



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:20 AM UTC

PDB ID : 8CQ3 / pdb_00008cq3
Title : Bifunctional chorismate mutase/cyclohexadienyl dehydratase from *Aequoribacter fuscus*
Authors : Khatanbaatar, T.; Cordara, G.; Kregel, U.
Deposited on : 2023-03-03
Resolution : 1.55 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

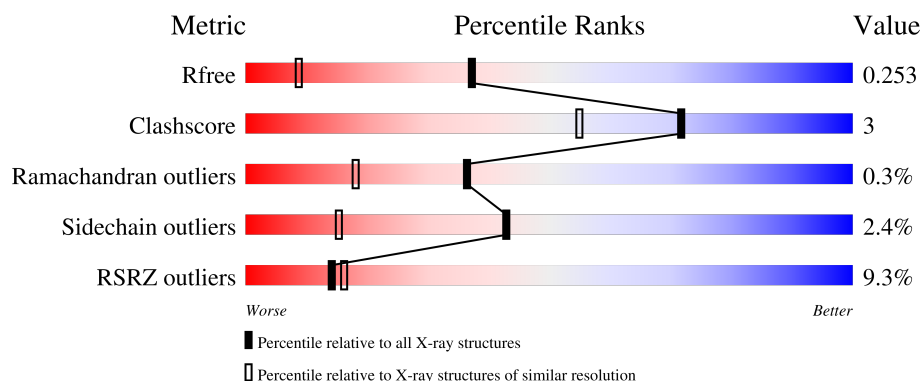
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	424	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3269 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.

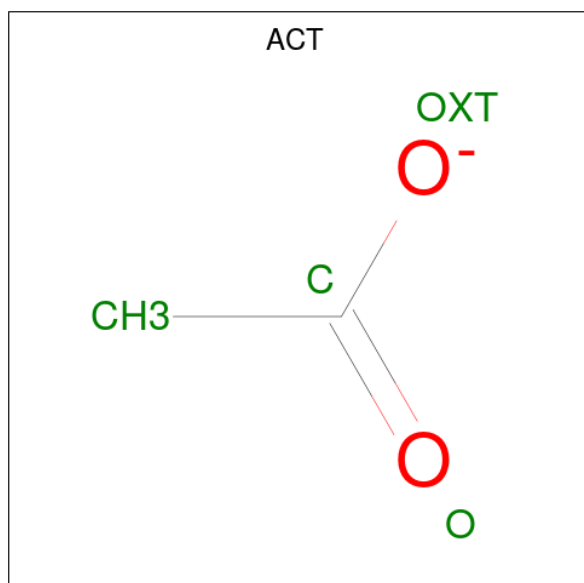
- Molecule 1 is a protein called chorismate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	3139	1981	551	597	10	0	7	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LEU	-	expression tag	UNP A0A7Z2NRM1
A	418	GLU	-	expression tag	UNP A0A7Z2NRM1
A	419	HIS	-	expression tag	UNP A0A7Z2NRM1
A	420	HIS	-	expression tag	UNP A0A7Z2NRM1
A	421	HIS	-	expression tag	UNP A0A7Z2NRM1
A	422	HIS	-	expression tag	UNP A0A7Z2NRM1
A	423	HIS	-	expression tag	UNP A0A7Z2NRM1
A	424	HIS	-	expression tag	UNP A0A7Z2NRM1

