



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 11:03 pm GMT

PDB ID : 8ORI
Title : Crystal structure of Rhizobium etli L-asparaginase ReAIV (orthorhombic)
Authors : Loch, J.I.; Worsztynowicz, P.; Sliwiak, J.; Imiolczyk, B.; Grzechowiak, M.;
Gilski, M.; Jaskolski, M.
Deposited on : 2023-04-14
Resolution : 1.35 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

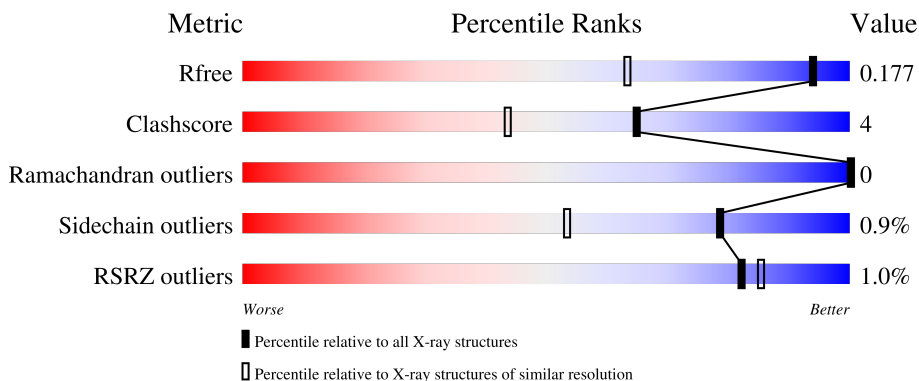
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

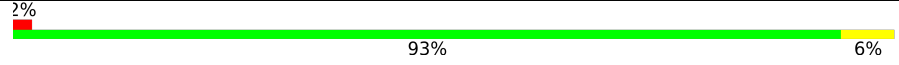
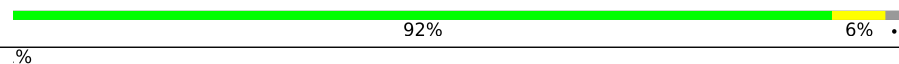
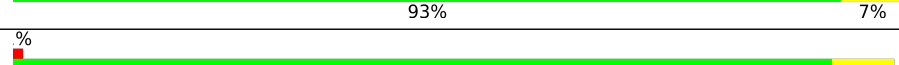

The reported resolution of this entry is 1.35 Å.

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}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	341	 2% 93% 6%
1	B	341	 92% 6%
1	C	341	 1% 93% 7%
1	D	341	 1% 92% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	702	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 12486 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 Putative L-asparaginase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2677	1660	483	503	31	0	21	0
1	B	335	2612	1617	472	494	29	0	18	0
1	C	340	2680	1660	485	506	29	0	22	0
1	D	341	2683	1665	480	509	29	0	21	0

There are 24 discrepancies between the modelled and reference sequences:

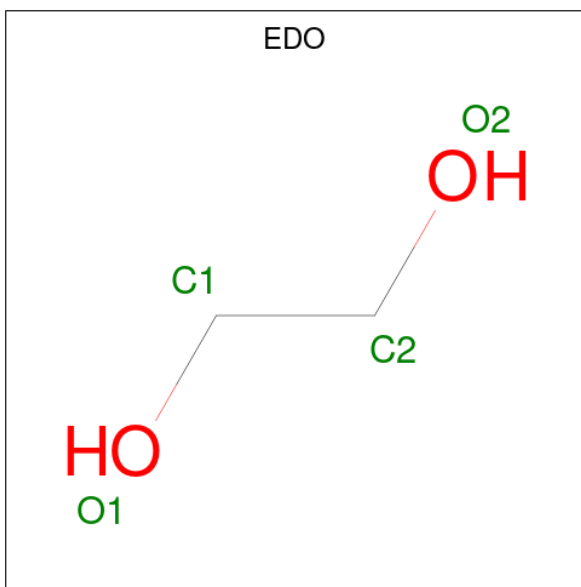
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q2KB35
A	-4	ILE	-	expression tag	UNP Q2KB35
A	-3	ASP	-	expression tag	UNP Q2KB35
A	-2	PRO	-	expression tag	UNP Q2KB35
A	-1	PHE	-	expression tag	UNP Q2KB35
A	0	THR	-	expression tag	UNP Q2KB35
B	-5	GLY	-	expression tag	UNP Q2KB35
B	-4	ILE	-	expression tag	UNP Q2KB35
B	-3	ASP	-	expression tag	UNP Q2KB35
B	-2	PRO	-	expression tag	UNP Q2KB35
B	-1	PHE	-	expression tag	UNP Q2KB35
B	0	THR	-	expression tag	UNP Q2KB35
C	-5	GLY	-	expression tag	UNP Q2KB35
C	-4	ILE	-	expression tag	UNP Q2KB35
C	-3	ASP	-	expression tag	UNP Q2KB35
C	-2	PRO	-	expression tag	UNP Q2KB35
C	-1	PHE	-	expression tag	UNP Q2KB35
C	0	THR	-	expression tag	UNP Q2KB35
D	-5	GLY	-	expression tag	UNP Q2KB35
D	-4	ILE	-	expression tag	UNP Q2KB35
D	-3	ASP	-	expression tag	UNP Q2KB35

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	expression tag	UNP Q2KB35
D	-1	PHE	-	expression tag	UNP Q2KB35
D	0	THR	-	expression tag	UNP Q2KB35

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

- 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	1	Total Zn 1 1	0	1
3	B	1	Total Zn 1 1	0	1
3	C	1	Total Zn 1 1	0	0

Continued on next page...

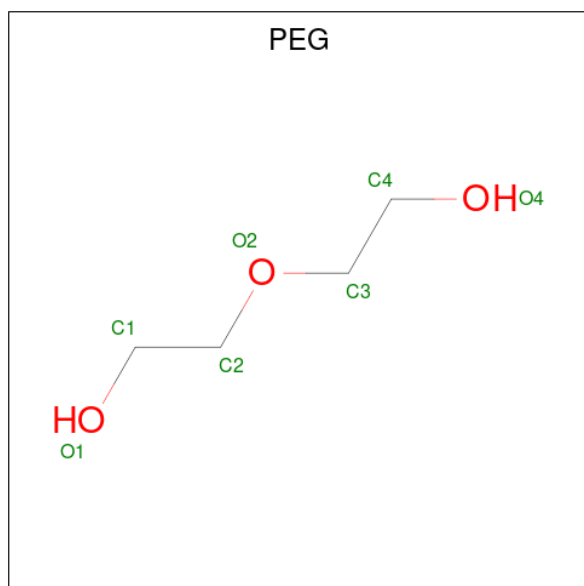
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	1
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

