	13	17
2	D	108/275 (39%)	99 (92%)	9 (8%)	10	12
All	All	521/1070 (49%)	468 (90%)	53 (10%)	7	6

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	VAL
1	A	288	LEU
1	A	299	THR
1	A	355	ARG
1	A	358	ARG
1	A	361	LEU

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Mol	Chain	Res	Type
1	A	364	ARG
1	A	384	LEU
1	A	400	LYS
1	A	402	THR
1	A	414	LEU
1	A	420	GLN
1	A	428	LEU
2	B	249	LEU
2	B	252	ILE
2	B	264	GLU
2	B	269	LEU
2	B	285	GLN
2	B	291	VAL
2	B	344	GLN
2	B	354	THR
1	C	260	LEU
1	C	269	VAL
1	C	270	LEU
1	C	288	LEU
1	C	296	VAL
1	C	328	LEU
1	C	334	ARG
1	C	351	GLU
1	C	361	LEU
1	C	379	LEU
1	C	381	GLU
1	C	384	LEU
1	C	400	LYS
1	C	402	THR
1	C	414	LEU
1	C	415	LEU
1	C	421	ARG
1	C	422	LEU
1	C	427	THR
1	C	431	ARG
1	C	433	TRP
1	C	452	SER
1	C	455	THR
2	D	264	GLU
2	D	285	GLN
2	D	287	VAL
2	D	291	VAL

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Mol	Chain	Res	Type
2	D	313	LEU
2	D	344	GLN
2	D	354	THR
2	D	366	GLN
2	D	414	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	HIS
1	A	322	ASN
1	A	352	GLN
1	A	420	GLN
2	B	268	GLN
2	B	344	GLN
2	B	366	GLN
1	C	304	HIS
1	C	330	HIS
1	C	352	GLN
1	C	420	GLN
2	D	268	GLN
2	D	344	GLN
2	D	366	GLN
2	D	416	GLN
2	D	424	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
4	A1IA4	A	603	3	25,25,25	0.33	0	32,35,35	0.65	0
4	A1IA4	C	603	3	25,25,25	0.33	0	32,35,35	0.73	1 (3%)

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	A1IA4	A	603	3	-	4/12/20/20	0/3/3/3
4	A1IA4	C	603	3	-	0/12/20/20	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	A1IA4	C1-C5-C4	-2.00	116.23	118.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

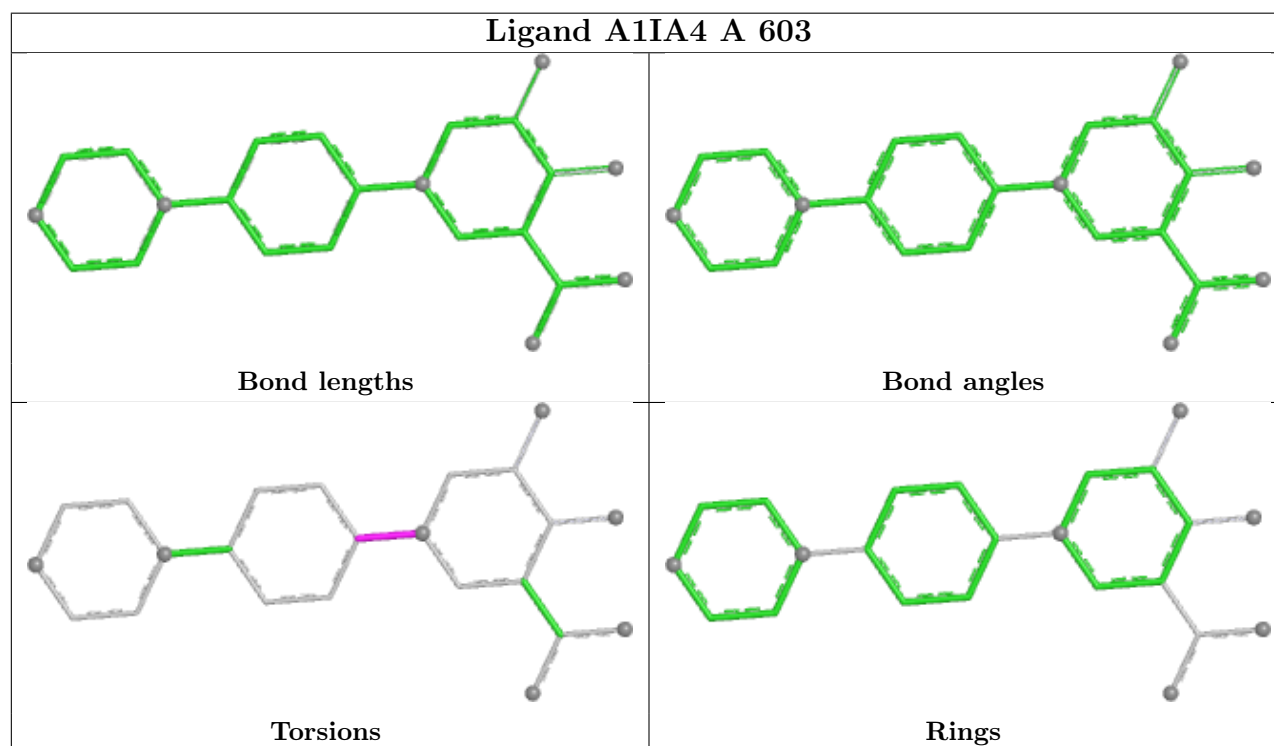
Mol	Chain	Res	Type	Atoms
4	A	603	A1IA4	C7-C6-N-C2
4	A	603	A1IA4	C11-C6-N-C2
4	A	603	A1IA4	C7-C6-N-C3
4	A	603	A1IA4	C11-C6-N-C3

