



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7LZ3 / pdb_00007lz3
Title : Computational design of constitutively active cGAS
Authors : Dowling, Q.; Volkman, H.E.; Gray, E.E.; Ovchinnikov, S.; Cambier, S.; Bera, A.K.; Bick, M.; Kang, A.; Stetson, D.B.; King, N.P.
Deposited on : 2021-03-08
Resolution : 2.18 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
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

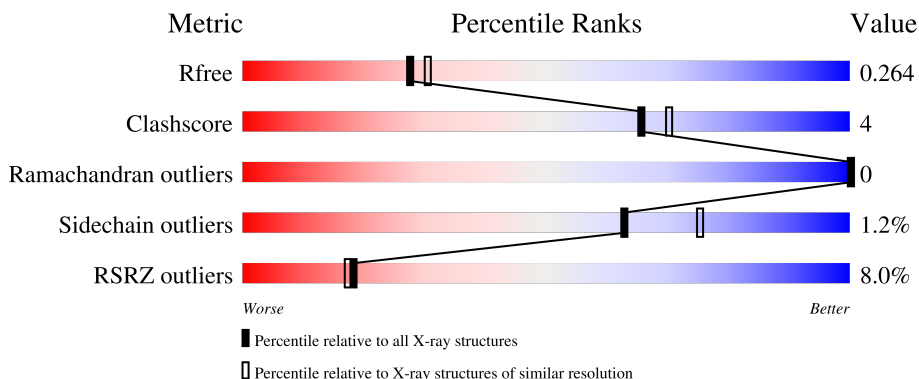
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	362	4% 90% 9%
1	B	362	12% 81% 13% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6011 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.

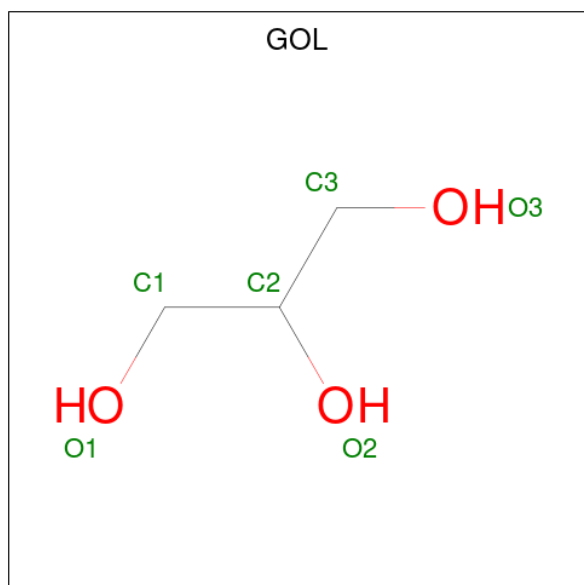
- Molecule 1 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	2	0
			2969	1912	500	542	15			
1	B	339	Total	C	N	O	S	0	0	0
			2815	1820	474	506	15			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

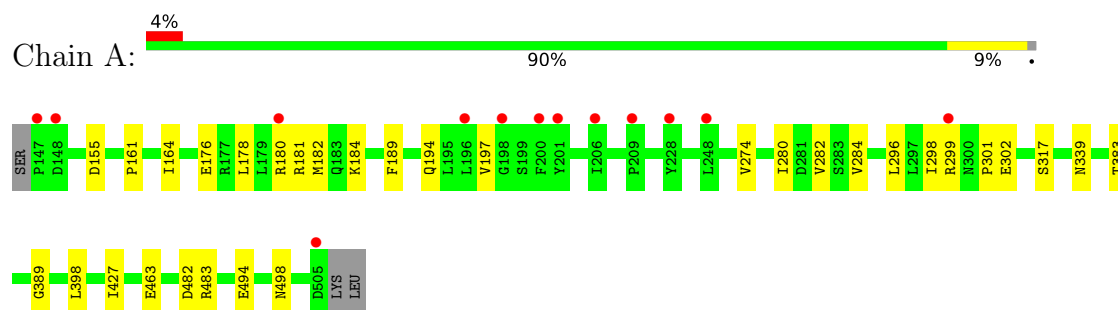
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	94	Total	O	0	0
			94	94		

