



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:27 PM UTC

PDB ID : 7XBS / pdb_00007xbs
Title : Crystal structure of the adenylation domain of CmnG
Authors : Chen, I.H.; Wang, Y.L.; Chang, C.Y.
Deposited on : 2022-03-22
Resolution : 1.64 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

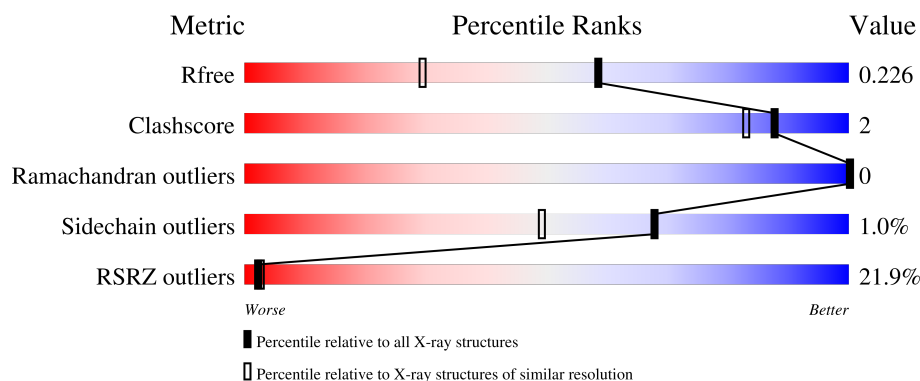
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	513	21% 89% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4034 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.

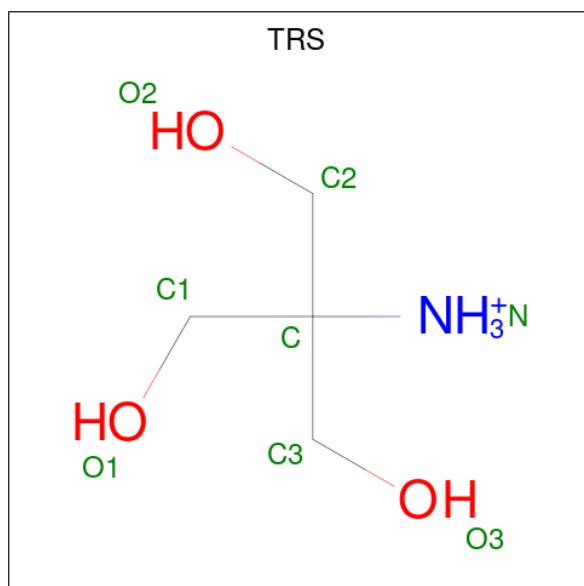
- Molecule 1 is a protein called CmnG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	484	3751	2369	689	686	7	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	conflict	UNP A6YEH8

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0

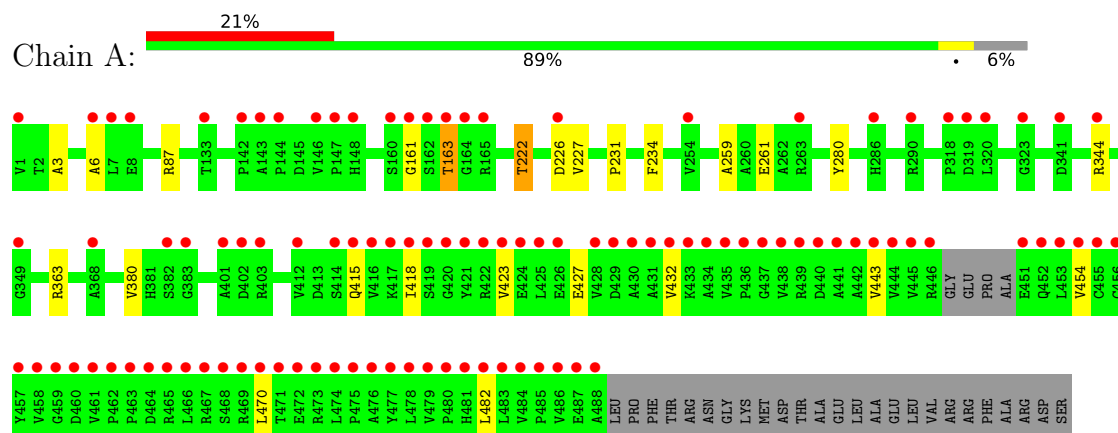
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	275	Total 275	O 275	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: CmnG



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.41 Å 77.41 Å 191.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.37 – 1.64 27.37 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.37-1.64) 99.9 (27.37-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 1.64 Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.205 , 0.228 0.205 , 0.226	Depositor DCC
R_{free} test set	3609 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4034	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: TRS

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	0/3855	0.53	0/5290

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	3751	0	3686	15	0
2	A	8	0	12	0	0
3	A	275	0	0	2	0
All	All	4034	0	3698	15	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 2.