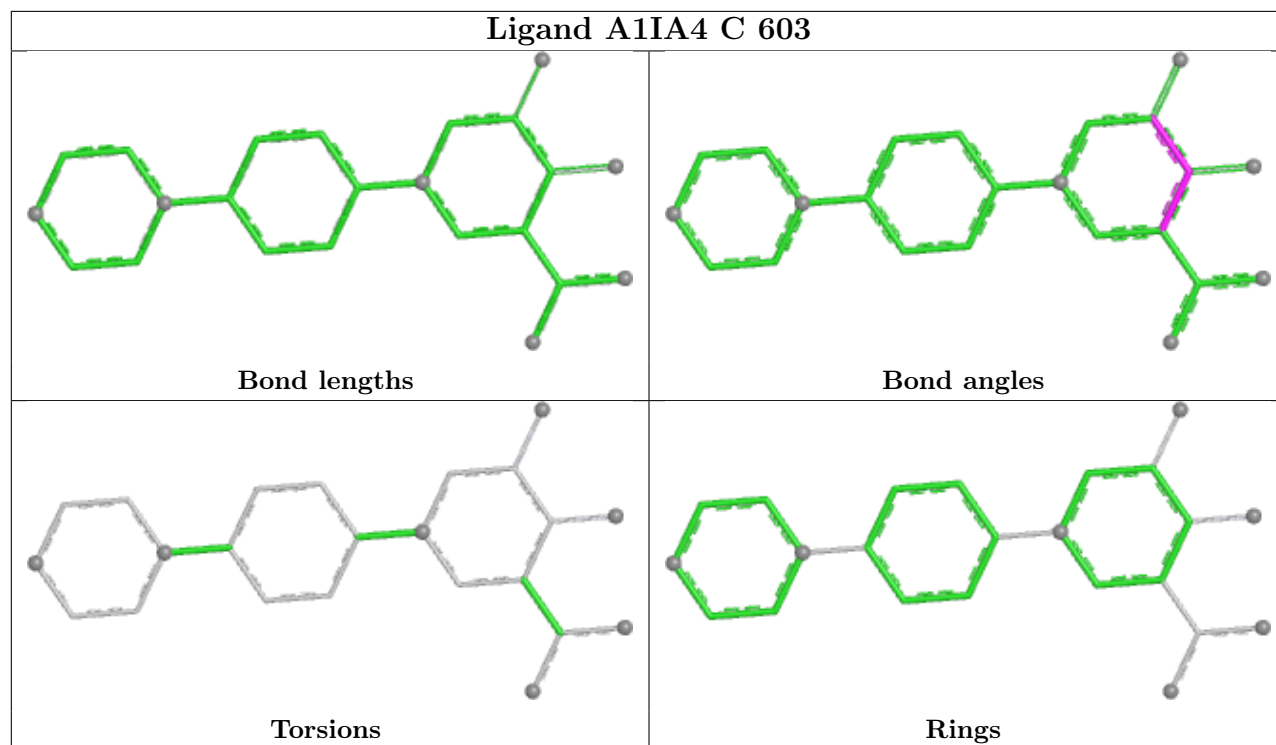
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	A1IA4	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 [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	179/308 (58%)	1.65	53 (29%) 1 1	47, 79, 102, 124	0
1	C	183/308 (59%)	1.50	49 (26%) 1 1	46, 78, 100, 120	0
2	B	139/326 (42%)	1.34	26 (18%) 3 2	59, 74, 95, 101	0
2	D	137/326 (42%)	1.16	23 (16%) 4 3	54, 71, 92, 101	0
All	All	638/1268 (50%)	1.44	151 (23%) 2 1	46, 75, 98, 124	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	VAL	6.3
1	A	287	LEU	5.9
1	C	433	TRP	5.8
1	A	462	GLY	4.8
1	C	300	VAL	4.6
1	C	435	THR	4.6
1	C	269	VAL	4.5
1	C	270	LEU	4.4
1	C	299	THR	4.2
1	C	324	GLY	4.1
1	A	316	ASN	4.0
1	A	262	LEU	4.0
1	C	285	PRO	3.9
1	C	296	VAL	3.9
1	A	289	ARG	3.8
1	C	260	LEU	3.7
1	A	299	THR	3.7
1	A	389	THR	3.7
1	A	270	LEU	3.7
1	C	447	PRO	3.7
2	B	328	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	295	HIS	3.6
2	B	249	LEU	3.6
1	C	434	GLY	3.6
1	C	288	LEU	3.6
1	A	447	PRO	3.5
2	B	280	CYS	3.5
1	A	324	GLY	3.5
1	C	292	GLN	3.5
1	A	433	TRP	3.5
1	A	448	ASN	3.4
1	A	318	ARG	3.4
1	A	311	VAL	3.4
1	A	288	LEU	3.3
2	D	318	ALA	3.3
1	C	432	PRO	3.3
1	A	296	VAL	3.3
1	C	318	ARG	3.3
2	B	279	ARG	3.3
1	A	291	LEU	3.2
1	A	294	LEU	3.2
1	A	298	HIS	3.2
1	C	320	PRO	3.2
1	A	434	GLY	3.2
2	D	315	LEU	3.2
2	B	342	THR	3.2
1	A	328	LEU	3.1
1	A	428	LEU	3.1
1	C	316	ASN	3.1
2	B	366	GLN	3.0
1	A	260	LEU	3.0
2	B	446	ALA	3.0
2	D	404	SER	3.0
1	C	448	ASN	3.0
1	C	273	VAL	2.9
1	A	297	THR	2.9
1	C	294	LEU	2.9
1	C	280	GLY	2.9
2	D	435	PHE	2.8
2	B	325	ILE	2.8
1	C	263	ARG	2.8
1	C	420	GLN	2.8
1	C	287	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	315	THR	2.7
2	D	364	VAL	2.7
1	A	417	ARG	2.7
1	C	317	PRO	2.6
1	A	300	VAL	2.6
1	A	405	ILE	2.6
1	A	390	ASN	2.6
1	C	266	GLU	2.6
1	C	297	THR	2.6
1	A	267	TYR	2.6
1	C	428	LEU	2.6
1	A	435	THR	2.6
1	C	279	ARG	2.5
1	A	459	PHE	2.5
1	C	326	LEU	2.5
2	B	426	VAL	2.5
1	A	342	SER	2.5
1	C	298	HIS	2.5
2	D	250	LYS	2.5
1	A	293	ARG	2.5
2	B	278	CYS	2.5
2	D	263	MET	2.5
2	B	315	LEU	2.5
2	D	259	VAL	2.5
2	D	325	ILE	2.5
1	C	262	LEU	2.5
1	C	328	LEU	2.5
1	C	265	GLY	2.4
2	B	411	ALA	2.4
2	D	446	ALA	2.4
1	A	290	GLU	2.4
2	B	321	PHE	2.4
1	A	337	LEU	2.4
1	C	377	LEU	2.4
2	B	405	ARG	2.4
2	D	362	VAL	2.4
1	A	430	SER	2.3
1	A	279	ARG	2.3
1	C	275	ILE	2.3
2	B	273	LEU	2.3
2	D	412	LEU	2.3
2	D	289	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	432	PRO	2.3
2	D	342	THR	2.3
1	C	276	GLY	2.3
1	A	264	PRO	2.3
2	D	408	ALA	2.3
2	B	412	LEU	2.3
2	D	317	ARG	2.3
2	D	328	GLY	2.3
2	B	407	ASP	2.3
1	C	456	PHE	2.3
1	A	320	PRO	2.3
1	C	322	ASN	2.2
2	D	354	THR	2.2
1	C	319	ASP	2.2
1	C	431	ARG	2.2
1	C	315	THR	2.2
1	C	271	LEU	2.2
2	D	321	PHE	2.2
1	C	295	HIS	2.2
1	A	416	THR	2.2
2	D	432	LEU	2.2
2	B	445	GLU	2.2
1	C	301	ARG	2.2
2	B	306	TRP	2.2
1	A	273	VAL	2.1
2	B	408	ALA	2.1
2	D	344	GLN	2.1
2	D	411	ALA	2.1
1	A	278	THR	2.1
2	B	348	THR	2.1
1	A	378	SER	2.1
2	B	251	HIS	2.1
1	C	321	ALA	2.1
1	C	414	LEU	2.1
1	A	341	CYS	2.1
1	A	323	PRO	2.1
1	A	456	PHE	2.1
2	B	318	ALA	2.1
2	D	405	ARG	2.1
1	A	259	PRO	2.1
2	B	320	ALA	2.1
1	A	263	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	343	LEU	2.1
1	A	415	LEU	2.0
1	C	286	GLU	2.0
2	B	261	LEU	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](#)

