



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2022 – 06:07 PM EDT

PDB ID : 7TL7  
Title : 1.90Å resolution structure of independent phosphoglycerate mutase from *C. elegans* in complex with a macrocyclic peptide inhibitor (Sa-D2)  
Authors : Liu, L.; Lovell, S.; Battaile, K.P.; Dranchak, P.; Queme, B.; Aitha, M.; van Neer, R.H.P.; Kimura, H.; Katho, T.; Suga, H.; Inglese, J.  
Deposited on : 2022-01-18  
Resolution : 1.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

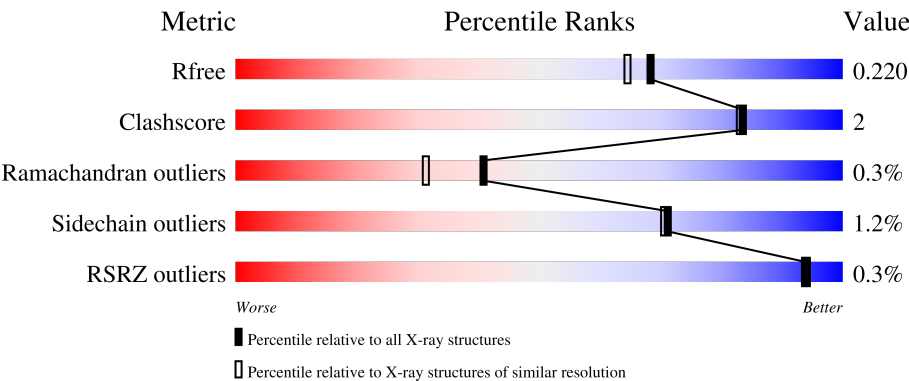
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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 <sub>free</sub>	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	534	<div><div></div><div>93%6%.</div></div>
1	B	534	<div><div>%</div><div>90%8%.</div></div>
1	C	534	<div><div></div><div>91%6%..</div></div>
1	D	534	<div><div></div><div>91%7%.</div></div>
2	a	15	<div><div></div><div>80%20%</div></div>

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Mol	Chain	Length	Quality of chain
2	b	15	 87%13%
2	c	15	 80%20%
2	d	15	 87%13%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17471 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 2,3-bisphosphoglycerate-independent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	1	0
			4039	2551	700	759	29			
1	B	526	Total	C	N	O	S	0	2	0
			3994	2525	688	752	29			
1	C	522	Total	C	N	O	S	0	2	0
			3977	2513	684	750	30			
1	D	521	Total	C	N	O	S	0	1	0
			3917	2482	675	731	29			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	LYS	-	expression tag	UNP G5EFZ1
A	541	LEU	-	expression tag	UNP G5EFZ1
A	542	ALA	-	expression tag	UNP G5EFZ1
A	543	ALA	-	expression tag	UNP G5EFZ1
A	544	ALA	-	expression tag	UNP G5EFZ1
A	545	LEU	-	expression tag	UNP G5EFZ1
A	546	GLU	-	expression tag	UNP G5EFZ1
A	547	HIS	-	expression tag	UNP G5EFZ1
A	548	HIS	-	expression tag	UNP G5EFZ1
A	549	HIS	-	expression tag	UNP G5EFZ1
A	550	HIS	-	expression tag	UNP G5EFZ1
A	551	HIS	-	expression tag	UNP G5EFZ1
A	552	HIS	-	expression tag	UNP G5EFZ1
B	540	LYS	-	expression tag	UNP G5EFZ1
B	541	LEU	-	expression tag	UNP G5EFZ1
B	542	ALA	-	expression tag	UNP G5EFZ1
B	543	ALA	-	expression tag	UNP G5EFZ1
B	544	ALA	-	expression tag	UNP G5EFZ1
B	545	LEU	-	expression tag	UNP G5EFZ1
B	546	GLU	-	expression tag	UNP G5EFZ1
B	547	HIS	-	expression tag	UNP G5EFZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	548	HIS	-	expression tag	UNP G5EFZ1
B	549	HIS	-	expression tag	UNP G5EFZ1
B	550	HIS	-	expression tag	UNP G5EFZ1
B	551	HIS	-	expression tag	UNP G5EFZ1
B	552	HIS	-	expression tag	UNP G5EFZ1
C	540	LYS	-	expression tag	UNP G5EFZ1
C	541	LEU	-	expression tag	UNP G5EFZ1
C	542	ALA	-	expression tag	UNP G5EFZ1
C	543	ALA	-	expression tag	UNP G5EFZ1
C	544	ALA	-	expression tag	UNP G5EFZ1
C	545	LEU	-	expression tag	UNP G5EFZ1
C	546	GLU	-	expression tag	UNP G5EFZ1
C	547	HIS	-	expression tag	UNP G5EFZ1
C	548	HIS	-	expression tag	UNP G5EFZ1
C	549	HIS	-	expression tag	UNP G5EFZ1
C	550	HIS	-	expression tag	UNP G5EFZ1
C	551	HIS	-	expression tag	UNP G5EFZ1
C	552	HIS	-	expression tag	UNP G5EFZ1
D	540	LYS	-	expression tag	UNP G5EFZ1
D	541	LEU	-	expression tag	UNP G5EFZ1
D	542	ALA	-	expression tag	UNP G5EFZ1
D	543	ALA	-	expression tag	UNP G5EFZ1
D	544	ALA	-	expression tag	UNP G5EFZ1
D	545	LEU	-	expression tag	UNP G5EFZ1
D	546	GLU	-	expression tag	UNP G5EFZ1
D	547	HIS	-	expression tag	UNP G5EFZ1
D	548	HIS	-	expression tag	UNP G5EFZ1
D	549	HIS	-	expression tag	UNP G5EFZ1
D	550	HIS	-	expression tag	UNP G5EFZ1
D	551	HIS	-	expression tag	UNP G5EFZ1
D	552	HIS	-	expression tag	UNP G5EFZ1

- Molecule 2 is a protein called peptide Sa-D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	15	Total	C	N	O	S	0	0	1
			127	86	16	23	2			
2	b	15	Total	C	N	O	S	0	0	1
			127	86	16	23	2			
2	c	15	Total	C	N	O	S	0	0	1
			123	83	15	23	2			
2	d	15	Total	C	N	O	S	0	0	1
			124	84	15	23	2			

