



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:23 PM UTC

PDB ID : 4U5N / pdb_00004u5n
Title : IMPORTIN-ALPHA MINOR NLS SITE INHIBITOR
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Deposited on : 2014-07-25
Resolution : 2.31 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

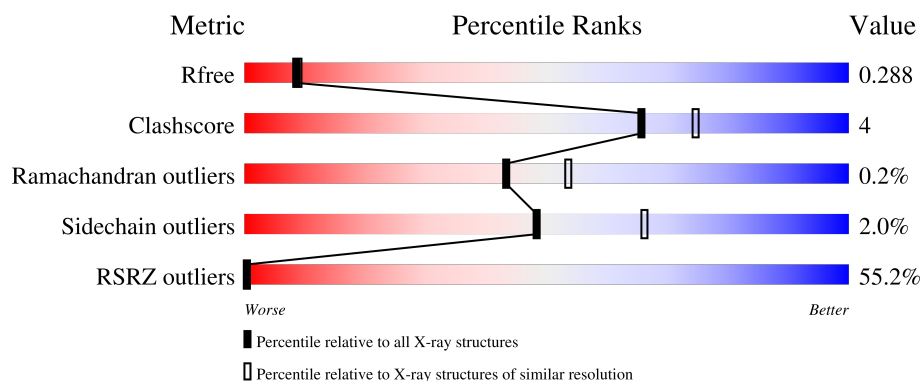
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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.

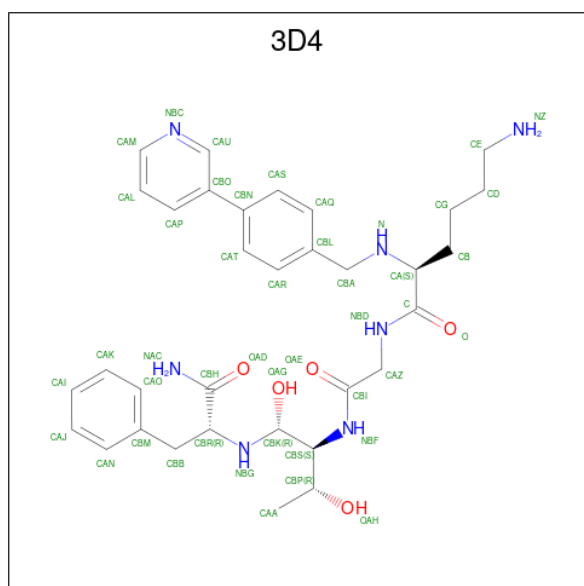
Mol	Chain	Length	Quality of chain
1	A	426	55% 89% 10%

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 Importin subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3254	2072	551	621	10			

- Molecule 2 is N 2 -[4-(pyridin-3-yl)benzyl]-L-lysyl-N-[(1R,2S,3R)-1-{[(2R)-1-amino-1-oxo-3-phenylpropan-2-yl]amino}-1,3-dihydroxybutan-2-yl]glycinamide (CCD ID: 3D4) (formula: C₃₃H₄₅N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			45	33	7	5		