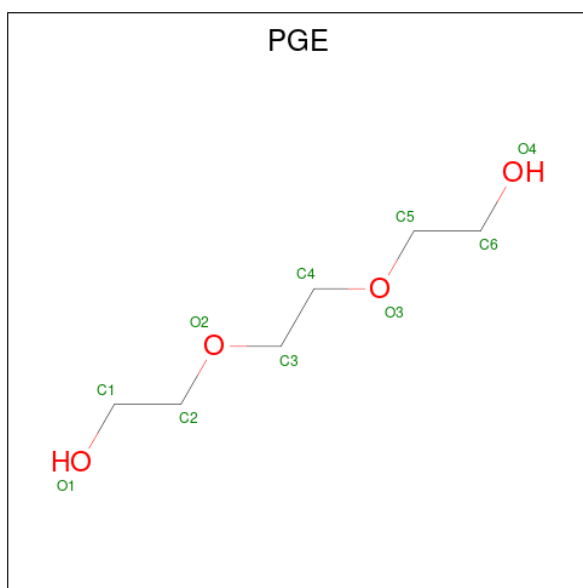


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	C O	0	0
			10	6 4		

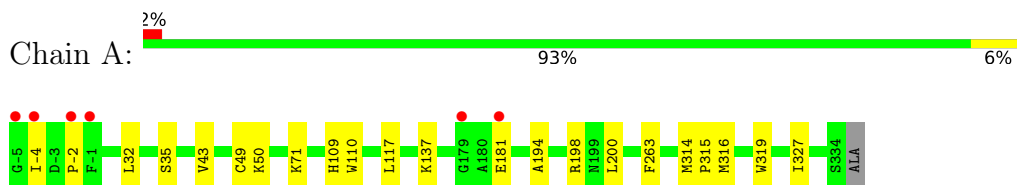
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	401	Total	O	0	10
			402	402		
8	B	456	Total	O	0	10
			460	460		
8	C	455	Total	O	0	12
			458	458		
8	D	462	Total	O	0	15
			466	466		

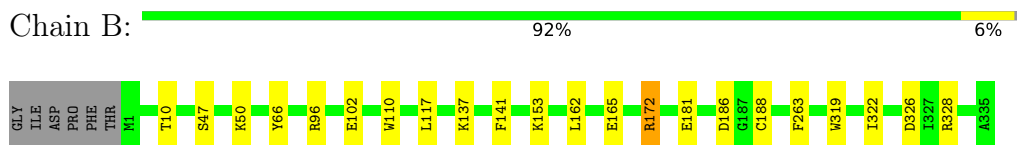
3 Residue-property plots [i](#)

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.

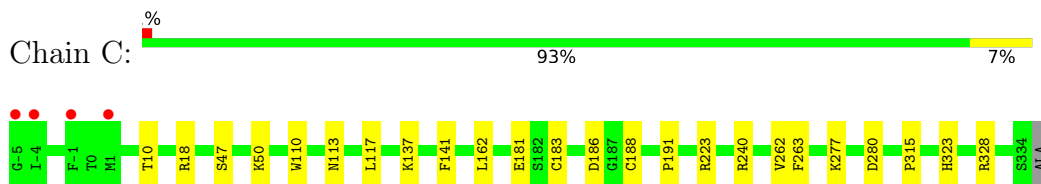
- Molecule 1: Putative L-asparaginase II protein



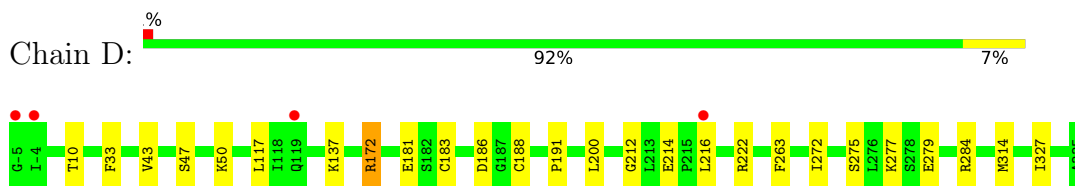
- Molecule 1: Putative L-asparaginase II protein



- Molecule 1: Putative L-asparaginase II protein



- Molecule 1: Putative L-asparaginase II protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.20Å 89.88Å 169.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.42 – 1.35 84.90 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.42-1.35) 99.9 (84.90-1.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.35Å)	Xtrriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.130 , 0.177 0.131 , 0.177	Depositor DCC
R_{free} test set	2771 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12486	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 29.85 % 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 1.4455e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PGE, ZN, PEG, CL, CSO, EDO, MG

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	0.67	0/2709	0.75	0/3659
1	B	0.69	0/2642	0.77	0/3567
1	C	0.67	0/2712	0.77	0/3663
1	D	0.65	0/2715	0.75	0/3667
All	All	0.67	0/10778	0.76	0/14556