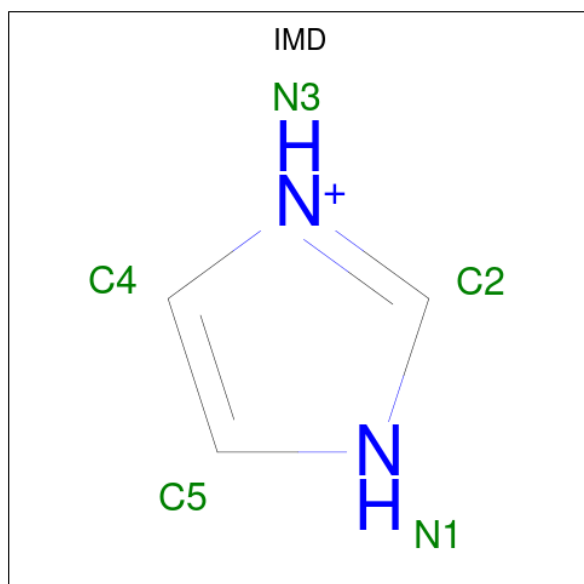
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0

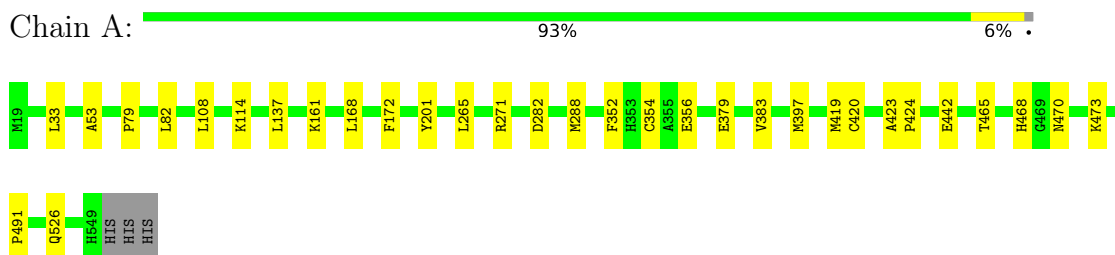
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	273	Total O 273 273	0	0
6	B	253	Total O 253 253	0	0
6	C	269	Total O 269 269	0	0
6	D	174	Total O 174 174	0	0
6	a	13	Total O 13 13	0	0
6	b	14	Total O 14 14	0	0
6	c	14	Total O 14 14	0	0
6	d	11	Total O 11 11	0	0

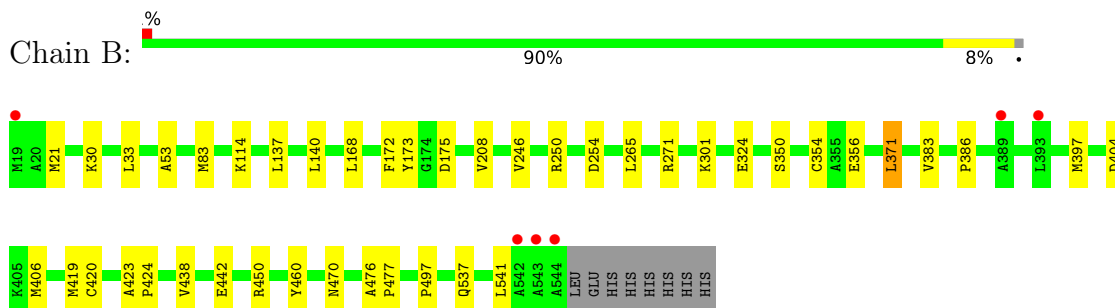
### 3 Residue-property plots

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.

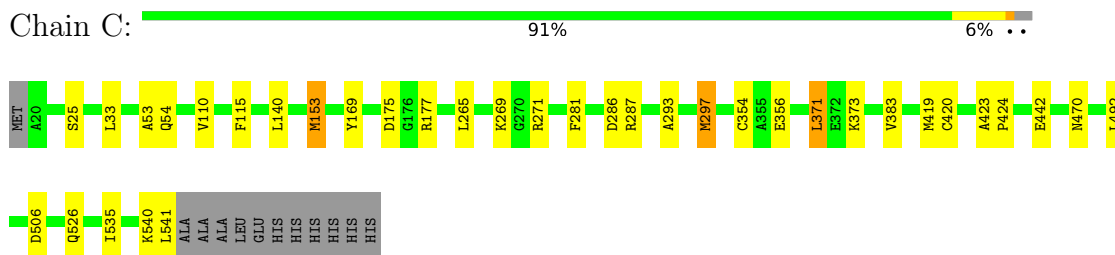
- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase



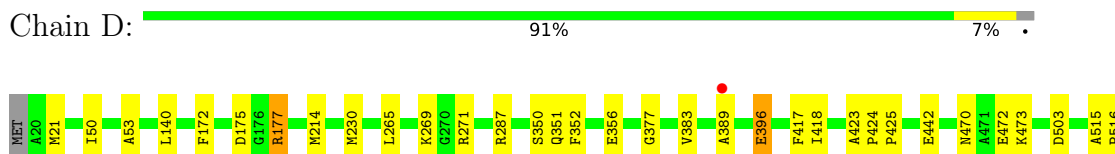
- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase



- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase



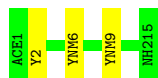
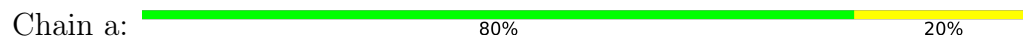
- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase







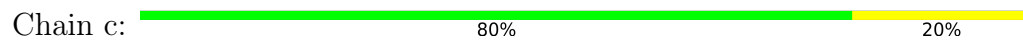
- Molecule 2: peptide Sa-D2



- Molecule 2: peptide Sa-D2



- Molecule 2: peptide Sa-D2



- Molecule 2: peptide Sa-D2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.00Å 87.62Å 151.34Å 90.00° 97.13° 90.00°	Depositor
Resolution (Å)	39.84 – 1.90 48.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.84-1.90) 99.7 (48.12-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.20rc2_4402	Depositor
R, $R_{free}$	0.171 , 0.216 0.177 , 0.220	Depositor DCC
$R_{free}$ test set	7975 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtrriage
Anisotropy	0.326	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9809e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DTY, IMD, ZN, ACE, NA, YNM, NH2

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	0.28	0/4133	0.54	0/5608
1	B	0.28	0/4086	0.55	0/5546
1	C	0.29	0/4072	0.55	0/5524
1	D	0.28	0/4009	0.53	0/5445
2	a	0.30	0/85	0.46	0/109
2	b	0.33	0/85	0.47	0/109
2	c	0.29	0/81	0.54	0/105
2	d	0.28	0/82	0.46	0/106
All	All	0.29	0/16633	0.54	0/22552

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	4039	0	3893	16	0
1	B	3994	0	3838	21	0
1	C	3977	0	3833	18	0
1	D	3917	0	3747	18	0
2	a	127	0	107	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	127	0	106	0	0
2	c	123	0	95	0	1
2	d	124	0	97	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	5	0	5	3	0
5	D	5	0	5	1	0
6	A	273	0	0	0	0
6	B	253	0	0	1	0
6	C	269	0	0	1	0
6	D	174	0	0	2	0
6	a	13	0	0	0	0
6	b	14	0	0	0	0
6	c	14	0	0	0	0
6	d	11	0	0	0	0
All	All	17471	0	15726	73	1