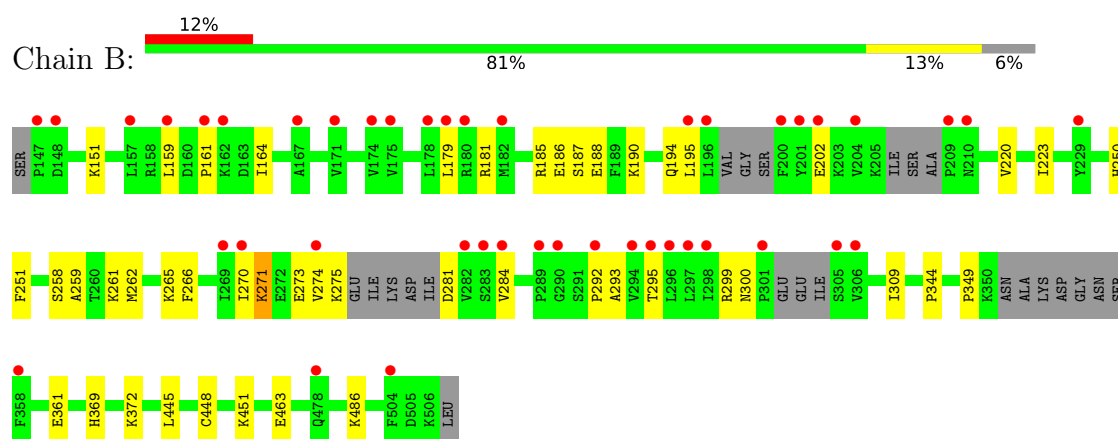
3 Residue-property plots

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: Cyclic GMP-AMP synthase



• Molecule 1: Cyclic GMP-AMP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.24Å 106.36Å 75.67Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	47.23 – 2.18 47.23 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.23-2.18) 99.8 (47.23-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.18Å)	Xtriage
Refinement program	PHENIX dev_3500	Depositor
R, R_{free}	0.211 , 0.265 0.211 , 0.264	Depositor DCC
R_{free} test set	1910 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6011	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: GOL, ZN

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	0.10	0/3040	0.28	0/4083
1	B	0.10	0/2875	0.28	0/3852
All	All	0.10	0/5915	0.28	0/7935

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

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	2969	0	3018	17	0
1	B	2815	0	2861	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	16	1	0
3	B	6	0	8	0	0
4	A	113	0	0	0	0
4	B	94	0	0	0	0
All	All	6011	0	5903	45	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 (45) 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:B:186:GLU:HA	1:B:190:LYS:HE2	1.70	0.73
1:B:258:SER:HA	1:B:361:GLU:HG3	1.74	0.69
1:B:259:ALA:HB1	1:B:349:PRO:HB3	1.74	0.68
1:B:179:LEU:HD11	1:B:194:GLN:HG3	1.81	0.63
1:A:339:ASN:HB3	3:A:603:GOL:H2	1.84	0.60
1:A:494:GLU:O	1:A:498:ASN:ND2	2.36	0.58
1:B:202:GLU:N	1:B:202:GLU:OE2	2.38	0.56
1:A:463:GLU:OE2	1:A:483:ARG:HG2	2.05	0.56
1:A:274:VAL:HG21	1:A:284:VAL:HG23	1.88	0.55
1:B:195:LEU:HD21	1:B:369:HIS:HB3	1.89	0.54
1:B:151:LYS:HG2	1:B:445:LEU:HD13	1.89	0.53
1:B:274:VAL:HG12	1:B:275:LYS:HD2	1.90	0.53
1:A:178:LEU:O	1:A:182:MET:HG2	2.09	0.51
1:B:292:PRO:HB3	1:B:349:PRO:O	2.10	0.51
1:A:194:GLN:HB3	1:A:197:VAL:HG22	1.92	0.51
1:B:293:ALA:HB2	1:B:309:ILE:HG12	1.94	0.50
1:A:182:MET:HE3	1:A:189:PHE:HB2	1.94	0.50
1:A:181:ARG:HA	1:A:184:LYS:HE3	1.95	0.49
1:B:344:PRO:O	1:B:369:HIS:NE2	2.45	0.49
1:B:159:LEU:HD11	1:B:164:ILE:HD12	1.95	0.48
1:B:181:ARG:HB3	1:B:273:GLU:OE2	2.14	0.47
1:A:282:VAL:HG22	1:A:298:ILE:HG12	1.97	0.47
1:B:188:GLU:HG2	1:B:250:HIS:CE1	2.50	0.47
1:B:188:GLU:H	1:B:188:GLU:CD	2.23	0.46
1:B:220:VAL:HB	1:B:223:ILE:HG23	1.97	0.46
1:B:161:PRO:HA	1:B:164:ILE:HG22	1.98	0.45
1:B:187:SER:O	1:B:190:LYS:HG3	2.16	0.45
1:A:176:GLU:O	1:A:180[B]:ARG:HG2	2.18	0.44
1:B:271:LYS:HE2	1:B:284:VAL:HG11	1.99	0.44
1:B:251:PHE:CD1	1:B:262:MET:HG2	2.53	0.44
1:B:463:GLU:HG2	1:B:486:LYS:HD3	1.99	0.44
1:A:299:ARG:HG2	1:A:301:PRO:O	2.18	0.43
1:B:202:GLU:HG2	1:B:372:LYS:HE3	2.00	0.43
1:A:161:PRO:HA	1:A:164:ILE:HG22	2.00	0.43
1:B:270:ILE:O	1:B:274:VAL:HG23	2.19	0.43
1:B:281:ASP:OD2	1:B:300:ASN:HA	2.19	0.42
1:B:266:PHE:O	1:B:270:ILE:HG12	2.19	0.42
1:A:398:LEU:HB2	1:A:427:ILE:HD13	2.01	0.42
1:B:185:ARG:NH1	1:B:187:SER:OG	2.53	0.41
1:B:448:CYS:HA	1:B:451:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:PHE:CZ	1:B:265:LYS:HD2	2.55	0.41
1:A:482:ASP:OD1	1:A:483:ARG:N	2.54	0.41
1:A:383:THR:O	1:A:389:GLY:HA3	2.21	0.40
1:A:161:PRO:HB3	1:B:161:PRO:HB3	2.03	0.40
1:A:178:LEU:HD11	1:A:296:LEU:HD11	2.03	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	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
1	B	327/362 (90%)	312 (95%)	15 (5%)	0	100	100
All	All	686/724 (95%)	660 (96%)	26 (4%)	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	334/335 (100%)	330 (99%)	4 (1%)	63	75
1	B	316/335 (94%)	312 (99%)	4 (1%)	61	74
All	All	650/670 (97%)	642 (99%)	8 (1%)	63	75