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

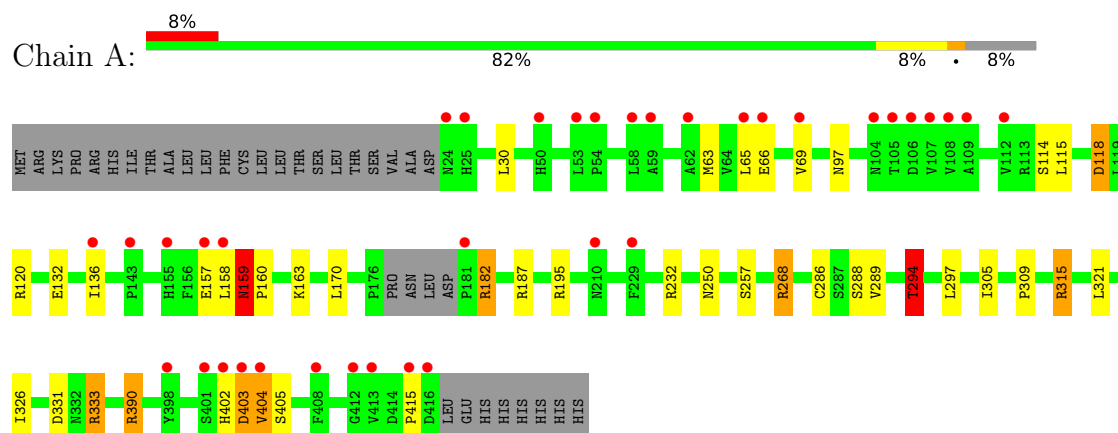
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	117	Total O 117 117	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: chorismate mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.42Å 98.76Å 55.34Å 90.00° 108.52° 90.00°	Depositor
Resolution (Å)	52.47 – 1.55 52.47 – 1.55	Depositor EDS
% Data completeness (in resolution range)	61.7 (52.47-1.55) 61.8 (52.47-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.198 , 0.251 0.207 , 0.253	Depositor DCC
R_{free} test set	1578 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3269	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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: CL, ACT

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	0.64	0/3201	1.07	3/4345 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	118	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	159	ASN	CB-CA-C	5.21	117.66	109.27
1	A	294	THR	N-CA-CB	-5.00	102.22	111.52

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	A	187	ARG	Sidechain
1	A	195	ARG	Sidechain
1	A	232	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	309	PRO	Peptide
1	A	315[A]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	333	ARG	Sidechain
1	A	390	ARG	Sidechain
1	A	402	HIS	Peptide
1	A	403	ASP	Peptide
1	A	415	PRO	Peptide

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	3139	0	3124	21	0
2	A	12	0	9	0	0
3	A	1	0	0	0	0
4	A	117	0	0	1	0
All	All	3269	0	3133	21	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 3.

All (21) 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:294:THR:HG22	1:A:297:LEU:H	1.35	0.89
1:A:65:LEU:O	1:A:69:VAL:HG13	1.92	0.69
1:A:97:ASN:ND2	1:A:157:GLU:HG3	2.08	0.67
1:A:97:ASN:HD22	1:A:157:GLU:HG3	1.61	0.65
1:A:132:GLU:O	1:A:136:ILE:HD13	1.96	0.65
1:A:315[B]:ARG:HD3	4:A:611:HOH:O	1.97	0.62
1:A:158:LEU:HB2	1:A:163:LYS:HE2	1.90	0.54
1:A:66:GLU:O	1:A:69:VAL:HG22	2.09	0.53
1:A:182:ARG:NH1	1:A:250:ASN:HB2	2.27	0.50
1:A:30:LEU:HD21	1:A:170:LEU:HD11	1.93	0.49
1:A:305:ILE:HB	1:A:326[A]:ILE:HD13	1.97	0.47
1:A:182:ARG:HH12	1:A:250:ASN:HB2	1.81	0.46
1:A:321:LEU:HD12	1:A:326[A]:ILE:HD11	1.98	0.46
1:A:294:THR:HG22	1:A:297:LEU:N	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:CYS:HA	1:A:289:VAL:HG23	2.00	0.43
1:A:159:ASN:HA	1:A:160:PRO:HD3	1.87	0.42
1:A:331:ASP:OD1	1:A:333:ARG:HB2	2.20	0.42
1:A:66:GLU:HA	1:A:69:VAL:HG22	2.01	0.42
1:A:114:SER:O	1:A:118:ASP:HB3	2.20	0.41
1:A:404:VAL:O	1:A:405:SER:C	2.64	0.40
1:A:115:LEU:O	1:A:120:ARG:HB2	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	392/424 (92%)	376 (96%)	15 (4%)	1 (0%)	36 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	SER

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	347/373 (93%)	339 (98%)	8 (2%)	44 16

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

Mol	Chain	Res	Type
1	A	63	MET
1	A	159	ASN
1	A	268	ARG
1	A	288	SER
1	A	294	THR
1	A	390	ARG
1	A	403	ASP
1	A	404	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	97	ASN
1	A	133	GLN
1	A	152	HIS
1	A	213	ASN
1	A	266	GLN
1	A	267	HIS
1	A	357	GLN
1	A	376	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 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	ACT	A	501	-	3,3,3	1.06	0	3,3,3	0.68	0
2	ACT	A	503	-	3,3,3	0.89	0	3,3,3	1.03	0
2	ACT	A	502	-	3,3,3	0.99	0	3,3,3	0.74	0

There are no bond length outliers.