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 (73) 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:D:214:MET:HB3	1:D:287:ARG:HB3	1.72	0.72
1:D:50:ILE:HD12	1:D:472:GLU:HB3	1.85	0.58
1:A:265:LEU:O	1:A:271:ARG:NH2	2.36	0.58
1:B:324:GLU:OE1	1:B:324:GLU:N	2.37	0.56
1:C:53:ALA:HB1	1:C:442:GLU:HG3	1.86	0.56
1:A:282:ASP:HB2	1:A:288:MET:SD	2.47	0.55
5:C:601:IMD:H2	6:C:874:HOH:O	2.09	0.53
1:D:265:LEU:O	1:D:271:ARG:NH2	2.42	0.52
1:A:53:ALA:HB1	1:A:442:GLU:HG3	1.92	0.52
1:C:356:GLU:HA	1:C:383:VAL:O	2.10	0.51
1:B:21:MET:HG3	1:B:350:SER:HB3	1.91	0.51
1:B:265:LEU:O	1:B:271:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ALA:N	1:C:424:PRO:CD	2.74	0.51
1:D:423:ALA:N	1:D:424:PRO:CD	2.74	0.51
1:B:371:LEU:HD21	6:B:873:HOH:O	2.10	0.50
1:B:404:ASP:OD1	1:B:450:ARG:NH2	2.32	0.50
1:C:265:LEU:O	1:C:271:ARG:NH2	2.45	0.49
1:B:137:LEU:HG	1:B:168:LEU:HD11	1.93	0.49
1:A:397:MET:HB2	1:A:424:PRO:HG3	1.94	0.49
1:B:423:ALA:N	1:B:424:PRO:CD	2.75	0.49
5:D:601:IMD:H2	6:D:828:HOH:O	2.11	0.49
1:A:356:GLU:HA	1:A:383:VAL:O	2.13	0.48
1:A:137:LEU:HG	1:A:168:LEU:HD11	1.96	0.48
1:A:423:ALA:N	1:A:424:PRO:CD	2.76	0.48
1:D:396:GLU:H	1:D:396:GLU:CD	2.17	0.48
1:B:386:PRO:HG3	1:B:397:MET:HA	1.94	0.47
1:D:21:MET:SD	1:D:377:GLY:HA3	2.55	0.47
1:B:497:PRO:HG2	1:B:541:LEU:HD12	1.96	0.47
1:C:140:LEU:HD11	1:C:175:ASP:HA	1.97	0.47
1:B:114:LYS:NZ	1:D:503:ASP:OD2	2.36	0.47
1:A:526:GLN:O	5:C:601:IMD:H5	2.15	0.47
1:A:108:LEU:HD13	1:C:506:ASP:HA	1.96	0.46
1:D:527:PRO:HG2	1:D:530:MET:HG3	1.97	0.46
1:D:518:VAL:O	1:D:522:MET:HG3	2.16	0.46
1:B:53:ALA:HB1	1:B:442:GLU:HG3	1.98	0.46
1:D:356:GLU:HA	1:D:383:VAL:O	2.16	0.45
1:A:79:PRO:HG2	1:A:82:LEU:HD22	1.98	0.45
1:C:540:LYS:O	1:C:541:LEU:CB	2.64	0.45
1:B:406:MET:SD	1:B:420:CYS:HB3	2.57	0.45
1:D:177:ARG:NH1	6:D:709:HOH:O	2.50	0.45
1:B:354:CYS:O	1:B:420:CYS:HA	2.18	0.44
1:B:140:LEU:HD11	1:B:175:ASP:HA	1.99	0.44
1:C:354:CYS:O	1:C:420:CYS:HA	2.18	0.44
1:D:21:MET:HG3	1:D:350:SER:HB3	1.99	0.44
1:B:356:GLU:HA	1:B:383:VAL:O	2.17	0.43
1:D:515:ALA:HB3	1:D:516:PRO:HD3	2.00	0.43
1:B:173:TYR:HA	1:B:208:VAL:O	2.19	0.43
1:C:169:TYR:OH	1:C:269:LYS:HG2	2.18	0.43
1:C:293:ALA:HA	1:C:297:MET:HG3	2.00	0.43
1:C:54:GLN:HG3	1:C:442:GLU:OE2	2.19	0.43
1:D:140:LEU:HD11	1:D:175:ASP:HA	2.00	0.43
1:A:465:THR:HA	1:A:491:PRO:O	2.19	0.42
1:B:476:ALA:HB1	1:B:477:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:PHE:HB3	1:D:418:ILE:HG22	2.01	0.42
1:C:110:VAL:HG22	1:C:115:PHE:CE2	2.54	0.42
1:A:114:LYS:HA	1:A:114:LYS:HE2	2.01	0.42
1:C:492:LEU:HD23	1:C:535:ILE:HD11	2.01	0.42
1:B:30:LYS:HE2	1:B:460:TYR:CZ	2.55	0.42
1:C:153[A]:MET:HG3	1:C:281:PHE:CE2	2.55	0.41
1:D:53:ALA:HB1	1:D:442:GLU:HG3	2.02	0.41
1:C:371:LEU:CD2	1:C:373:LYS:HB3	2.50	0.41
1:B:53:ALA:HB2	1:B:438:VAL:HG13	2.03	0.41
1:D:424:PRO:HB2	1:D:425:PRO:HD3	2.02	0.41
1:B:33:LEU:O	1:B:419:MET:HA	2.20	0.41
1:A:354:CYS:O	1:A:420:CYS:HA	2.20	0.41
1:B:246:VAL:O	1:B:250:ARG:HG2	2.20	0.41
1:C:33:LEU:O	1:C:419:MET:HA	2.20	0.41
1:C:286:ASP:OD1	1:C:287:ARG:N	2.54	0.41
1:D:351:GLN:HA	1:D:417:PHE:O	2.21	0.41
1:C:526:GLN:O	5:C:601:IMD:H4	2.21	0.40
1:A:33:LEU:O	1:A:419:MET:HA	2.21	0.40
1:A:161:LYS:HB2	1:A:201:TYR:CD2	2.57	0.40
1:A:352:PHE:HA	1:A:379:GLU:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:2:DTY:OH	2:c:5:GLU:OE1[2_655]	2.09	0.11

