



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 6TN2 / pdb_00006tn2
Title : Rapid optimisation of fragments and hits to lead compounds from screening of crude reaction mixtures
Authors : Baker, L.M.; Aimon, A.; Murray, J.B.; Surgenor, A.E.; Matassova, N.; Roughley, S.D.; von Delft, F.; Hubbard, R.E.
Deposited on : 2019-12-05
Resolution : 1.77 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

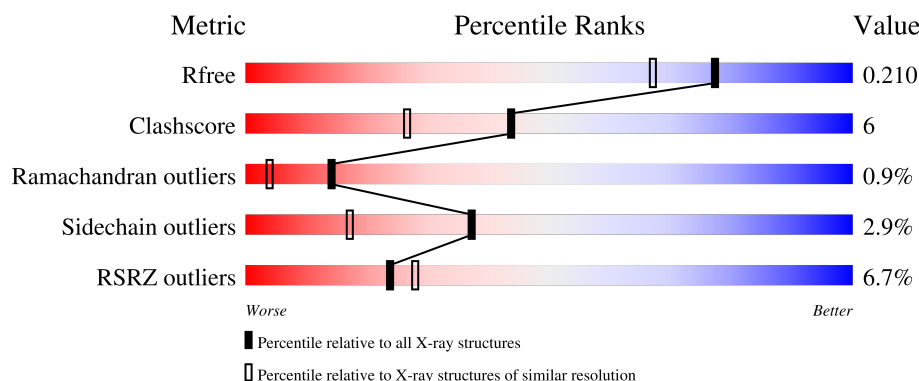
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

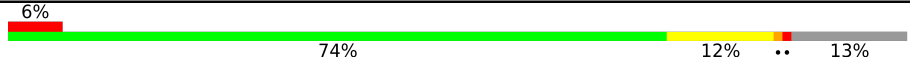
The reported resolution of this entry is 1.77 Å.

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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	394	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	AAA	403	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5794 atoms, of which 2784 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.

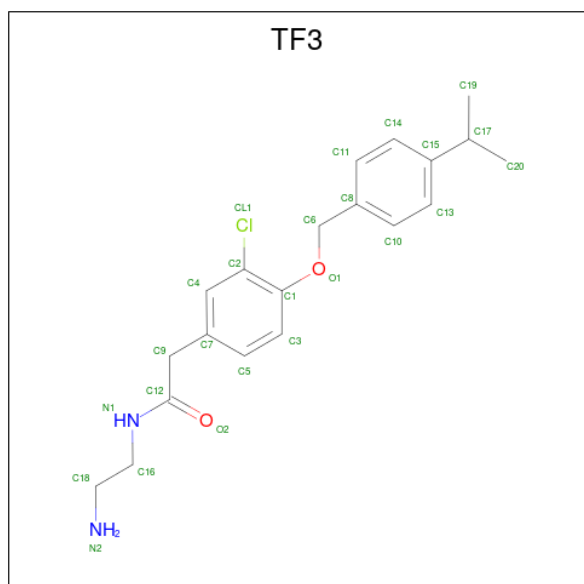
- Molecule 1 is a protein called [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	341	Total	C	H	N	O	S	140	3	0
			5494	1768	2739	452	519	16			

There are 2 discrepancies between the modelled and reference sequences:

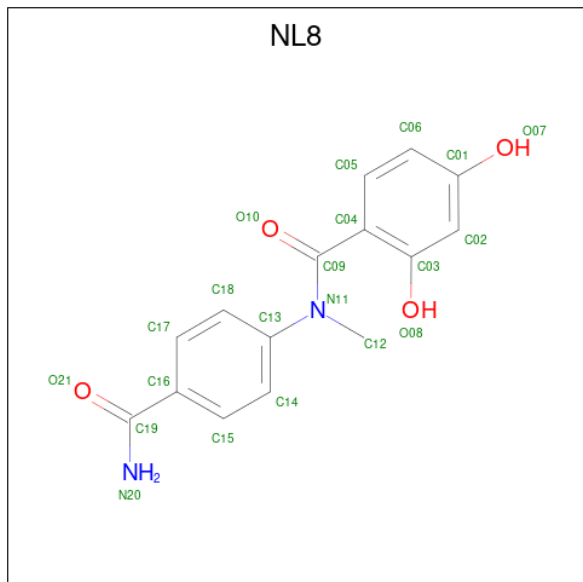
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	6	GLY	ALA	conflict	UNP Q15119
AAA	7	SER	GLY	conflict	UNP Q15119

- Molecule 2 is N-(2-AMINOETHYL)-2-{3-CHLORO-4-[(4-ISOPROPYLBENZYL)OXY]PHENYL} ACETAMIDE (CCD ID: TF3) (formula: C₂₀H₂₅ClN₂O₂).