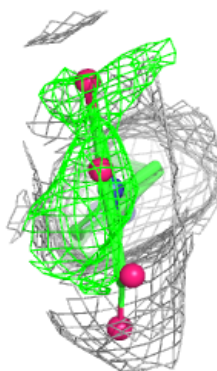
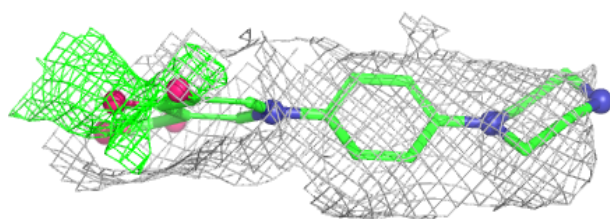
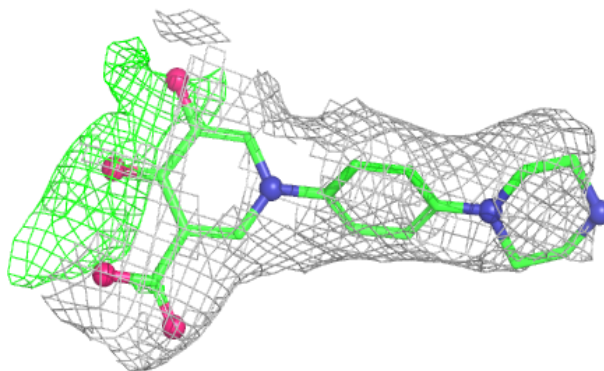
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	602	1/1	0.74	0.17	97,97,97,97	0
3	MG	A	601	1/1	0.79	0.26	72,72,72,72	0
4	A1IA4	C	603	23/23	0.80	0.18	97,99,102,102	0
4	A1IA4	A	603	23/23	0.83	0.15	89,91,95,95	0
3	MG	C	601	1/1	0.88	0.23	69,69,69,69	0
3	MG	C	602	1/1	0.97	0.15	76,76,76,76	0