There are no bond angle outliers.

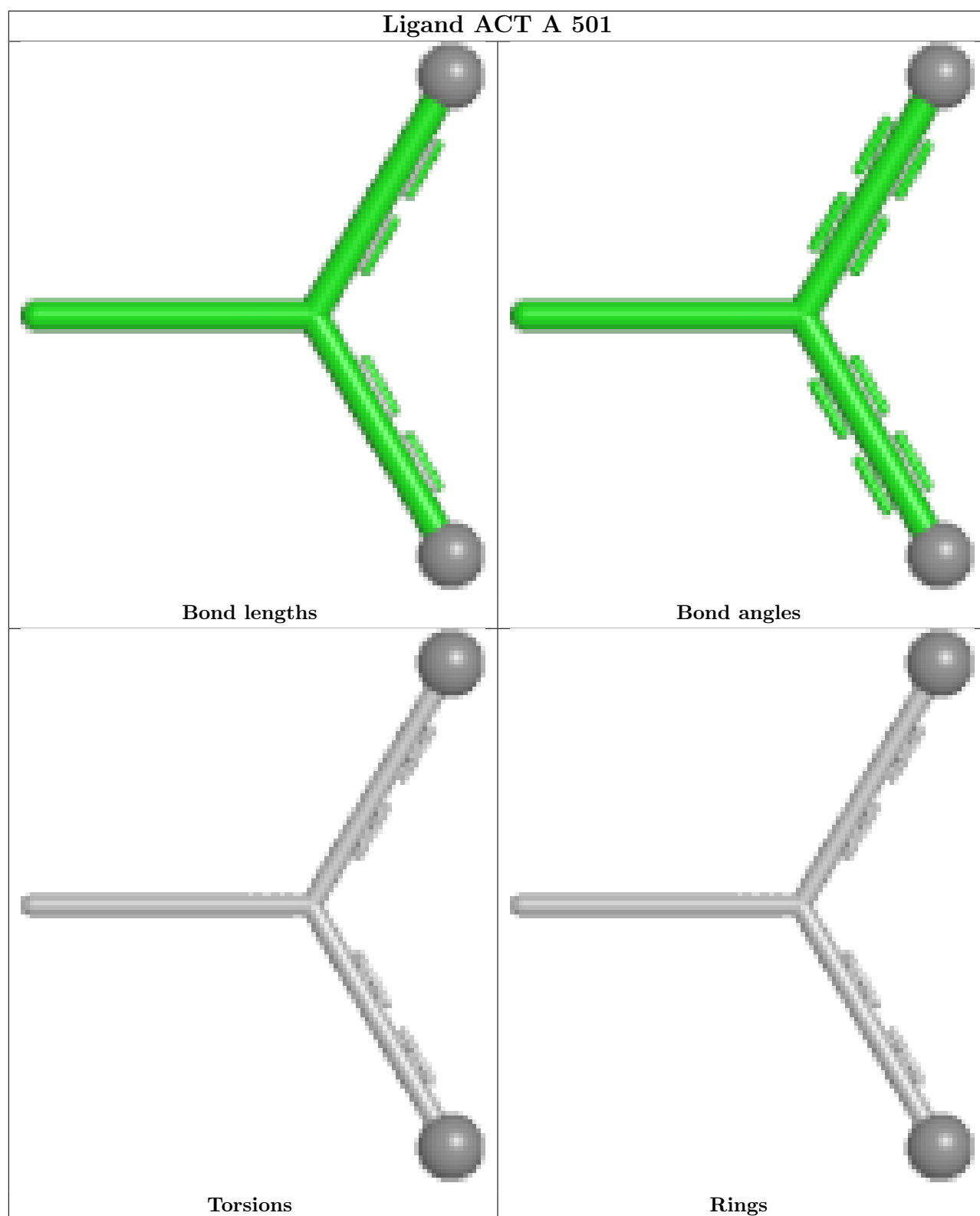
There are no chirality outliers.