## 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	530/534 (99%)	520 (98%)	8 (2%)	2 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	526/534 (98%)	516 (98%)	9 (2%)	1 (0%)	47	38
1	C	522/534 (98%)	513 (98%)	8 (2%)	1 (0%)	47	38
1	D	520/534 (97%)	507 (98%)	11 (2%)	2 (0%)	34	24
2	a	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
2	b	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
2	c	10/15 (67%)	8 (80%)	2 (20%)	0	100	100
2	d	10/15 (67%)	8 (80%)	2 (20%)	0	100	100
All	All	2138/2196 (97%)	2090 (98%)	42 (2%)	6 (0%)	41	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	389	ALA
1	A	468	HIS
1	B	470	ASN
1	C	470	ASN
1	D	470	ASN
1	A	470	ASN

### 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	414/432 (96%)	412 (100%)	2 (0%)	88	89
1	B	406/432 (94%)	400 (98%)	6 (2%)	65	62
1	C	409/432 (95%)	403 (98%)	6 (2%)	65	62
1	D	393/432 (91%)	387 (98%)	6 (2%)	65	62
2	a	9/10 (90%)	9 (100%)	0	100	100
2	b	9/10 (90%)	9 (100%)	0	100	100
2	c	8/10 (80%)	8 (100%)	0	100	100
2	d	8/10 (80%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1656/1768 (94%)	1636 (99%)	20 (1%)	71 70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	PHE
1	A	473	LYS
1	B	83	MET
1	B	172	PHE
1	B	254	ASP
1	B	301	LYS
1	B	371	LEU
1	B	537	GLN
1	C	25	SER
1	C	153[A]	MET
1	C	153[B]	MET
1	C	177	ARG
1	C	297	MET
1	C	371	LEU
1	D	172	PHE
1	D	177	ARG
1	D	230	MET
1	D	269	LYS
1	D	396	GLU
1	D	473	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	508	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues are 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	YNM	c	9	2	12,13,14	0.57	0	15,16,18	1.26	2 (13%)
2	YNM	c	6	2	12,13,14	0.59	0	15,16,18	1.11	1 (6%)
2	DTY	d	2	2	11,12,13	0.37	0	12,15,17	0.32	0
2	YNM	d	9	2	12,13,14	0.60	0	15,16,18	1.20	3 (20%)
2	DTY	b	2	2	11,12,13	0.35	0	12,15,17	0.40	0
2	YNM	b	6	2	12,13,14	0.55	0	15,16,18	1.14	1 (6%)
2	YNM	a	6	2	12,13,14	0.59	0	15,16,18	1.15	2 (13%)
2	DTY	c	2	2	11,12,13	0.39	0	12,15,17	0.46	0
2	YNM	a	9	2	12,13,14	0.63	0	15,16,18	1.38	3 (20%)
2	YNM	b	9	2	12,13,14	0.62	0	15,16,18	1.08	2 (13%)
2	YNM	d	6	2	12,13,14	0.54	0	15,16,18	1.08	1 (6%)
2	DTY	a	2	2	11,12,13	0.39	0	12,15,17	0.48	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	YNM	c	9	2	-	0/5/8/10	0/1/1/1
2	YNM	c	6	2	-	0/5/8/10	0/1/1/1
2	DTY	d	2	2	-	0/5/6/8	0/1/1/1
2	YNM	d	9	2	-	0/5/8/10	0/1/1/1
2	DTY	b	2	2	-	0/5/6/8	0/1/1/1
2	YNM	b	6	2	-	0/5/8/10	0/1/1/1
2	YNM	a	6	2	-	0/5/8/10	0/1/1/1
2	DTY	c	2	2	-	0/5/6/8	0/1/1/1
2	YNM	a	9	2	-	0/5/8/10	0/1/1/1
2	YNM	b	9	2	-	0/5/8/10	0/1/1/1
2	YNM	d	6	2	-	0/5/8/10	0/1/1/1
2	DTY	a	2	2	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	9	YNM	CG-CB-CA	-3.26	108.97	113.63
2	a	9	YNM	CG-CB-CA	-2.98	109.37	113.63
2	c	6	YNM	CG-CB-CA	-2.39	110.20	113.63
2	a	9	YNM	CM-N-CA	2.39	121.09	113.64
2	d	9	YNM	CM-N-CA	2.39	121.08	113.64
2	d	9	YNM	CB-CA-C	-2.36	107.17	111.65
2	a	6	YNM	CM-N-CA	2.25	120.64	113.64
2	b	9	YNM	CM-N-CA	2.17	120.40	113.64
2	a	6	YNM	CG-CB-CA	-2.12	110.60	113.63
2	b	9	YNM	O-C-CA	-2.11	119.26	124.78
2	a	9	YNM	O-C-CA	-2.11	119.26	124.78
2	b	6	YNM	CM-N-CA	2.09	120.15	113.64
2	d	6	YNM	CG-CB-CA	-2.02	110.75	113.63
2	c	9	YNM	CM-N-CA	2.01	119.91	113.64
2	d	9	YNM	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	2	DTY	0	1

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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
5	IMD	C	601	-	3,5,5	0.42	0	4,5,5	0.60	0
5	IMD	D	601	-	3,5,5	0.40	0	4,5,5	0.60	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
5	IMD	C	601	-	-	-	0/1/1/1
5	IMD	D	601	-	-	-	0/1/1/1

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	IMD	3	0
5	D	601	IMD	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	531/534 (99%)	-0.43	0 100 100	17, 26, 40, 66	0
1	B	526/534 (98%)	-0.34	6 (1%) 80 82	17, 28, 48, 83	0
1	C	522/534 (97%)	-0.43	0 100 100	16, 26, 41, 54	0
1	D	521/534 (97%)	-0.31	1 (0%) 95 95	19, 32, 49, 76	0
2	a	10/15 (66%)	-0.50	0 100 100	21, 24, 38, 41	0
2	b	10/15 (66%)	-0.50	0 100 100	21, 26, 35, 36	0
2	c	10/15 (66%)	-0.58	0 100 100	25, 31, 40, 40	0
2	d	10/15 (66%)	-0.34	0 100 100	28, 32, 39, 40	0
All	All	2140/2196 (97%)	-0.38	7 (0%) 94 94	16, 28, 45, 83	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	ALA	4.3
1	B	543	ALA	3.1
1	B	393	LEU	2.9
1	D	389	ALA	2.8
1	B	544	ALA	2.4
1	B	19	MET	2.2
1	B	389	ALA	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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	DTY	c	2	12/13	0.92	0.17	31,59,73,77	0
2	DTY	d	2	12/13	0.93	0.10	28,38,45,54	0
2	YNM	c	9	13/14	0.93	0.10	26,32,39,41	0
2	YNM	c	6	13/14	0.94	0.11	25,33,43,45	0
2	DTY	a	2	12/13	0.94	0.13	24,37,50,57	0
2	YNM	a	6	13/14	0.96	0.08	21,23,32,32	0
2	YNM	d	6	13/14	0.96	0.10	23,31,39,41	0
2	YNM	b	9	13/14	0.96	0.09	20,26,31,36	0
2	YNM	b	6	13/14	0.96	0.10	22,26,34,36	0
2	YNM	d	9	13/14	0.96	0.08	28,33,38,40	0
2	YNM	a	9	13/14	0.97	0.07	21,24,33,40	0
2	DTY	b	2	12/13	0.97	0.08	19,30,39,46	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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.