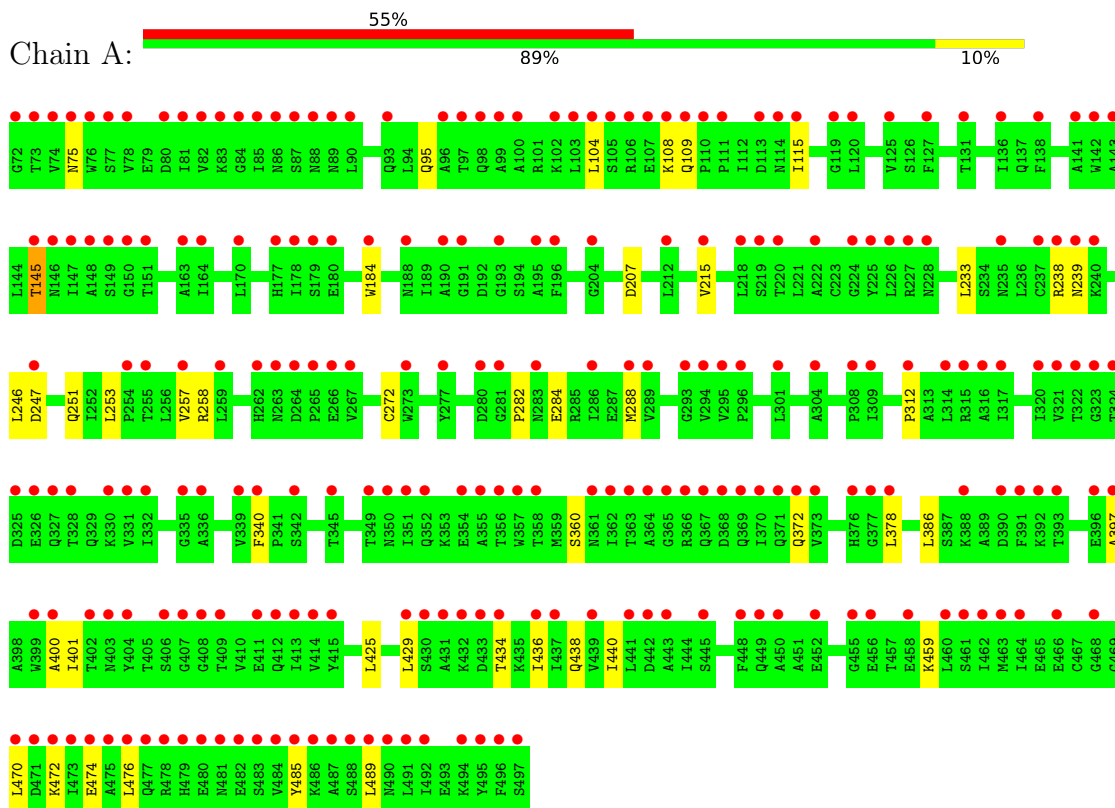
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	113	Total O 113 113	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: Importin subunit alpha-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 91.08Å 98.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.54 – 2.31 45.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.54-2.31) 97.1 (45.54-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.187 , 0.221 0.303 , 0.288	Depositor DCC
R_{free} test set	1256 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3412	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: 3D4

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	0.56	0/3318	0.85	3/4522 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	PHE	CA-C-N	-6.13	112.25	119.05
1	A	340	PHE	C-N-CA	-6.13	112.25	119.05
1	A	75	ASN	N-CA-C	5.75	120.24	113.23

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	3254	0	3330	24	0
2	A	45	0	45	1	0
3	A	113	0	0	0	0
All	All	3412	0	3375	25	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 (25) 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:108:LYS:HG3	1:A:109:GLN:HG3	1.79	0.63
1:A:284:GLU:H	1:A:284:GLU:CD	2.09	0.61
1:A:246:LEU:HD22	1:A:288:MET:HE1	1.84	0.59
1:A:145:THR:HG21	1:A:184:TRP:HD1	1.68	0.57
1:A:207:ASP:OD1	1:A:251:GLN:NE2	2.39	0.55
1:A:429:LEU:HD22	1:A:476:LEU:HD11	1.87	0.55
1:A:145:THR:HG21	1:A:184:TRP:CD1	2.43	0.53
1:A:470:LEU:O	1:A:474:GLU:HG3	2.11	0.51
1:A:104:LEU:HD21	1:A:115:ILE:HG13	1.94	0.50
2:A:501:3D4:H31	2:A:501:3D4:OAG	2.12	0.49
1:A:282:PRO:HB2	1:A:284:GLU:OE1	2.12	0.49
1:A:386:LEU:HD21	1:A:425:LEU:HD13	1.94	0.49
1:A:360:SER:HA	1:A:400:ALA:HA	1.95	0.49
1:A:215:VAL:O	1:A:258:ARG:NH2	2.44	0.49
1:A:397:ALA:O	1:A:401:ILE:HG12	2.13	0.48
1:A:425:LEU:HG	1:A:440:ILE:HG23	1.98	0.46
1:A:472:LYS:O	1:A:476:LEU:HG	2.16	0.45
1:A:246:LEU:CD2	1:A:288:MET:HE1	2.47	0.44
1:A:145:THR:CG2	1:A:184:TRP:CD1	3.01	0.43
1:A:272:CYS:HB3	1:A:312:PRO:HB2	2.01	0.42
1:A:238:ARG:O	1:A:239:ASN:HB2	2.20	0.42
1:A:434:THR:O	1:A:438:GLN:HG3	2.19	0.42
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.85	0.41
1:A:253:LEU:O	1:A:257:VAL:HG23	2.21	0.41
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.89	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	426/426 (100%)	414 (97%)	11 (3%)	1 (0%)	43 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	TYR