All (15) 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:6:ALA:HB2	1:A:344:ARG:HH21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:O	3:A:701:HOH:O	2.18	0.55
1:A:161:GLY:HA3	1:A:415:GLN:NE2	2.24	0.51
1:A:163:THR:HB	1:A:427:GLU:HB2	1.94	0.49
1:A:454:VAL:HG22	1:A:482:LEU:HD21	1.93	0.49
1:A:87:ARG:HH11	1:A:222:THR:HG22	1.78	0.48
1:A:227:VAL:HG13	1:A:234:PHE:HA	1.95	0.48
1:A:226:ASP:OD1	1:A:227:VAL:HG23	2.13	0.47
1:A:161:GLY:HA3	1:A:415:GLN:HE21	1.81	0.45
1:A:363:ARG:NH2	3:A:702:HOH:O	2.35	0.44
1:A:432:VAL:HG12	1:A:470:LEU:HD11	2.00	0.43
1:A:3:ALA:HB3	1:A:380:VAL:HA	2.00	0.43
1:A:454:VAL:HG13	1:A:482:LEU:HD21	2.00	0.43
1:A:231:PRO:HB2	1:A:259:ALA:HB2	2.03	0.41
1:A:418:ILE:HD12	1:A:423:VAL:HG11	2.02	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	481/513 (94%)	468 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	385/407 (95%)	381 (99%)	4 (1%)	68 49

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	THR
1	A	222	THR
1	A	280	TYR
1	A	443	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	208	GLN
1	A	209	GLN
1	A	310	ASN

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](#)

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	TRS	A	601	-	7,7,7	0.32	0	9,9,9	0.61	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	TRS	A	601	-	-	0/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

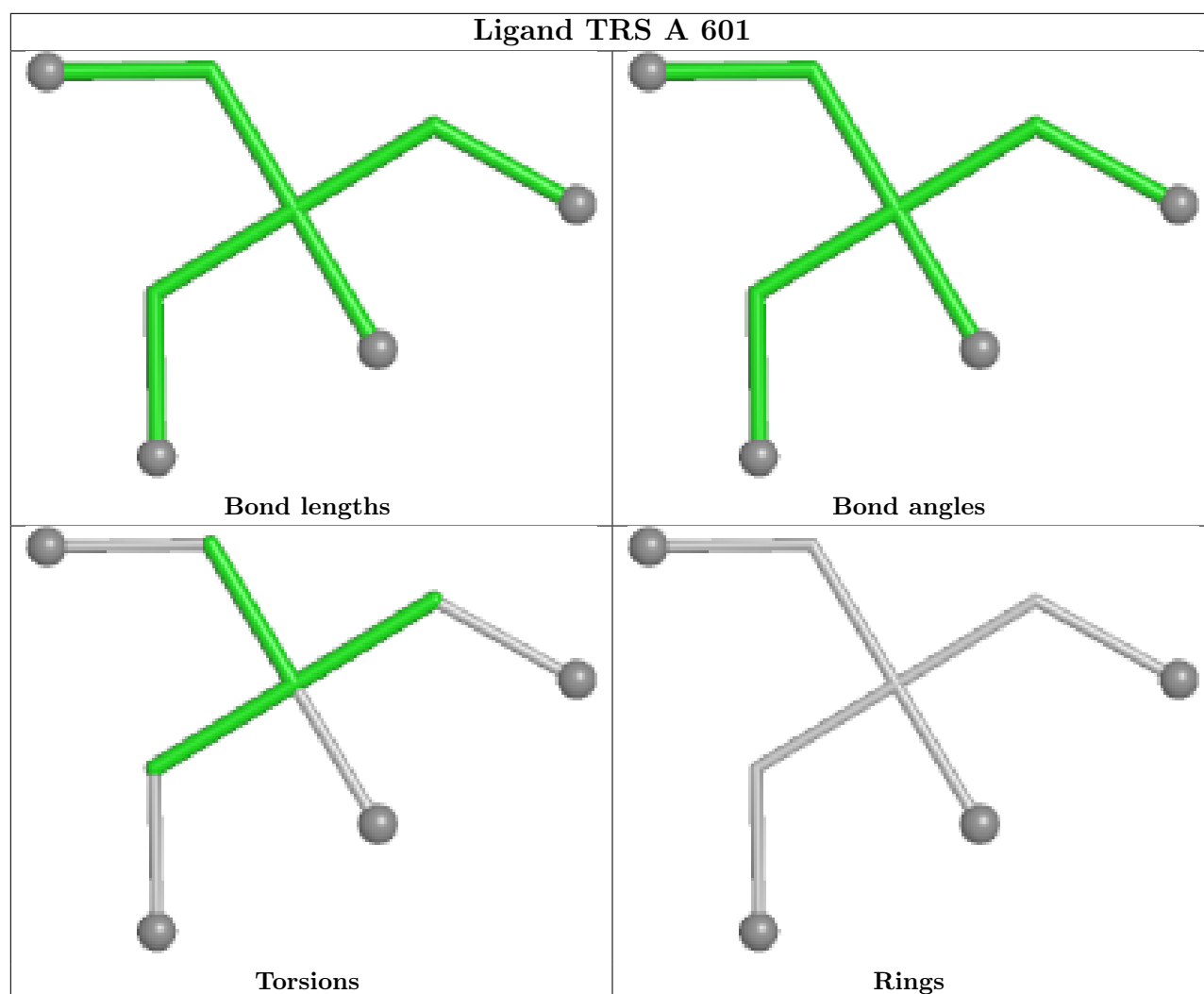
There are no chirality outliers.