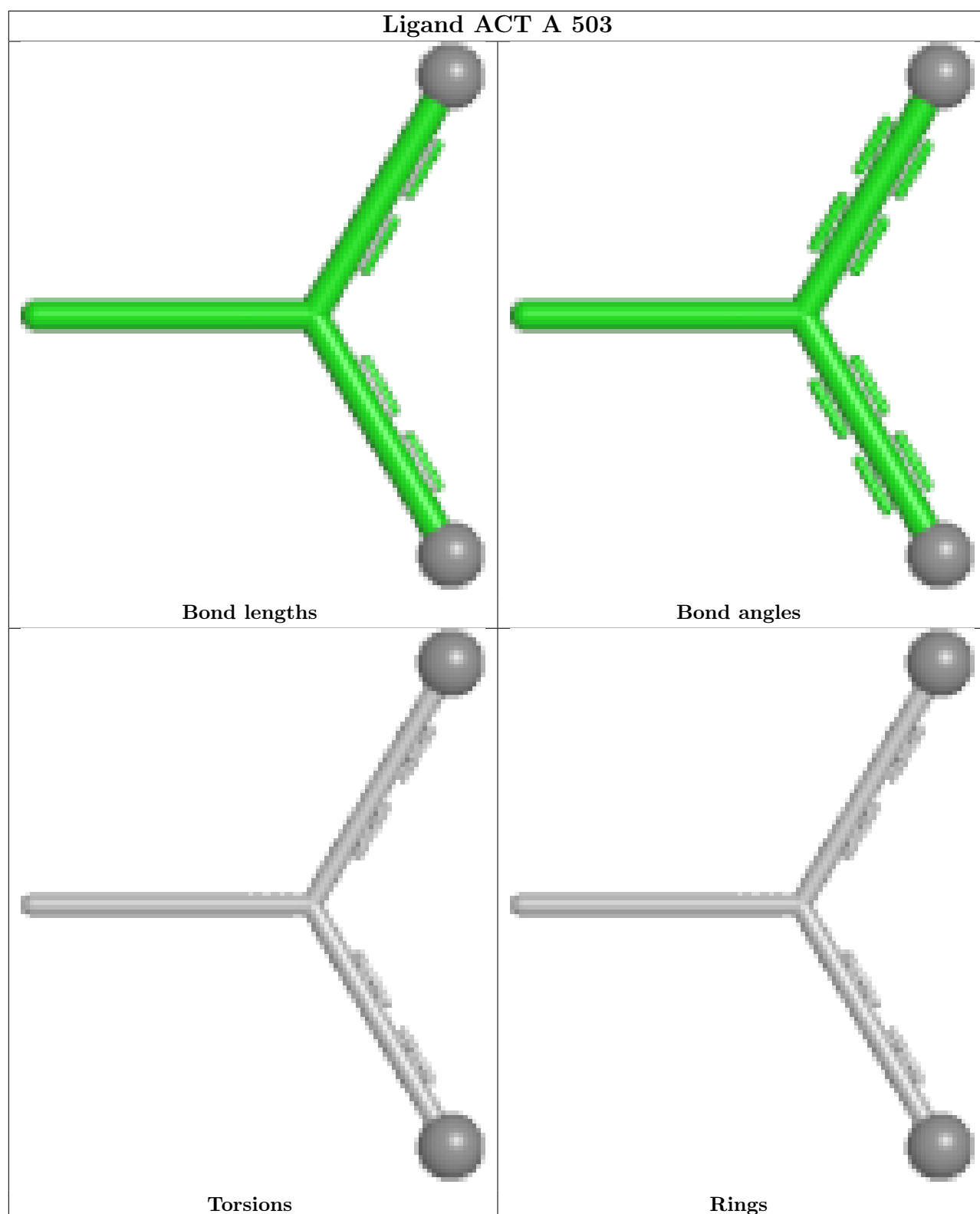
There are no torsion outliers.