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	359/357 (101%)	351 (98%)	8 (2%)	45 63

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	145	THR
1	A	247[A]	ASP
1	A	247[B]	ASP
1	A	372	GLN
1	A	436	ILE
1	A	459	LYS
1	A	489	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	477	GLN
1	A	479	HIS

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	3D4	A	501	-	45,47,47	1.89	8 (17%)	53,61,61	1.42	8 (15%)

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	3D4	A	501	-	-	17/46/47/47	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	3D4	CBH-NAC	5.71	1.46	1.32
2	A	501	3D4	CBI-NBF	5.66	1.46	1.34
2	A	501	3D4	C-NBD	5.46	1.46	1.33
2	A	501	3D4	CAA-CBP	-5.11	1.37	1.51
2	A	501	3D4	OAH-CBP	3.88	1.53	1.43
2	A	501	3D4	OAD-CBH	-2.56	1.19	1.23
2	A	501	3D4	O-C	-2.21	1.19	1.23
2	A	501	3D4	OAE-CBI	-2.15	1.19	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	3D4	CBS-NBF-CBI	3.89	128.63	122.90
2	A	501	3D4	OAE-CBI-NBF	-3.83	116.47	122.95
2	A	501	3D4	CAZ-CBI-NBF	3.56	124.63	116.16
2	A	501	3D4	CBB-CBR-NBG	3.29	117.01	109.35
2	A	501	3D4	CAM-NBC-CAU	2.53	121.29	116.85
2	A	501	3D4	CBR-CBH-NAC	2.46	120.94	116.76
2	A	501	3D4	CAQ-CAS-CBN	-2.27	118.21	121.12
2	A	501	3D4	CAT-CBN-CAS	2.11	121.45	117.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	3D4	NBG-CBK-CBS-CBP
2	A	501	3D4	CAA-CBP-CBS-CBK
2	A	501	3D4	CAA-CBP-CBS-NBF
2	A	501	3D4	OAH-CBP-CBS-NBF
2	A	501	3D4	CBB-CBR-NBG-CBK
2	A	501	3D4	CBK-CBS-NBF-CBI
2	A	501	3D4	OAE-CBI-NBF-CBS
2	A	501	3D4	CAZ-CBI-NBF-CBS
2	A	501	3D4	CBM-CBB-CBR-NBG
2	A	501	3D4	CA-CB-CG-CD
2	A	501	3D4	CBR-CBB-CBM-CAN
2	A	501	3D4	CBM-CBB-CBR-CBH
2	A	501	3D4	CBR-CBB-CBM-CAO
2	A	501	3D4	OAH-CBP-CBS-CBK
2	A	501	3D4	CBH-CBR-NBG-CBK
2	A	501	3D4	CBP-CBS-NBF-CBI
2	A	501	3D4	CBI-CAZ-NBD-C