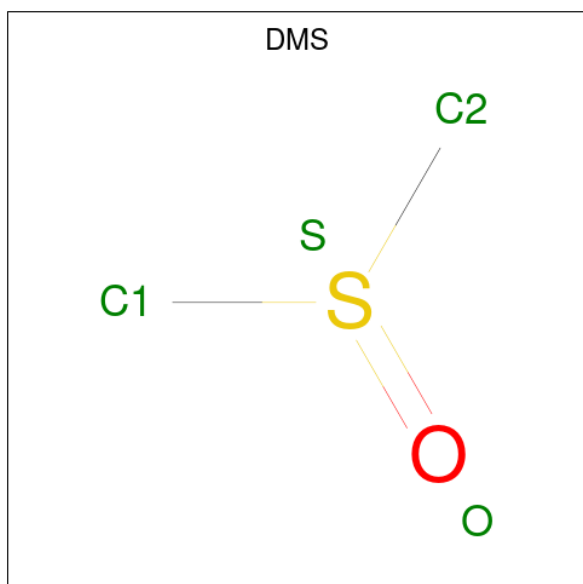
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	Cl	H	N	O	0	0
			50	20	1	25	2	2		

- Molecule 3 is {N}-(4-aminocarbonylphenyl)- {N}-methyl-2,4-bis(oxidanyl)benzamide (CCD ID: NL8) (formula: C₁₅H₁₄N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	2	0
			35	15	14	2	4		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total 1	Cl 1	0	0

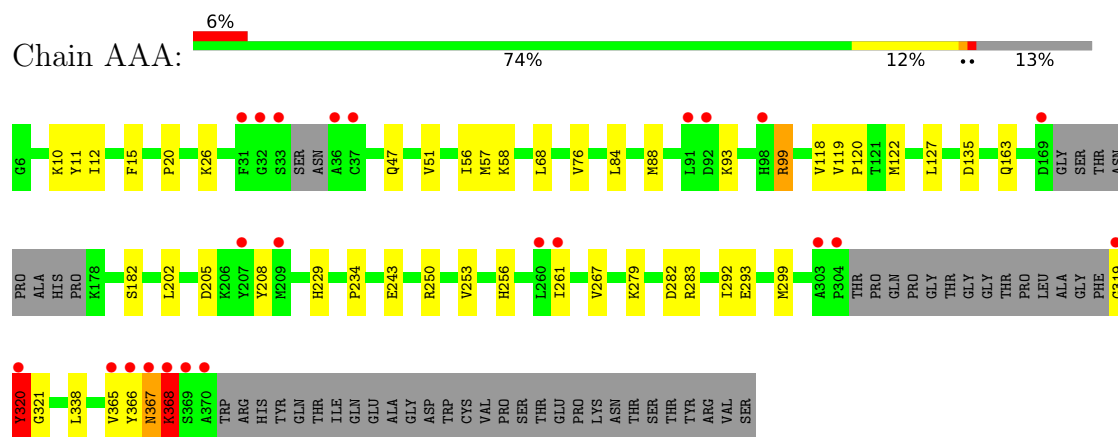
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	204	Total 204	O 204	0	0

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: [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	108.52Å 108.52Å 83.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.49 – 1.77 62.49 – 1.77	Depositor EDS
% Data completeness (in resolution range)	55.3 (62.49-1.77) 56.0 (62.49-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.171 , 0.210 0.171 , 0.210	Depositor DCC
R_{free} test set	1530 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5794	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: NL8, CL, DMS, TF3

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	1.03	0/2820	1.35	3/3816 (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	AAA	10	LYS	CA-C-N	5.12	127.44	120.54
1	AAA	10	LYS	C-N-CA	5.12	127.44	120.54
1	AAA	282	ASP	CA-CB-CG	5.09	117.69	112.60

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	AAA	2755	2739	2719	33	0
2	AAA	25	25	25	0	0
3	AAA	21	14	0	1	0
4	AAA	4	6	6	4	0
5	AAA	1	0	0	0	0
6	AAA	204	0	0	5	0
All	All	3010	2784	2750	34	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 6.