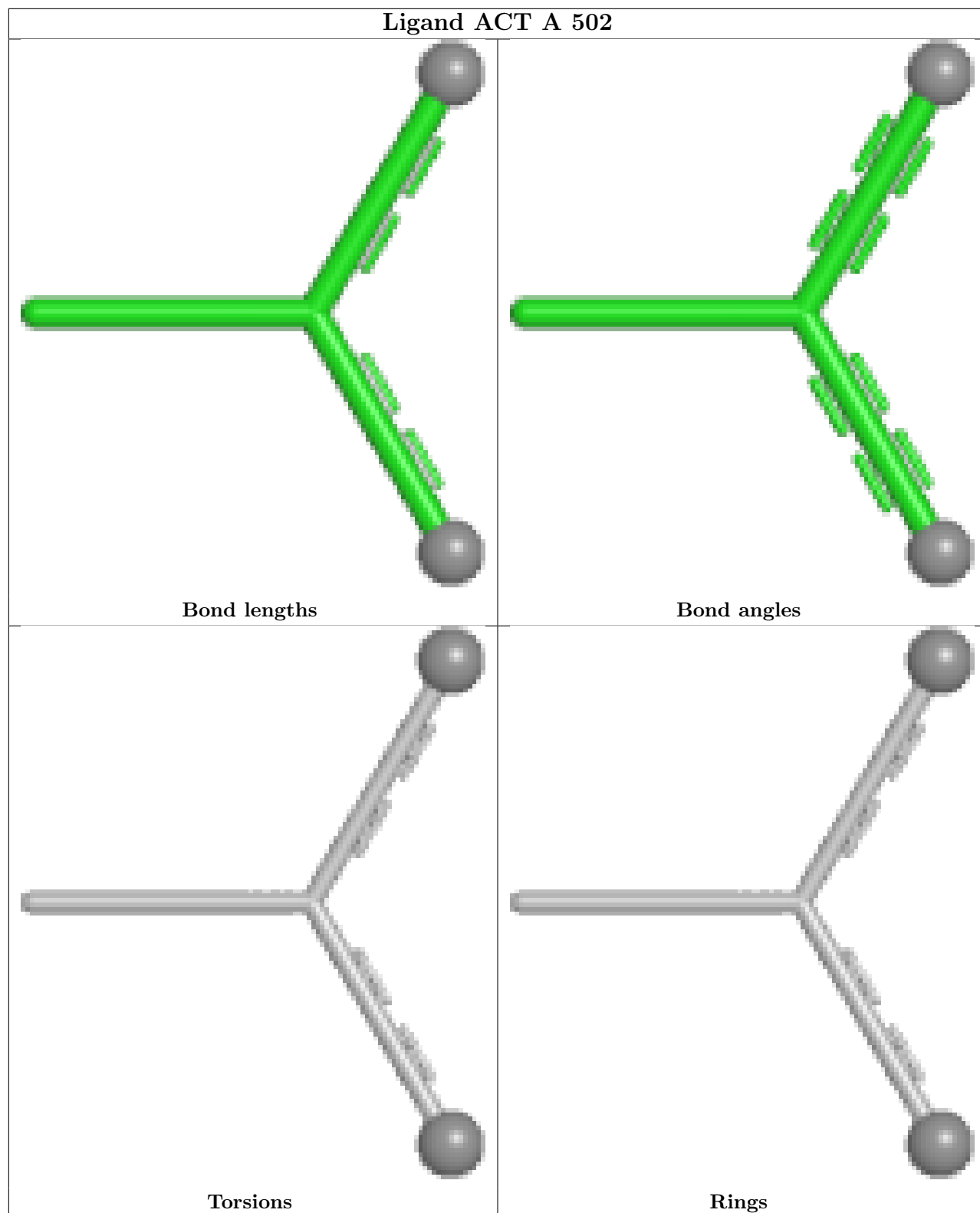
There are no ring outliers.