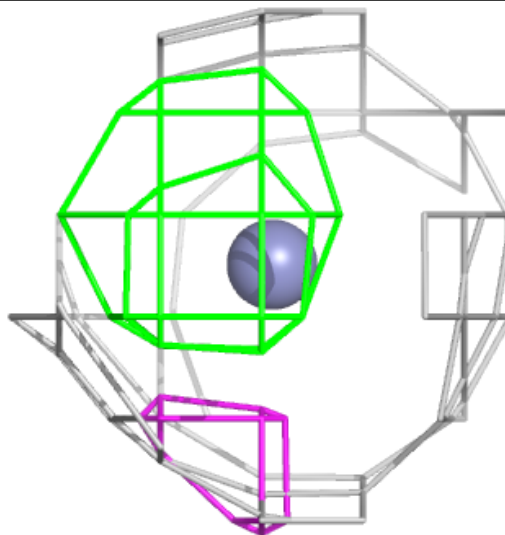
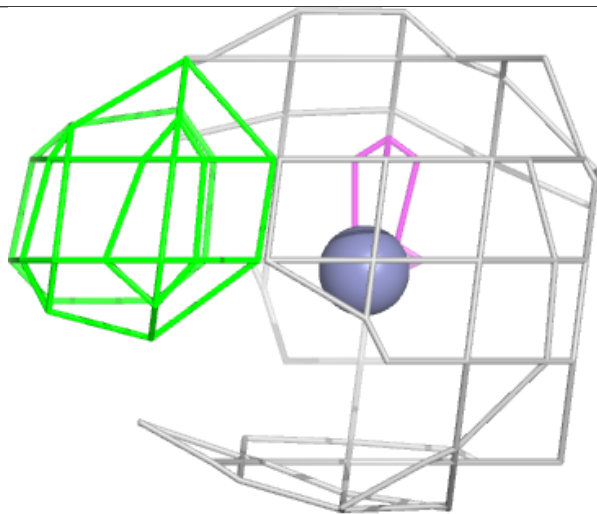
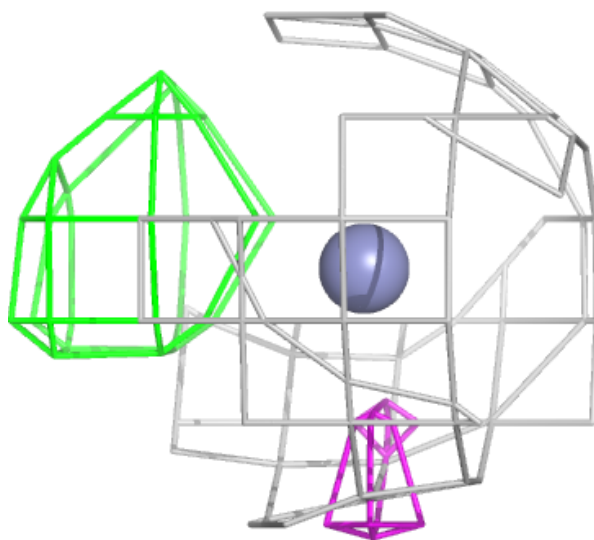
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	B	603	1/1	0.82	0.14	44,44,44,44	0
4	NA	D	604	1/1	0.89	0.08	48,48,48,48	0
4	NA	A	603	1/1	0.94	0.06	28,28,28,28	0
5	IMD	C	601	5/5	0.96	0.09	18,18,22,23	0
5	IMD	D	601	5/5	0.96	0.10	19,20,22,24	0
4	NA	C	604	1/1	0.98	0.04	27,27,27,27	0
3	ZN	B	601	1/1	0.99	0.07	28,28,28,28	0
3	ZN	B	602	1/1	0.99	0.06	34,34,34,34	0
3	ZN	D	602	1/1	0.99	0.06	27,27,27,27	0
3	ZN	C	602	1/1	1.00	0.07	19,19,19,19	0
3	ZN	C	603	1/1	1.00	0.04	25,25,25,25	0
3	ZN	A	601	1/1	1.00	0.08	23,23,23,23	0
3	ZN	D	603	1/1	1.00	0.03	32,32,32,32	0
3	ZN	A	602	1/1	1.00	0.02	28,28,28,28	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.

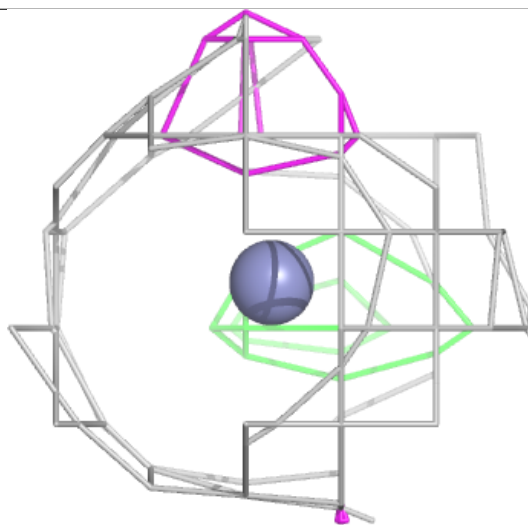
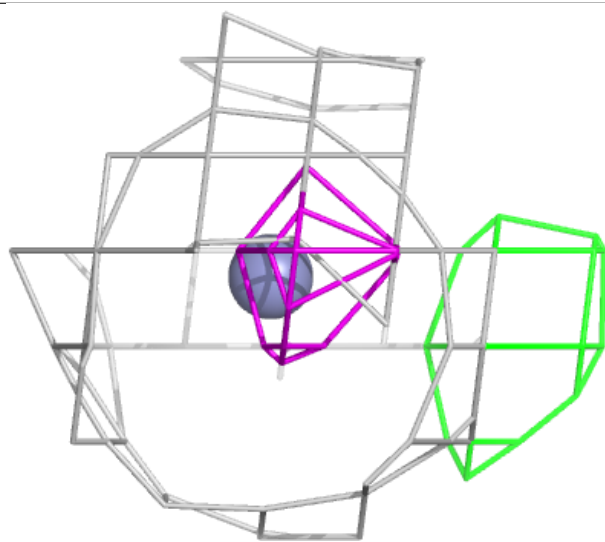
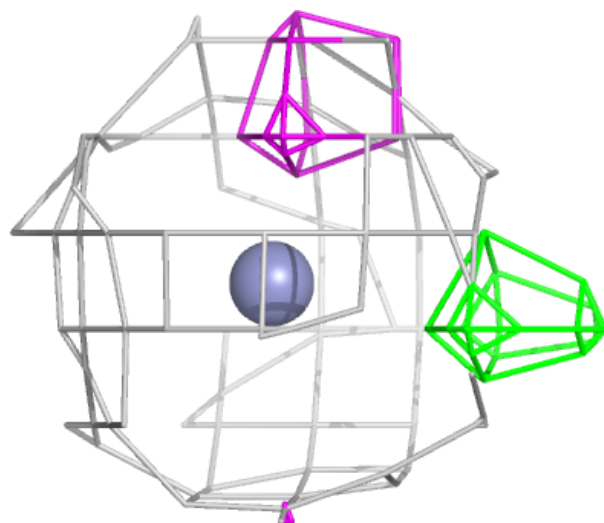
**Electron density around ZN B 601:**