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	2677	0	2631	18	0
1	B	2612	0	2563	24	0
1	C	2680	0	2627	27	0
1	D	2683	0	2634	20	0
2	A	8	0	12	2	0
2	B	4	0	6	4	0
2	C	4	0	6	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	1	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	B	7	0	10	0	0
6	C	1	0	0	0	0
7	D	10	0	14	0	0
8	A	402	0	0	3	0
8	B	460	0	0	11	0
8	C	458	0	0	14	0
8	D	466	0	0	8	0
All	All	12486	0	10503	87	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 (87) 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:49[B]:CYS:SG	1:A:200:LEU:HD11	2.15	0.87
1:B:186[B]:ASP:OD2	8:B:1083[B]:HOH:O	1.94	0.84
1:B:110:TRP:H	2:B:702:EDO:H12	1.43	0.83
1:C:18[B]:ARG:NE	1:D:279[B]:GLU:OE1	2.19	0.73
1:C:18[B]:ARG:NH1	8:C:502:HOH:O	2.21	0.72
1:B:110:TRP:N	2:B:702:EDO:H12	2.08	0.69
1:A:198[B]:ARG:NH2	8:A:501:HOH:O	2.21	0.67
1:B:137:LYS:NZ	8:B:805[B]:HOH:O	2.28	0.67
1:D:137:LYS:NZ	8:D:503[B]:HOH:O	2.29	0.65
1:A:110:TRP:HB3	1:A:117[A]:LEU:HD13	1.80	0.64
1:B:153:LYS:NZ	8:B:806:HOH:O	2.30	0.64
1:C:137:LYS:NZ	8:C:508[B]:HOH:O	2.31	0.63
1:C:18[B]:ARG:NH2	8:C:507:HOH:O	2.30	0.63
1:D:47[B]:SER:OG	8:D:501[B]:HOH:O	2.15	0.63
1:B:326[B]:ASP:OD2	1:B:328:ARG:HD3	1.98	0.62
1:B:10:THR:HG23	8:B:837:HOH:O	1.99	0.62
1:C:223[A]:ARG:NE	8:C:504:HOH:O	2.26	0.61
1:C:328:ARG:HD3	8:C:583:HOH:O	2.01	0.60
1:C:50:LYS:HE2	1:C:137:LYS:HE2	1.83	0.59
1:C:328:ARG:HG2	8:C:571:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:PRO:HB3	1:A:198[C]:ARG:NH2	2.19	0.58
1:A:71:LYS:NZ	8:A:508:HOH:O	2.36	0.56
8:C:507:HOH:O	1:D:279[B]:GLU:HG3	2.05	0.56
1:C:10:THR:HG23	8:C:571:HOH:O	2.04	0.56
1:B:172:ARG:NH2	4:B:705:CL:CL	2.76	0.56
1:C:315:PRO:HB3	1:C:323:HIS:CD2	2.40	0.56
1:B:110:TRP:H	2:B:702:EDO:C1	2.18	0.55
1:C:47[B]:SER:HB3	8:C:505[B]:HOH:O	2.07	0.55
1:D:172:ARG:NH2	1:D:212:GLY:O	2.40	0.54
1:D:10:THR:HG23	8:D:676:HOH:O	2.07	0.54
1:C:186[A]:ASP:OD1	1:C:188[A]:CYS:SG	2.65	0.54
1:A:109:HIS:HB2	2:A:401:EDO:H12	1.88	0.53
1:C:113:ASN:HA	2:C:401:EDO:H22	1.89	0.53
1:D:200:LEU:HD23	1:D:275[C]:SER:OG	2.09	0.53
1:C:47[B]:SER:CB	8:C:505[B]:HOH:O	2.56	0.52
1:B:50:LYS:HE2	1:B:137:LYS:HE2	1.92	0.51
1:D:183:CYS:SG	1:D:191:PRO:HB3	2.51	0.51
1:C:18[B]:ARG:CZ	8:C:507:HOH:O	2.57	0.51
1:B:165[B]:GLU:OE2	8:B:801:HOH:O	2.20	0.50
1:D:137:LYS:CE	8:D:503[B]:HOH:O	2.60	0.50
1:B:50:LYS:HG2	1:B:137:LYS:HD3	1.93	0.50
1:B:66:TYR:O	1:B:96[A]:ARG:HD2	2.12	0.49
1:A:32[A]:LEU:HD21	1:A:35[A]:SER:HB3	1.95	0.49
1:C:223[A]:ARG:HG3	8:C:504:HOH:O	2.12	0.49