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

Mol	Chain	Res	Type
1	A	155	ASP
1	A	280	ILE
1	A	302	GLU
1	A	317	SER
1	B	261	LYS
1	B	271	LYS
1	B	295	THR
1	B	299	ARG

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	351	ASN
1	A	407	GLN
1	A	444	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](#)

Of 5 ligands modelled in this entry, 2 are 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
3	GOL	B	602	-	5,5,5	0.56	0	5,5,5	0.33	0
3	GOL	A	602	-	5,5,5	0.58	0	5,5,5	0.28	0
3	GOL	A	603	-	5,5,5	0.55	0	5,5,5	0.27	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
3	GOL	B	602	-	-	3/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-O2
3	A	603	GOL	O2-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	GOL	1	0

5.7 Other polymers ⓘ

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	359/362 (99%)	0.40	13 (3%) 46 45	18, 46, 73, 88	9 (2%)
1	B	339/362 (93%)	0.74	43 (12%) 8 7	27, 49, 86, 99	19 (5%)
All	All	698/724 (96%)	0.56	56 (8%) 18 17	18, 47, 82, 99	28 (4%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	LEU	6.1
1	B	297	LEU	6.0
1	B	201	TYR	5.8
1	A	209	PRO	5.1
1	B	147	PRO	5.1
1	B	282	VAL	4.2
1	B	200	PHE	4.2
1	B	202	GLU	3.9
1	B	301	PRO	3.8
1	B	196	LEU	3.8
1	A	200	PHE	3.7
1	B	292	PRO	3.6
1	B	358	PHE	3.6
1	A	147	PRO	3.6
1	B	269	ILE	3.4
1	B	204	VAL	3.4
1	B	209	PRO	3.4
1	B	294	VAL	3.3
1	B	229	TYR	3.2
1	B	270	ILE	3.1
1	B	274	VAL	3.1
1	B	178	LEU	3.0
1	A	206	ILE	2.9
1	B	283	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	284	VAL	2.9
1	A	198	GLY	2.9
1	B	195	LEU	2.8
1	A	196	LEU	2.8
1	B	298	ILE	2.8
1	B	296	LEU	2.7
1	B	148	ASP	2.7
1	A	148	ASP	2.7
1	A	299	ARG	2.7
1	A	505	ASP	2.6
1	B	157	LEU	2.6
1	B	289	PRO	2.5
1	B	174	VAL	2.5
1	B	175	VAL	2.4
1	B	167	ALA	2.4
1	A	248	LEU	2.3
1	B	171	VAL	2.3
1	B	295	THR	2.3
1	A	228	TYR	2.3
1	B	161	PRO	2.3
1	B	290	GLY	2.3
1	A	201	TYR	2.3
1	B	478	GLN	2.2
1	A	180[A]	ARG	2.2
1	B	162	LYS	2.2
1	B	306	VAL	2.2
1	B	180	ARG	2.1
1	B	305	SER	2.1
1	B	210	ASN	2.1
1	B	179	LEU	2.1
1	B	182	MET	2.1
1	B	504	PHE	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