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 ⓘ

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	389/424 (91%)	0.58	36 (9%) 14 16	9, 22, 49, 75	7 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	VAL	5.3
1	A	108	VAL	5.1
1	A	404	VAL	4.7
1	A	181	PRO	4.5
1	A	25[A]	HIS	4.3
1	A	415	PRO	4.2
1	A	58	LEU	3.6
1	A	62	ALA	3.4
1	A	109	ALA	3.3
1	A	112	VAL	3.2
1	A	65	LEU	2.9
1	A	402	HIS	2.9
1	A	413	VAL	2.9
1	A	416	ASP	2.8
1	A	401	SER	2.8
1	A	24	ASN	2.7
1	A	53	LEU	2.7
1	A	59	ALA	2.6
1	A	54	PRO	2.6
1	A	408	PHE	2.6
1	A	50	HIS	2.5
1	A	106	ASP	2.5
1	A	403	ASP	2.5
1	A	158	LEU	2.4
1	A	105	THR	2.4
1	A	69	VAL	2.3
1	A	136	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	143	PRO	2.3
1	A	66	GLU	2.3
1	A	398	TYR	2.3
1	A	412	GLY	2.2
1	A	104	ASN	2.1
1	A	210	ASN	2.1
1	A	229	PHE	2.0
1	A	155	HIS	2.0
1	A	157	GLU	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](#)

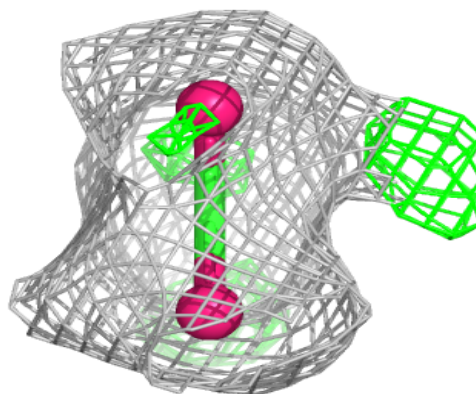
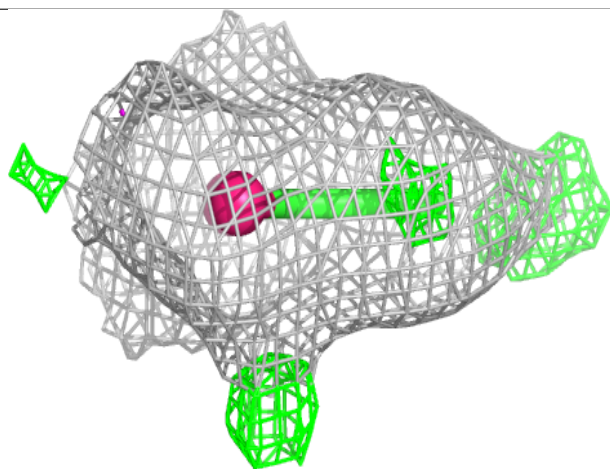
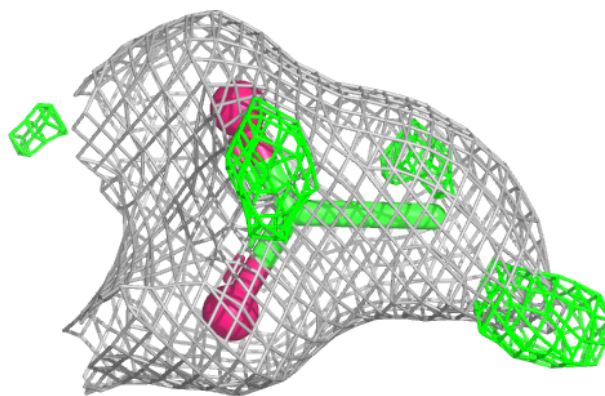
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	A	501	4/4	0.82	0.13	33,35,37,39	0
2	ACT	A	503	4/4	0.92	0.11	33,35,38,41	0
2	ACT	A	502	4/4	0.94	0.06	15,15,16,16	0
3	CL	A	504	1/1	0.98	0.03	15,15,15,15	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.