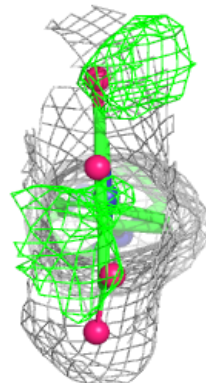
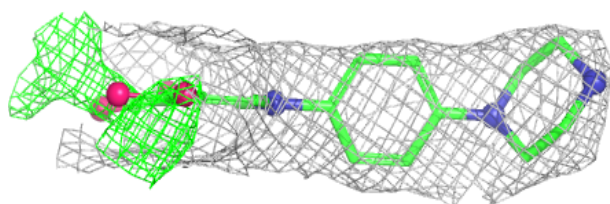
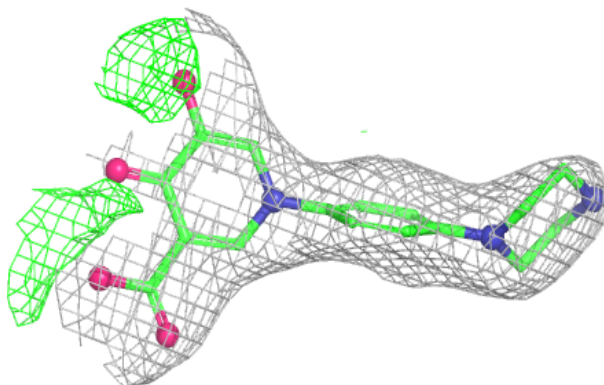
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IA4 C 603:

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

**Electron density around A1IA4 A 603:**

$2mF_o-DF_c$ (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.