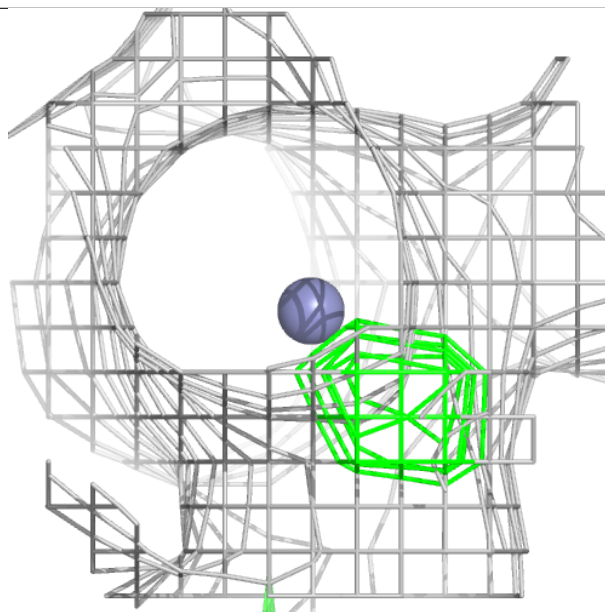
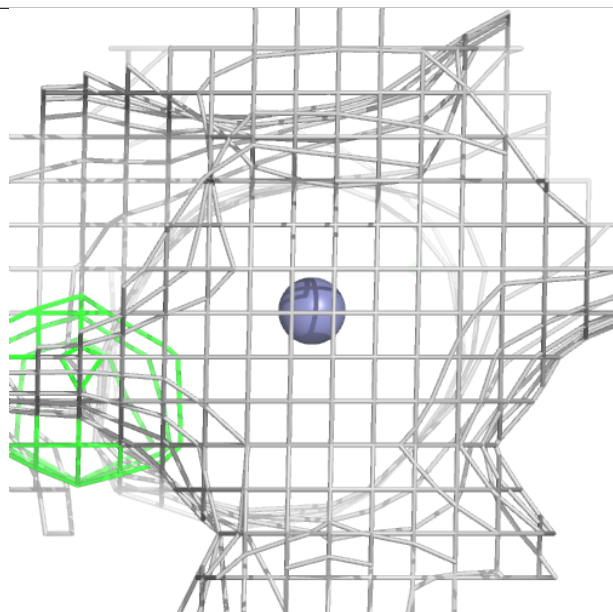
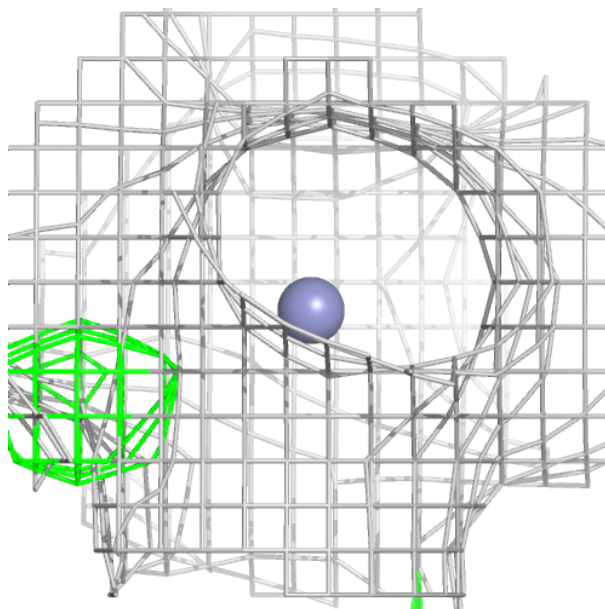
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	602	6/6	0.81	0.16	43,58,69,72	0
3	GOL	A	603	6/6	0.89	0.12	42,43,52,61	0
3	GOL	B	602	6/6	0.90	0.10	41,47,53,65	0
2	ZN	A	601	1/1	0.99	0.03	38,38,38,38	0
2	ZN	B	601	1/1	1.00	0.03	40,40,40,40	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.