There are no torsion outliers.

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	484/513 (94%)	1.01	106 (21%) 2 3	6, 19, 69, 92	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	PRO	8.3
1	A	430	ALA	7.3
1	A	444	VAL	6.8
1	A	421	TYR	6.8
1	A	458	VAL	6.7
1	A	416	VAL	6.6
1	A	445	VAL	6.6
1	A	462	PRO	6.6
1	A	482	LEU	6.5
1	A	161	GLY	6.4
1	A	477	TYR	6.4
1	A	412	VAL	6.2
1	A	435	VAL	6.2
1	A	486	VAL	6.1
1	A	162	SER	6.1
1	A	484	VAL	6.0
1	A	425	LEU	5.9
1	A	461	VAL	5.8
1	A	432	VAL	5.7
1	A	455	CYS	5.6
1	A	454	VAL	5.6
1	A	418	ILE	5.5
1	A	453	LEU	5.5
1	A	438	VAL	5.4
1	A	443	VAL	5.4
1	A	423	VAL	5.4
1	A	441	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	471	THR	5.2
1	A	1	VAL	5.1
1	A	401	ALA	5.1
1	A	483	LEU	5.0
1	A	442	ALA	5.0
1	A	422	ARG	5.0
1	A	437	GLY	4.9
1	A	460	ASP	4.9
1	A	488	ALA	4.8
1	A	419	SER	4.8
1	A	476	ALA	4.7
1	A	463	PRO	4.7
1	A	475	PRO	4.7
1	A	457	TYR	4.6
1	A	446	ARG	4.6
1	A	431	ALA	4.4
1	A	485	PRO	4.3
1	A	469	ARG	4.2
1	A	466	LEU	4.1
1	A	163	THR	4.1
1	A	434	ALA	4.1
1	A	479	VAL	4.0
1	A	472	GLU	4.0
1	A	452	GLN	4.0
1	A	414	SER	3.9
1	A	464	ASP	3.8
1	A	478	LEU	3.8
1	A	402	ASP	3.8
1	A	473	ARG	3.7
1	A	465	ARG	3.7
1	A	481	HIS	3.7
1	A	456	CYS	3.6
1	A	429	ASP	3.5
1	A	439	ARG	3.5
1	A	415	GLN	3.5
1	A	451	GLU	3.4
1	A	165	ARG	3.4
1	A	487	GLU	3.4
1	A	319	ASP	3.3
1	A	147	PRO	3.3
1	A	480	PRO	3.3
1	A	459	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	290	ARG	3.3
1	A	428	VAL	3.3
1	A	420	GLY	3.2
1	A	160	SER	3.2
1	A	164	GLY	3.1
1	A	440	ASP	3.1
1	A	474	LEU	3.0
1	A	344	ARG	3.0
1	A	470	LEU	3.0
1	A	320	LEU	2.9
1	A	146	VAL	2.8
1	A	226	ASP	2.7
1	A	341	ASP	2.7
1	A	318	PRO	2.7
1	A	468	SER	2.7
1	A	426	GLU	2.6
1	A	143	ALA	2.6
1	A	144	PRO	2.6
1	A	7	LEU	2.5
1	A	403	ARG	2.5
1	A	6	ALA	2.5
1	A	8	GLU	2.5
1	A	382	SER	2.5
1	A	383	GLY	2.4
1	A	467	ARG	2.4
1	A	148	HIS	2.4
1	A	263	ARG	2.3
1	A	433	LYS	2.3
1	A	417	LYS	2.2
1	A	424	GLU	2.1
1	A	323	GLY	2.1
1	A	349	GLY	2.1
1	A	142	PRO	2.1
1	A	368	ALA	2.0
1	A	133	THR	2.0
1	A	286	HIS	2.0
1	A	254	VAL	2.0