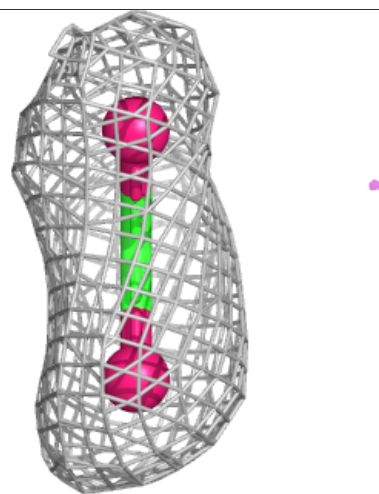
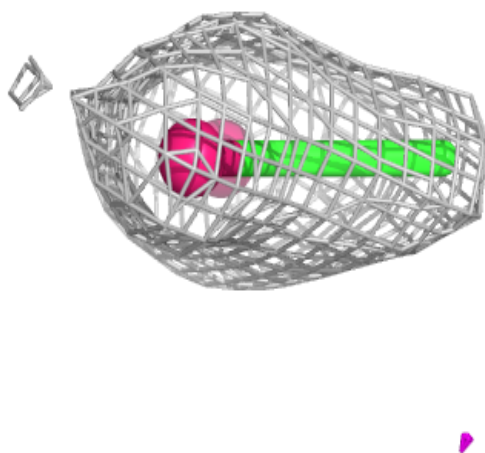
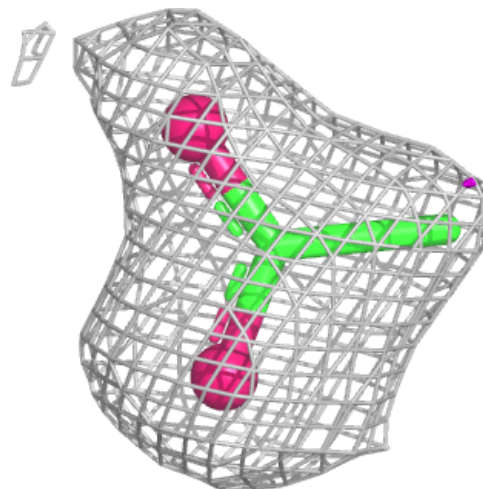
Electron density around ACT A 501:

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



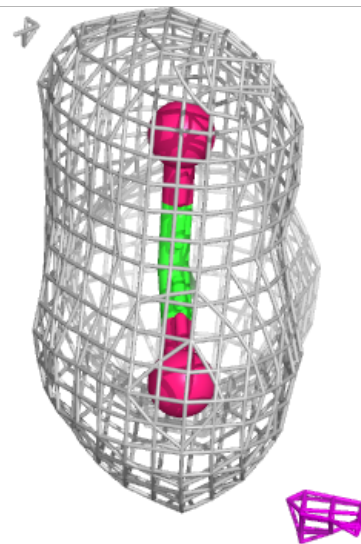
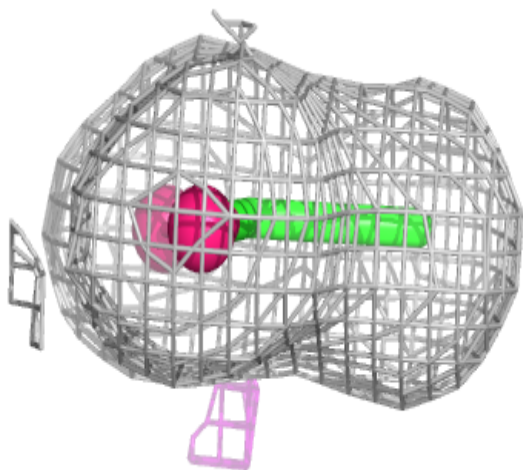
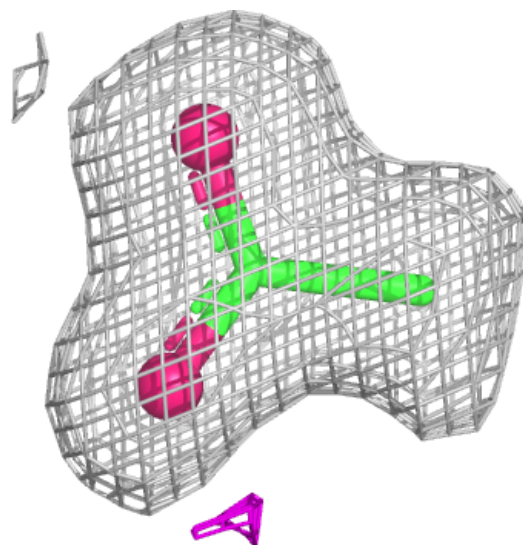
Electron density around ACT A 503:

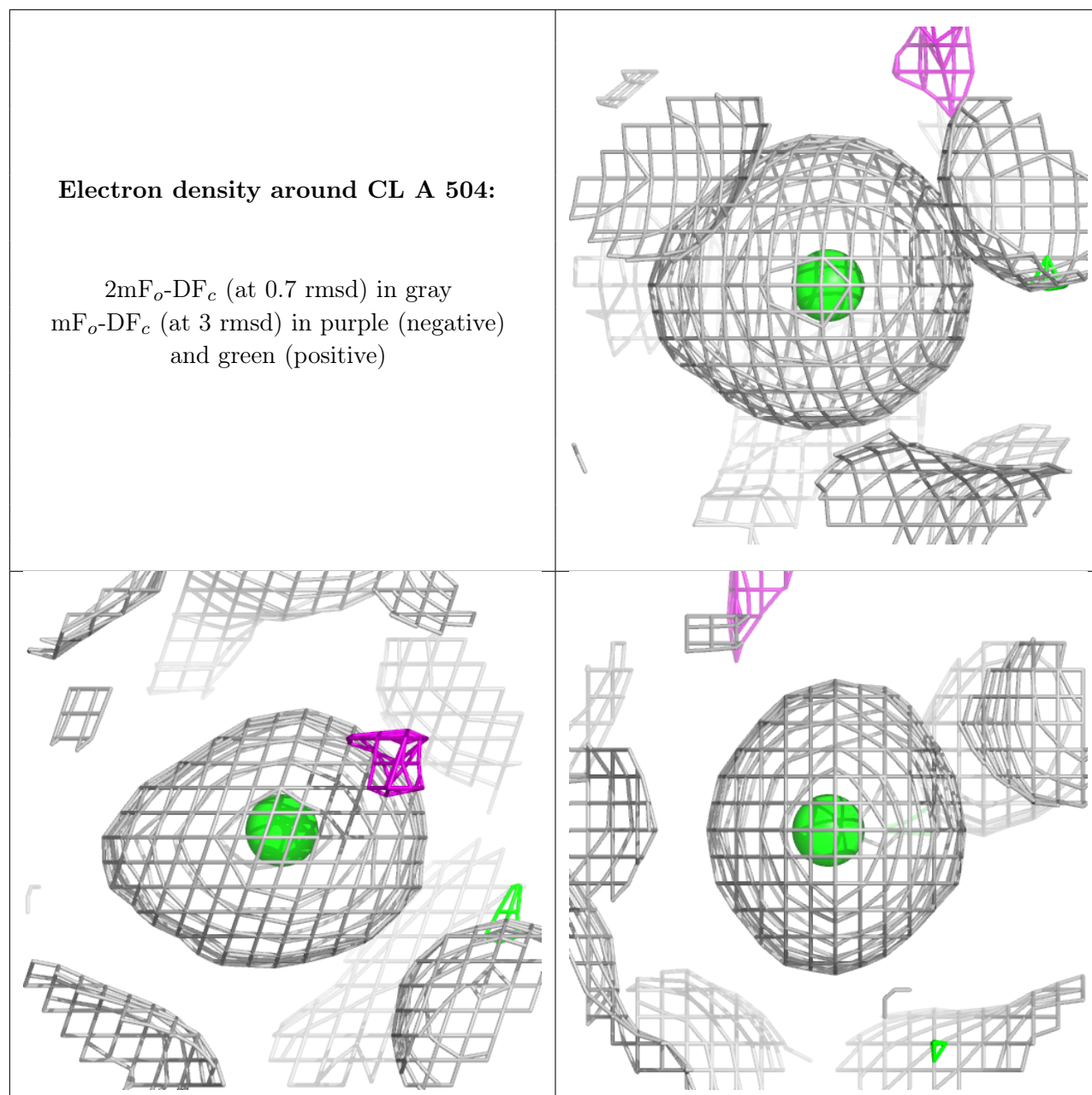
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ACT A 502:

$2mF_o-DF_c$ (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.