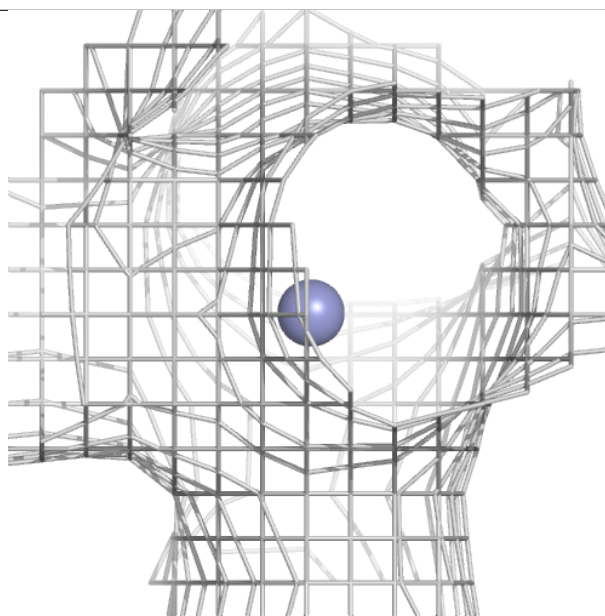
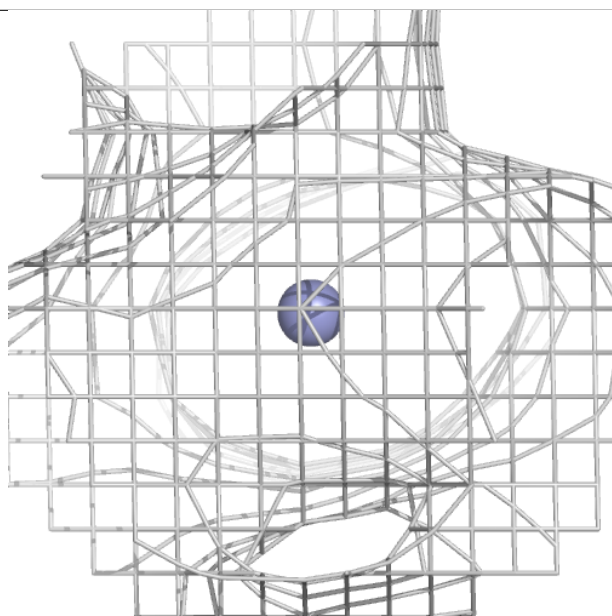
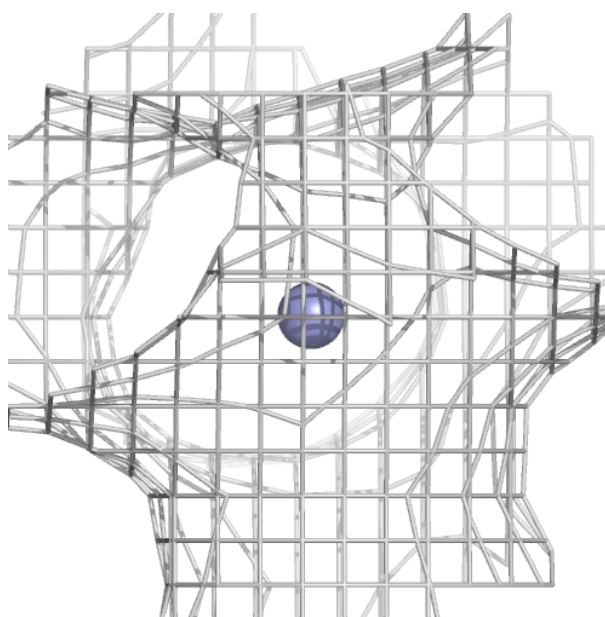
Electron density around ZN A 601:

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



Electron density around ZN B 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 ⓘ

There are no such residues in this entry.