All (34) 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:AAA:163:GLN:HE22	1:AAA:182:SER:H	1.14	0.94
1:AAA:118:VAL:HG21	6:AAA:509:HOH:O	1.89	0.71
1:AAA:292:ILE:HG21	4:AAA:403:DMS:C2	2.24	0.66
1:AAA:163:GLN:NE2	1:AAA:182:SER:H	1.91	0.65
1:AAA:20:PRO:HD2	1:AAA:365:VAL:HG12	1.80	0.63
1:AAA:76:VAL:HG11	1:AAA:122:MET:HE2	1.84	0.59
1:AAA:338:LEU:O	4:AAA:403:DMS:H23	2.03	0.58
1:AAA:292:ILE:CG2	4:AAA:403:DMS:H22	2.34	0.57
1:AAA:292:ILE:CG2	4:AAA:403:DMS:C2	2.85	0.55
1:AAA:250:ARG:NH1	6:AAA:504:HOH:O	2.39	0.52
1:AAA:11:TYR:CG	1:AAA:88:MET:CE	2.94	0.51
1:AAA:12:ILE:HD11	1:AAA:57:MET:HE2	1.93	0.49
1:AAA:321:GLY:HA2	6:AAA:671:HOH:O	2.14	0.48
3:AAA:402:NL8:C05	3:AAA:402:NL8:C13	2.92	0.47
1:AAA:243:GLU:CD	1:AAA:321:GLY:HA3	2.40	0.46
1:AAA:11:TYR:CG	1:AAA:88:MET:HE3	2.50	0.46
1:AAA:15:PHE:HE2	1:AAA:88:MET:HE1	1.80	0.46
1:AAA:205:ASP:O	1:AAA:208:TYR:O	2.35	0.45
1:AAA:267:VAL:HA	1:AAA:279:LYS:O	2.17	0.44
1:AAA:229:HIS:HB2	6:AAA:687:HOH:O	2.17	0.44
1:AAA:135:ASP:HB2	1:AAA:299:MET:HE3	1.99	0.43
1:AAA:256:HIS:HE1	1:AAA:283:ARG:O	2.01	0.43
1:AAA:58:LYS:HG2	1:AAA:366:TYR:CZ	2.54	0.43
1:AAA:367:ASN:O	1:AAA:368:LYS:HB2	2.19	0.43
1:AAA:319:GLY:O	1:AAA:320:TYR:HB2	2.18	0.43
1:AAA:163:GLN:HE22	1:AAA:182:SER:N	1.97	0.43
1:AAA:182:SER:O	1:AAA:234:PRO:HD2	2.18	0.43
1:AAA:26:LYS:HB3	6:AAA:506:HOH:O	2.18	0.43
1:AAA:47:GLN:O	1:AAA:51:VAL:HG23	2.19	0.42
1:AAA:56:ILE:HD12	1:AAA:56:ILE:HA	1.91	0.42
1:AAA:119:VAL:N	1:AAA:120:PRO:HD2	2.35	0.41
1:AAA:99:ARG:HE	1:AAA:99:ARG:HB2	1.60	0.41
1:AAA:84:LEU:O	1:AAA:88:MET:HG2	2.20	0.41
1:AAA:208:TYR:CG	1:AAA:253:VAL:HG11	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	336/394 (85%)	322 (96%)	11 (3%)	3 (1%)	14 4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	367	ASN
1	AAA	368	LYS
1	AAA	320	TYR

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	AAA	310/353 (88%)	301 (97%)	9 (3%)	37 17

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	68	LEU
1	AAA	93	LYS
1	AAA	99	ARG
1	AAA	127	LEU
1	AAA	202	LEU
1	AAA	261	ILE
1	AAA	293	GLU
1	AAA	320	TYR

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Mol	Chain	Res	Type
1	AAA	368	LYS