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

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](#)

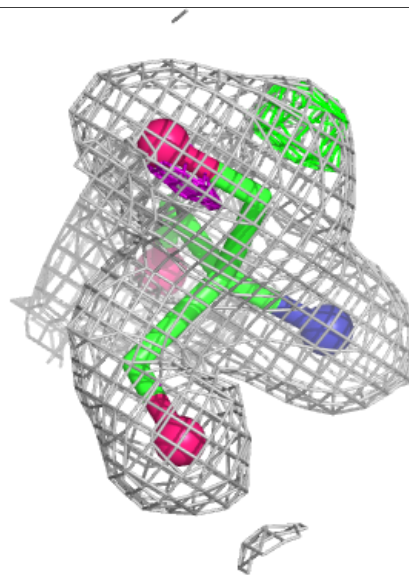
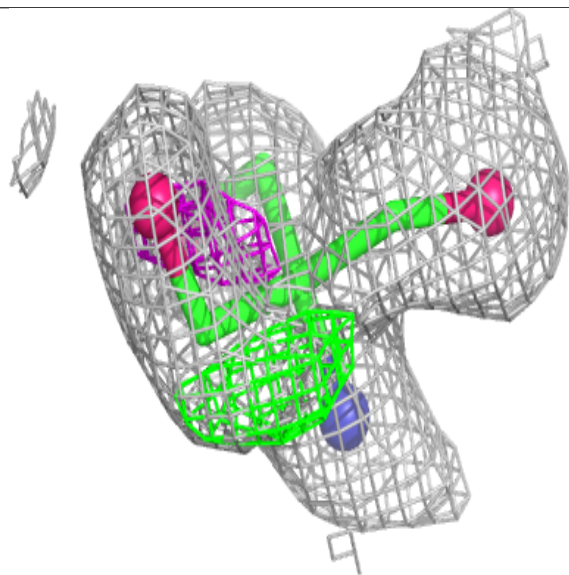
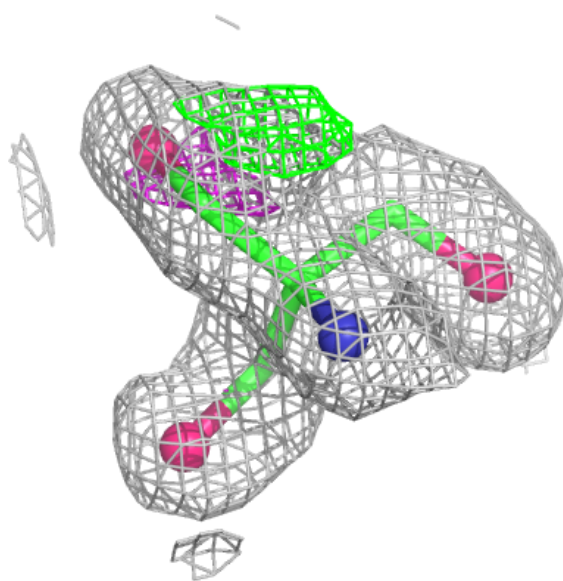
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TRS	A	601	8/8	0.92	0.12	16,19,23,25	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 TRS A 601:

$2mF_o-DF_c$ (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.