1:D:186[A]:ASP:OD1	1:D:188[A]:CYS:SG	2.71	0.49
1:B:47[B]:SER:HB3	8:B:813[B]:HOH:O	2.13	0.48
1:B:186[A]:ASP:OD1	1:B:188[A]:CYS:SG	2.72	0.48
1:C:181:GLU:H	1:C:181:GLU:CD	2.17	0.47
1:B:322:ILE:HD11	8:B:1110:HOH:O	2.14	0.47
1:A:319:TRP:CZ3	2:B:702:EDO:H21	2.49	0.47
1:B:102[B]:GLU:OE1	8:B:802:HOH:O	2.20	0.47
1:D:43:VAL:HG13	1:D:277[A]:LYS:HD3	1.96	0.47
1:D:50:LYS:HG2	1:D:137:LYS:HD3	1.96	0.47
1:A:-4:ILE:CG2	1:A:32[A]:LEU:HD23	2.44	0.47
1:D:216:LEU:HD23	8:D:861:HOH:O	2.14	0.46
1:C:137:LYS:CE	8:C:508[B]:HOH:O	2.64	0.46
1:D:214:GLU:HB2	8:D:781:HOH:O	2.15	0.46
1:A:137:LYS:CE	8:A:504[B]:HOH:O	2.62	0.45
2:A:401:EDO:H11	1:B:319:TRP:CH2	2.51	0.45
1:B:137:LYS:CE	8:B:805[B]:HOH:O	2.63	0.45
1:C:141:PHE:CG	1:C:162:LEU:HD21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:C	1:B:117:LEU:HD23	2.37	0.44
1:B:47[B]:SER:CB	8:B:813[B]:HOH:O	2.66	0.43
1:A:50:LYS:HG2	1:A:137:LYS:HD3	2.01	0.43
1:B:141:PHE:CG	1:B:162:LEU:HD21	2.54	0.43
1:C:137:LYS:HE3	8:C:508[B]:HOH:O	2.18	0.43
1:A:-4:ILE:HG23	1:A:32[A]:LEU:HD23	2.01	0.43
1:C:113:ASN:CA	2:C:401:EDO:H22	2.49	0.43
1:C:110:TRP:HB3	1:C:117:LEU:HD13	2.01	0.43
1:A:316[B]:MET:SD	1:A:327:ILE:HG13	2.59	0.42
1:C:240:ARG:HD3	2:C:401:EDO:H21	2.00	0.42
1:D:33:PHE:CE2	1:D:272[B]:ILE:HD11	2.54	0.42
1:C:183:CYS:SG	1:C:191:PRO:HB3	2.59	0.42
1:D:117:LEU:C	1:D:117:LEU:HD23	2.40	0.42
1:D:222:ARG:HH11	1:D:222:ARG:HD3	1.68	0.42
1:A:314[A]:MET:HA	1:A:315:PRO:HD3	1.91	0.42
1:D:284:ARG:HD2	1:D:327[B]:ILE:HD12	2.02	0.42
1:D:47[B]:SER:CB	8:D:501[B]:HOH:O	2.67	0.42
1:D:181:GLU:HB2	8:D:769:HOH:O	2.20	0.42
1:C:315:PRO:HB3	1:C:323:HIS:HD2	1.82	0.41
1:A:-2:PRO:CB	1:A:198[C]:ARG:NH2	2.82	0.41
1:C:262:VAL:HG22	1:C:277[B]:LYS:HD3	2.03	0.41
1:A:43[A]:VAL:O	1:A:194:ALA:HA	2.21	0.41
1:C:280[B]:ASP:N	1:C:280[B]:ASP:OD1	2.50	0.41
1:A:117[B]:LEU:HD22	1:B:117:LEU:HD22	2.03	0.40
1:A:117[B]:LEU:C	1:A:117[B]:LEU:HD23	2.40	0.40
1:B:137:LYS:HE3	8:B:805[B]:HOH:O	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	358/341 (105%)	352 (98%)	6 (2%)	0	100	100
1	B	349/341 (102%)	345 (99%)	4 (1%)	0	100	100
1	C	358/341 (105%)	353 (99%)	5 (1%)	0	100	100
1	D	359/341 (105%)	355 (99%)	4 (1%)	0	100	100
All	All	1424/1364 (104%)	1405 (99%)	19 (1%)	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	274/253 (108%)	272 (99%)	2 (1%)	84	64
1	B	265/253 (105%)	262 (99%)	3 (1%)	73	45
1	C	274/253 (108%)	273 (100%)	1 (0%)	91	81
1	D	274/253 (108%)	271 (99%)	3 (1%)	73	45
All	All	1087/1012 (107%)	1078 (99%)	9 (1%)	78	59