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	TF3	AAA	401	-	26,26,26	0.44	0	33,34,34	0.92	0
3	NL8	AAA	402	-	22,22,22	2.40	3 (13%)	31,31,31	0.97	1 (3%)
4	DMS	AAA	403	-	3,3,3	0.49	0	3,3,3	0.47	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
2	TF3	AAA	401	-	-	3/17/17/17	0/2/2/2
3	NL8	AAA	402	-	-	5/16/16/16	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	402	NL8	C16-C19	-6.83	1.40	1.50
3	AAA	402	NL8	C04-C09	-6.42	1.41	1.50
3	AAA	402	NL8	C13-N11	-5.60	1.34	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	402	NL8	O08-C03-C04	-3.03	116.10	121.71

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	401	TF3	N1-C16-C18-N2
3	AAA	402	NL8	C15-C16-C19-N20
3	AAA	402	NL8	C15-C16-C19-O21
3	AAA	402	NL8	C17-C16-C19-N20
3	AAA	402	NL8	C17-C16-C19-O21
2	AAA	401	TF3	C18-C16-N1-C12
3	AAA	402	NL8	C03-C04-C09-O10
2	AAA	401	TF3	C9-C12-N1-C16

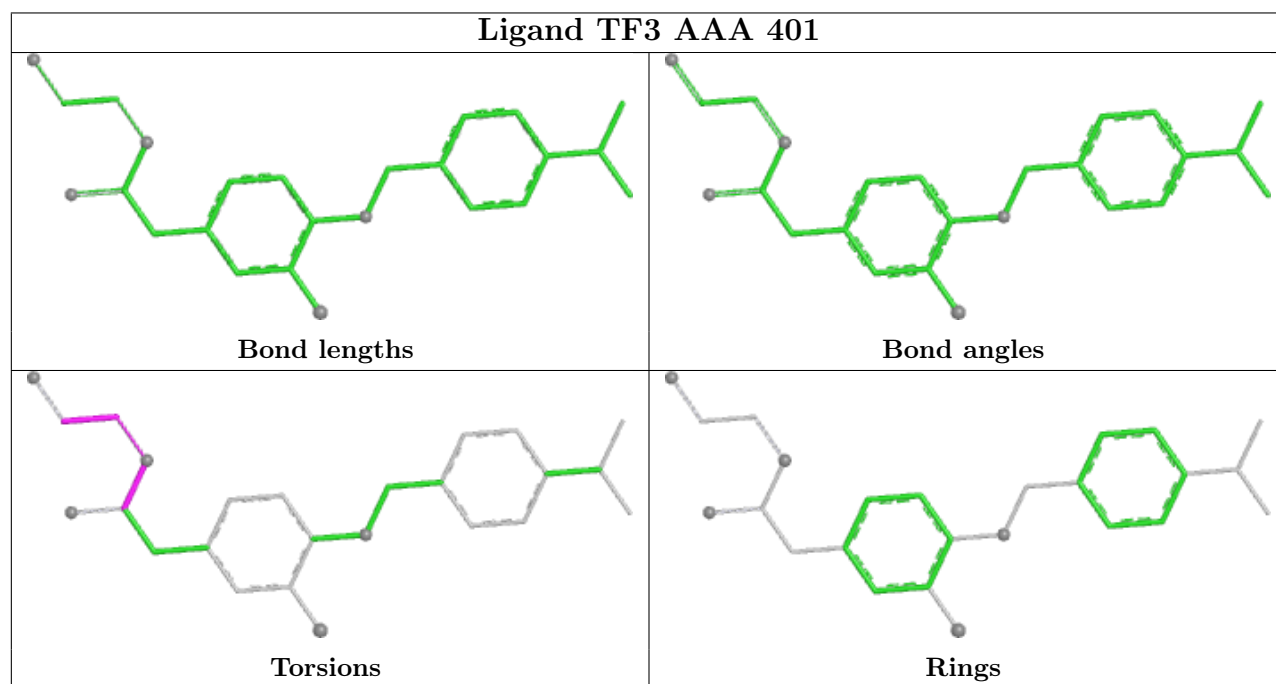
There are no ring outliers.