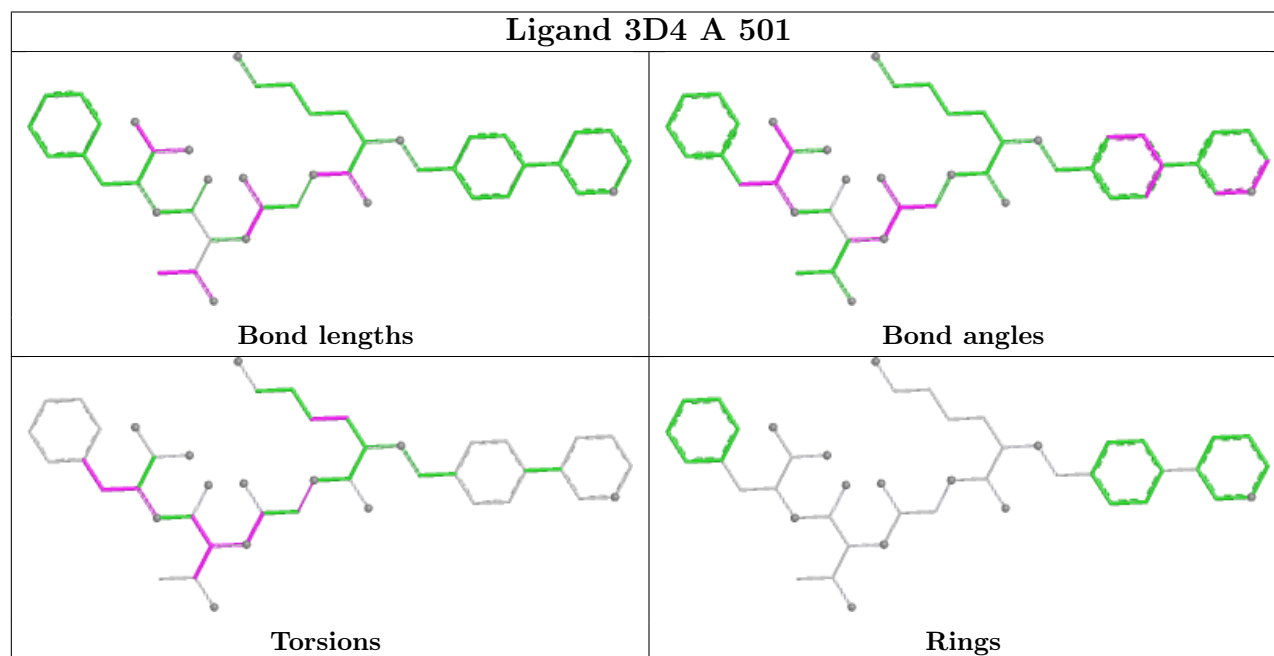
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	3D4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	426/426 (100%)	2.26	235 (55%) 0 0	28, 46, 87, 107	2 (0%)