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



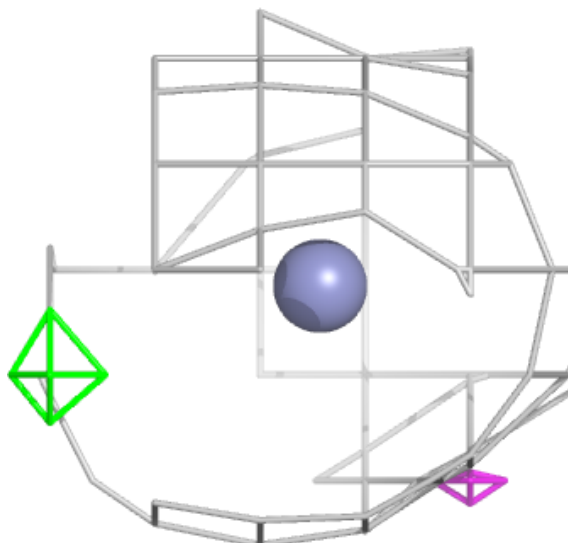
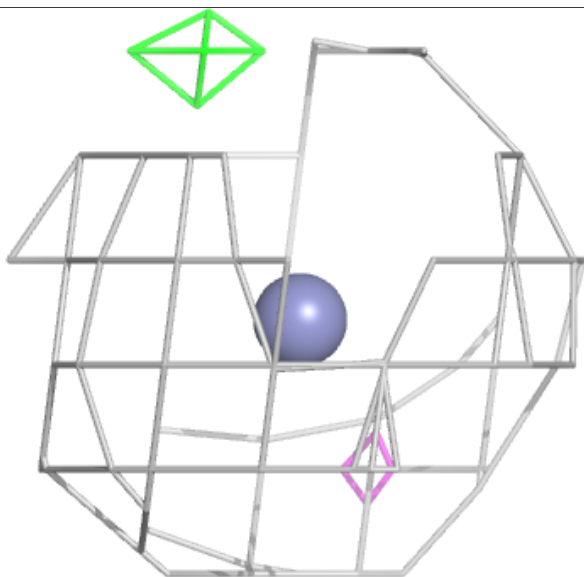
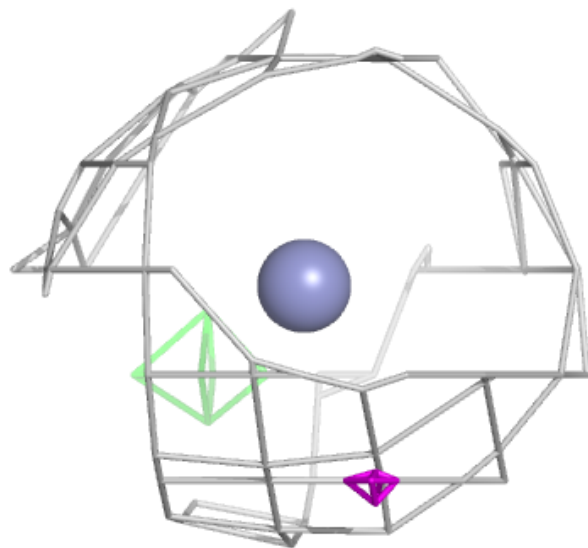
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and green (positive)



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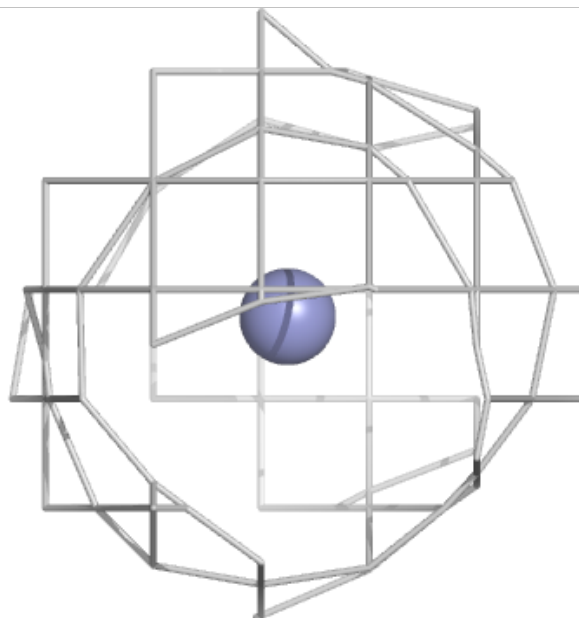
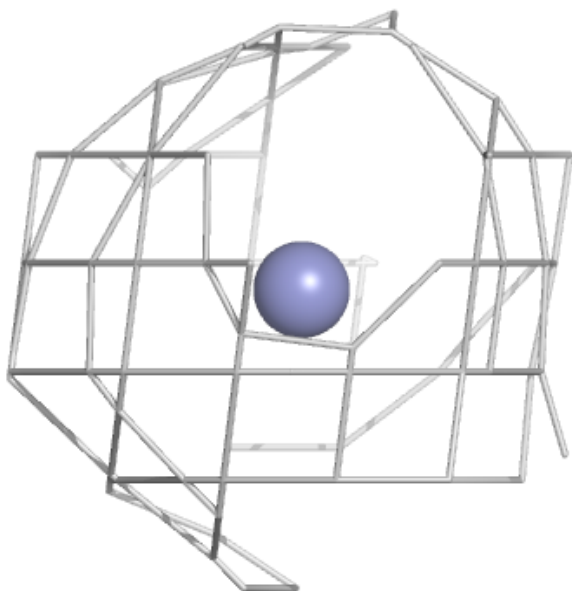
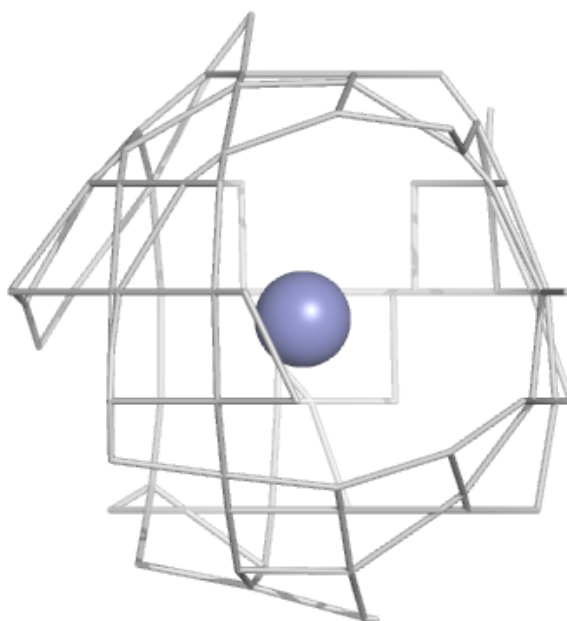
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and green (positive)