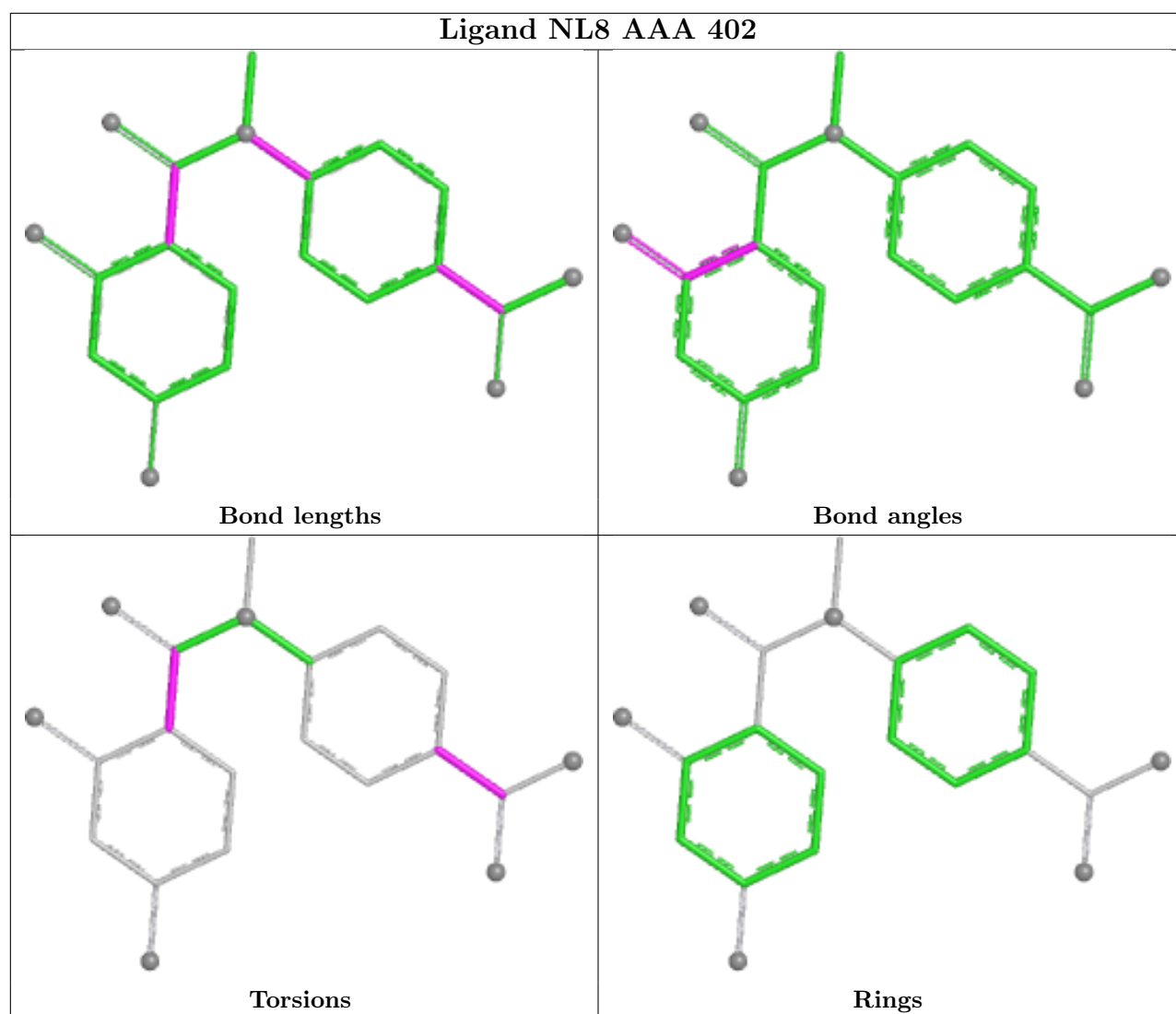
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	402	NL8	1	0
4	AAA	403	DMS	4	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	341/394 (86%)	0.19	23 (6%) 24 28	16, 39, 73, 127	3 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	370	ALA	8.3
1	AAA	36	ALA	7.2
1	AAA	320	TYR	5.1
1	AAA	209	MET	5.0
1	AAA	304	PRO	4.9
1	AAA	319	GLY	4.8
1	AAA	33	SER	4.5
1	AAA	365	VAL	4.4
1	AAA	369	SER	4.4
1	AAA	366	TYR	4.0
1	AAA	368	LYS	3.8
1	AAA	261	ILE	3.8
1	AAA	37	CYS	3.8
1	AAA	207	TYR	3.5
1	AAA	260	LEU	3.1
1	AAA	98	HIS	3.0
1	AAA	367	ASN	3.0
1	AAA	31	PHE	2.8
1	AAA	303	ALA	2.8
1	AAA	169	ASP	2.4
1	AAA	92[A]	ASP	2.3
1	AAA	32	GLY	2.1
1	AAA	91	LEU	2.1