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	VAL	8.2
1	A	484	VAL	7.3
1	A	485	TYR	6.4
1	A	72	GLY	5.8
1	A	184	TRP	5.5
1	A	73	THR	5.1
1	A	436	ILE	5.0
1	A	365	GLY	4.9
1	A	225	TYR	4.9
1	A	373	VAL	4.8
1	A	477	GLN	4.8
1	A	331	VAL	4.7
1	A	497	SER	4.6
1	A	488	SER	4.5
1	A	476	LEU	4.5
1	A	263	ASN	4.4
1	A	283	ASN	4.2
1	A	364	ALA	4.2
1	A	409	THR	4.2
1	A	489	LEU	4.0
1	A	358	THR	4.0
1	A	76	TRP	3.9
1	A	335	GLY	3.9
1	A	80	ASP	3.9
1	A	277	TYR	3.9
1	A	411	GLU	3.9
1	A	103	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	75	ASN	3.8
1	A	220	THR	3.8
1	A	88	ASN	3.8
1	A	115	ILE	3.7
1	A	442	ASP	3.7
1	A	492	ILE	3.7
1	A	109	GLN	3.7
1	A	327	GLN	3.7
1	A	363	THR	3.7
1	A	443	ALA	3.6
1	A	148	ALA	3.6
1	A	301	LEU	3.6
1	A	86	ASN	3.6
1	A	475	ALA	3.6
1	A	464	ILE	3.5
1	A	107	GLU	3.5
1	A	83	LYS	3.5
1	A	414	VAL	3.4
1	A	408	GLY	3.4
1	A	309	ILE	3.4
1	A	495	TYR	3.4
1	A	190	ALA	3.4
1	A	326	GLU	3.4
1	A	255	THR	3.4
1	A	460	LEU	3.4
1	A	357	TRP	3.4
1	A	478	ARG	3.4
1	A	437	ILE	3.3
1	A	77	SER	3.3
1	A	78	VAL	3.3
1	A	195	ALA	3.3
1	A	113	ASP	3.3
1	A	471	ASP	3.3
1	A	218	LEU	3.3
1	A	143	ALA	3.3
1	A	407	GLY	3.3
1	A	369	GLN	3.3
1	A	441	LEU	3.2
1	A	377	GLY	3.2
1	A	368	ASP	3.2
1	A	142	TRP	3.2
1	A	403	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	177	HIS	3.2
1	A	312	PRO	3.2
1	A	304	ALA	3.2
1	A	452	GLU	3.1
1	A	84	GLY	3.1
1	A	355	ALA	3.1
1	A	219	SER	3.1
1	A	433	ASP	3.1
1	A	470	LEU	3.1
1	A	491	LEU	3.1
1	A	362	ILE	3.1
1	A	222	ALA	3.1
1	A	108	LYS	3.1
1	A	308	PRO	3.1
1	A	376	HIS	3.0
1	A	399	TRP	3.0
1	A	483	SER	3.0
1	A	239	ASN	3.0
1	A	496	PHE	3.0
1	A	99	ALA	3.0
1	A	356	THR	3.0
1	A	400	ALA	3.0
1	A	240	LYS	3.0
1	A	87	SER	3.0
1	A	372	GLN	3.0
1	A	474	GLU	3.0
1	A	482	GLU	3.0
1	A	90	LEU	2.9
1	A	125	VAL	2.9
1	A	315	ARG	2.9
1	A	191	GLY	2.9
1	A	480	GLU	2.9
1	A	259	LEU	2.9
1	A	487	ALA	2.9
1	A	324	THR	2.9
1	A	228	ASN	2.9
1	A	96	ALA	2.9
1	A	120	LEU	2.9
1	A	340	PHE	2.9
1	A	412	GLN	2.9
1	A	321	VAL	2.9
1	A	456	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	390	ASP	2.8
1	A	193	GLY	2.8
1	A	354	GLU	2.8
1	A	466	GLU	2.8
1	A	450	ALA	2.8
1	A	391	PHE	2.8
1	A	330	LYS	2.8
1	A	151	THR	2.8
1	A	349	THR	2.8
1	A	479	HIS	2.8
1	A	415	TYR	2.7
1	A	352	GLN	2.7
1	A	102	LYS	2.7
1	A	448	PHE	2.7
1	A	289	VAL	2.7
1	A	396	GLU	2.7
1	A	266	GLU	2.7
1	A	339	VAL	2.6
1	A	238	ARG	2.6
1	A	490	ASN	2.6
1	A	81	ILE	2.6
1	A	288	MET	2.6
1	A	462	ILE	2.6
1	A	473	ILE	2.6
1	A	273	TRP	2.6
1	A	138	PHE	2.6
1	A	111	PRO	2.6
1	A	150	GLY	2.6
1	A	254	PRO	2.6
1	A	265	PRO	2.6
1	A	294	VAL	2.6
1	A	105	SER	2.6
1	A	147	ILE	2.6
1	A	224	GLY	2.6
1	A	486	LYS	2.6
1	A	180	GLU	2.5
1	A	332	ILE	2.5
1	A	227	ARG	2.5
1	A	212	LEU	2.5
1	A	204	GLY	2.5
1	A	82	VAL	2.5
1	A	413	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	325	ASP	2.5
1	A	149	SER	2.5
1	A	445	SER	2.5
1	A	336	ALA	2.5
1	A	264	ASP	2.4
1	A	293	GLY	2.4
1	A	366	ARG	2.4
1	A	434	THR	2.4
1	A	449	GLN	2.4
1	A	342	SER	2.4
1	A	430	SER	2.4
1	A	392	LYS	2.4
1	A	361	ASN	2.4
1	A	131	THR	2.4
1	A	402	THR	2.4
1	A	119	GLY	2.3
1	A	281	GLY	2.3
1	A	163	ALA	2.3
1	A	146	ASN	2.3
1	A	404	TYR	2.3
1	A	262	HIS	2.3
1	A	320	ILE	2.3
1	A	100	ALA	2.3
1	A	370	ILE	2.3
1	A	267	VAL	2.3
1	A	323	GLY	2.3
1	A	455	GLY	2.3
1	A	141	ALA	2.3
1	A	178	ILE	2.3
1	A	351	ILE	2.3
1	A	378	LEU	2.2
1	A	247[A]	ASP	2.2
1	A	481	ASN	2.2
1	A	406	SER	2.2
1	A	494	LYS	2.2
1	A	286	ILE	2.2
1	A	317	ILE	2.2
1	A	257	VAL	2.2
1	A	235	ASN	2.2
1	A	110	PRO	2.2
1	A	367	GLN	2.2
1	A	345	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	431	ALA	2.2
1	A	85	ILE	2.2
1	A	104	LEU	2.2
1	A	429	LEU	2.2
1	A	98	GLN	2.2
1	A	371	GLN	2.2
1	A	164	ILE	2.2
1	A	280	ASP	2.2
1	A	295	VAL	2.2
1	A	296	PRO	2.2
1	A	432	LYS	2.2
1	A	106	ARG	2.1
1	A	136	ILE	2.1
1	A	114	ASN	2.1
1	A	463	MET	2.1
1	A	127	PHE	2.1
1	A	237	CYS	2.1
1	A	322	THR	2.1
1	A	461	SER	2.1
1	A	472	LYS	2.1
1	A	188	ASN	2.1
1	A	93	GLN	2.1
1	A	145	THR	2.1
1	A	179	SER	2.1
1	A	393	THR	2.1
1	A	316	ALA	2.1
1	A	314	LEU	2.1
1	A	458	GLU	2.1
1	A	196	PHE	2.1
1	A	468	GLY	2.1
1	A	97	THR	2.1
1	A	170	LEU	2.1
1	A	215	VAL	2.1
1	A	226	LEU	2.0
1	A	439	VAL	2.0
1	A	328	THR	2.0
1	A	397	ALA	2.0
1	A	89	ASN	2.0
1	A	350[A]	ASN	2.0
1	A	388	LYS	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](#)