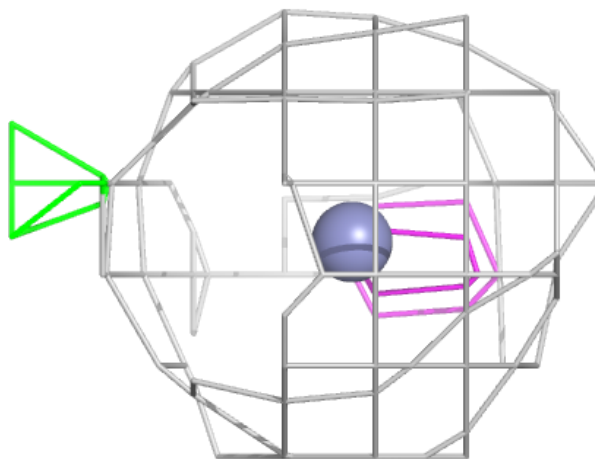
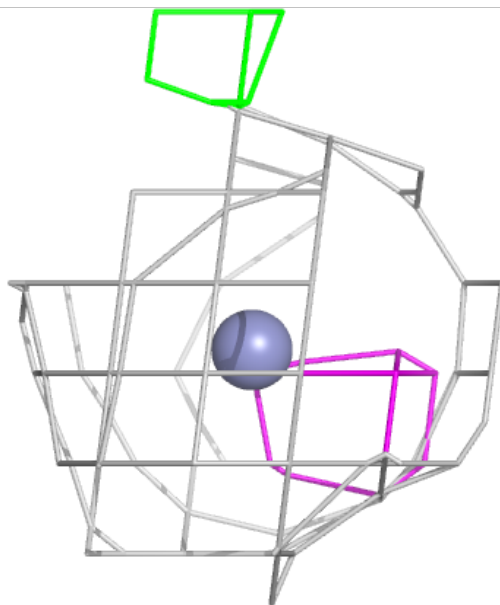
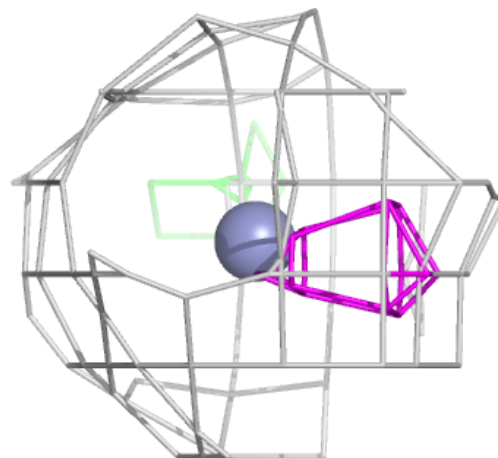
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and green (positive)



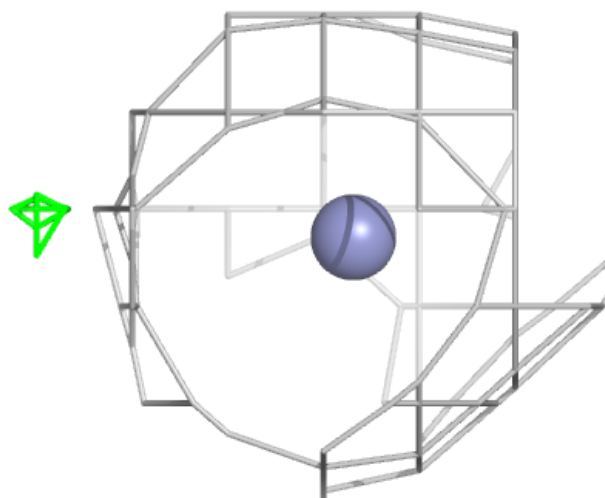
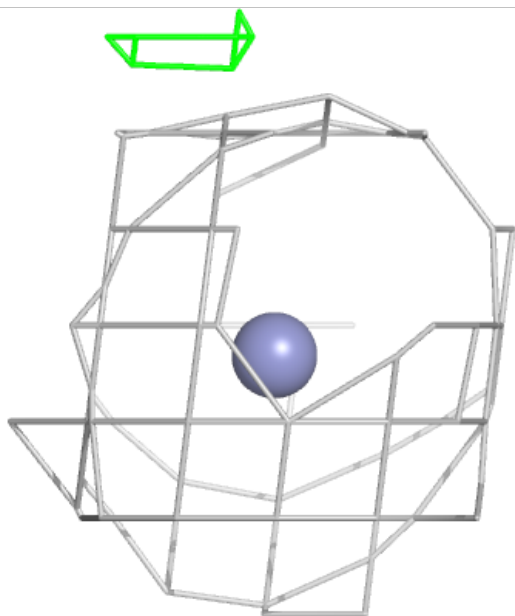
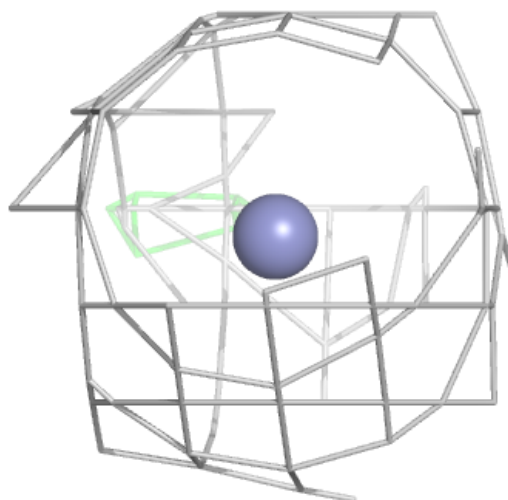
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and green (positive)