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](#)

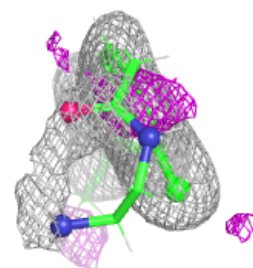
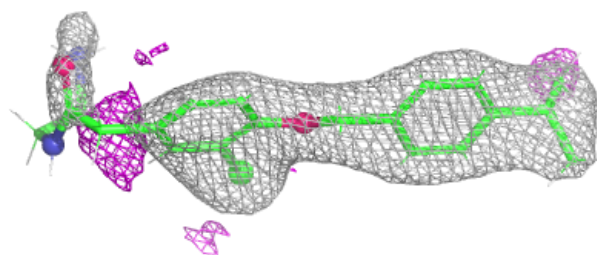
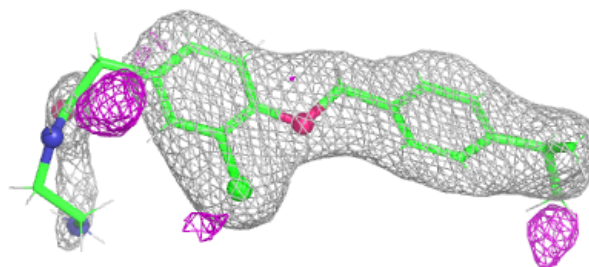
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TF3	AAA	401	25/25	0.91	0.14	34,53,97,99	0
5	CL	AAA	404	1/1	0.92	0.37	71,71,71,71	0
4	DMS	AAA	403	4/4	0.95	0.10	36,45,52,52	0
3	NL8	AAA	402	21/21	0.98	0.05	24,30,49,49	2

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.

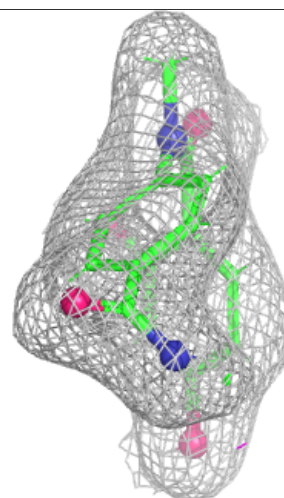
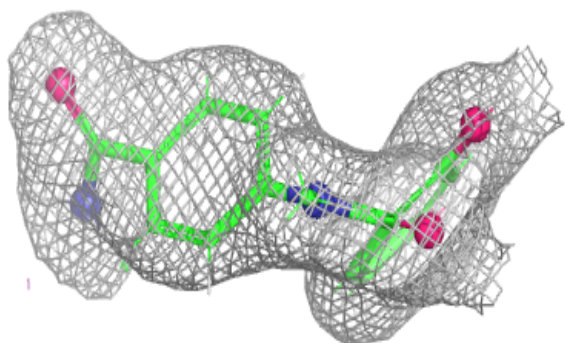
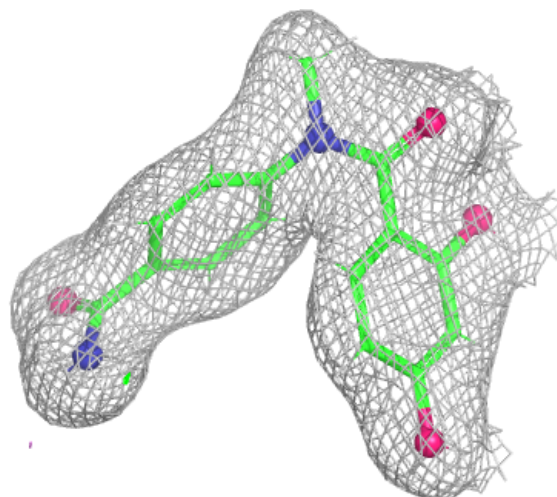
Electron density around TF3 AAA 401:

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



Electron density around NL8 AAA 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.