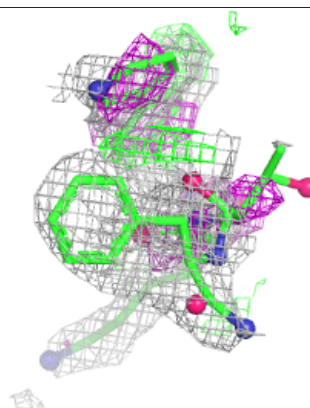
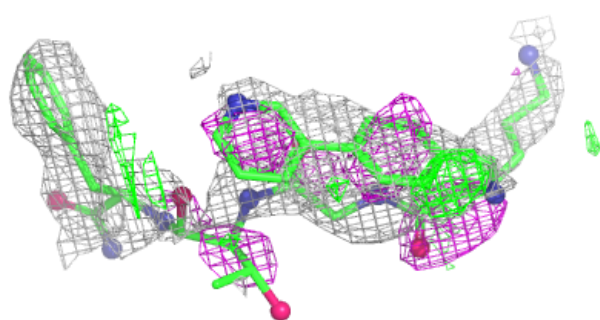
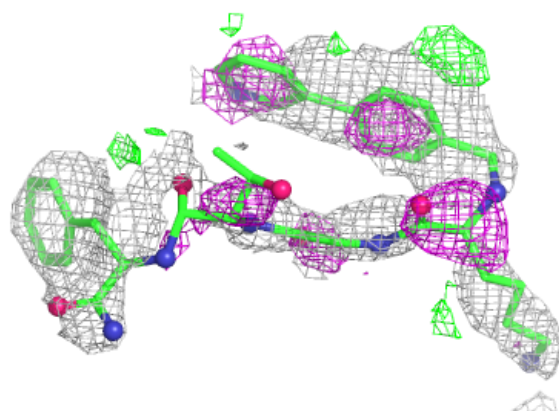
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	3D4	A	501	45/45	0.48	0.29	46,64,95,104	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 3D4 A 501:

$2mF_o-DF_c$ (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.