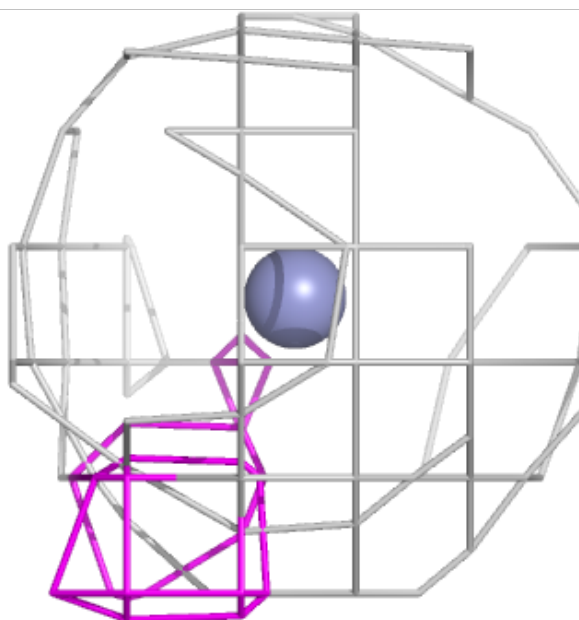
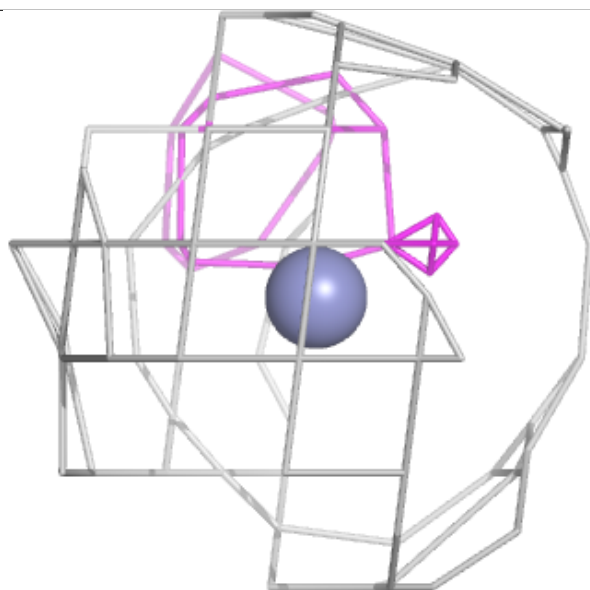
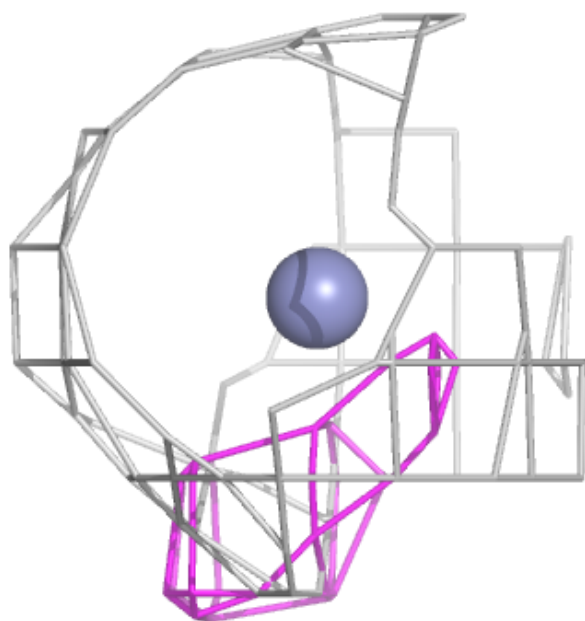
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



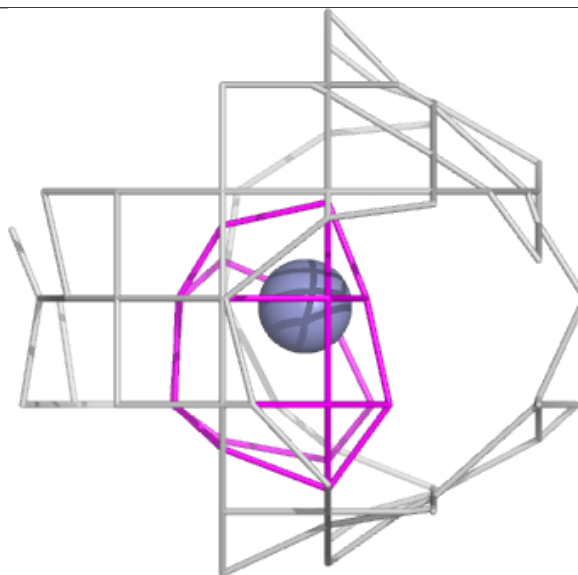
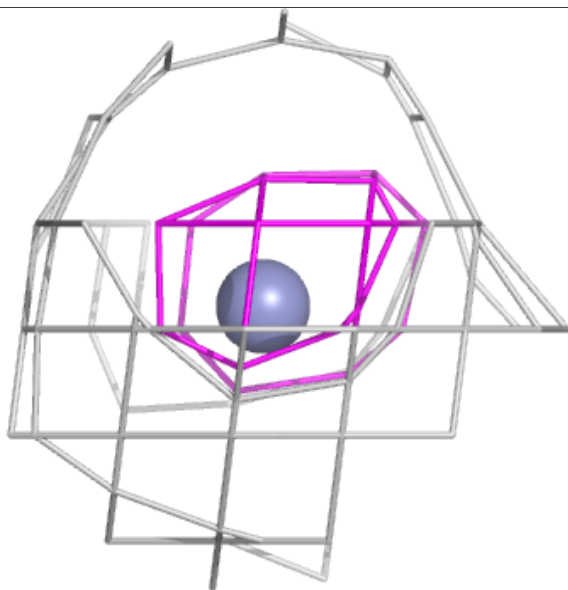
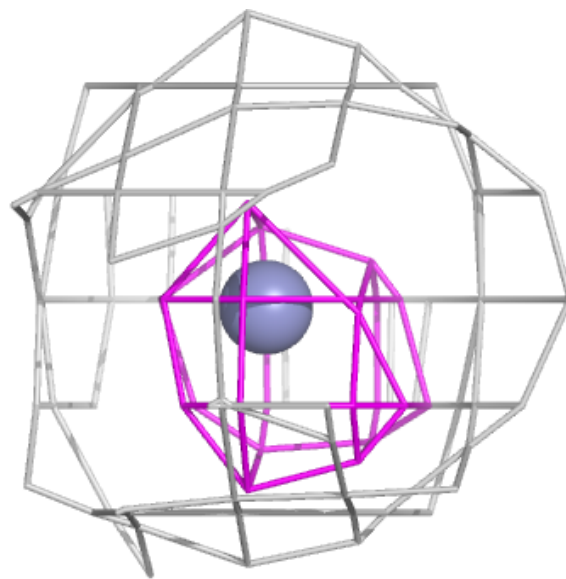
**Electron density around ZN D 603:**

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



**Electron density around ZN A 602:**

$2mF_o-DF_c$  (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.