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

Mol	Chain	Res	Type
1	A	181	GLU
1	A	263	PHE
1	B	172	ARG
1	B	181	GLU
1	B	263	PHE
1	C	263	PHE
1	D	172	ARG
1	D	263	PHE
1	D	314	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 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
1	CSO	D	242[A]	1	3,6,7	1.04	0	0,6,8	-	-
1	CSO	C	242[A]	1	3,6,7	0.97	0	0,6,8	-	-
1	CSO	A	242[B]	1	3,6,7	0.87	0	0,6,8	-	-
1	CSO	B	242[A]	1	3,6,7	0.81	0	0,6,8	-	-
1	CSO	D	242[B]	1	3,6,7	1.16	0	0,6,8	-	-
1	CSO	C	242[B]	1	3,6,7	1.27	0	0,6,8	-	-
1	CSO	B	242[B]	1	3,6,7	1.08	0	0,6,8	-	-
1	CSO	A	242[A]	1	3,6,7	1.21	0	0,6,8	-	-

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
1	CSO	D	242[A]	1	-	0/1/5/7	-
1	CSO	C	242[A]	1	-	0/1/5/7	-
1	CSO	A	242[B]	1	-	0/1/5/7	-
1	CSO	B	242[A]	1	-	0/1/5/7	-
1	CSO	D	242[B]	1	-	0/1/5/7	-
1	CSO	C	242[B]	1	-	0/1/5/7	-
1	CSO	B	242[B]	1	-	0/1/5/7	-
1	CSO	A	242[A]	1	-	0/1/5/7	-

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 15 are monoatomic - leaving 6 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
7	PGE	D	401	-	9,9,9	0.28	0	8,8,8	0.53	0
2	EDO	A	402	-	3,3,3	0.41	0	2,2,2	0.44	0
5	PEG	B	701	-	6,6,6	0.12	0	5,5,5	0.09	0
2	EDO	A	401	-	3,3,3	0.25	0	2,2,2	0.24	0
2	EDO	C	401	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	B	702	-	3,3,3	0.50	0	2,2,2	0.77	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
7	PGE	D	401	-	-	4/7/7/7	-
2	EDO	A	402	-	-	1/1/1/1	-
5	PEG	B	701	-	-	0/4/4/4	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	B	702	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	401	PGE	C4-C3-O2-C2
7	D	401	PGE	O2-C3-C4-O3
2	A	402	EDO	O1-C1-C2-O2
2	C	401	EDO	O1-C1-C2-O2
7	D	401	PGE	O1-C1-C2-O2
7	D	401	PGE	O3-C5-C6-O4
2	B	702	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	EDO	2	0
2	C	401	EDO	3	0
2	B	702	EDO	4	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, 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	339/341 (99%)	-0.47	6 (1%) 68 73	11, 16, 31, 55	0
1	B	334/341 (97%)	-0.56	0 100 100	10, 14, 25, 47	0
1	C	339/341 (99%)	-0.50	4 (1%) 79 83	10, 15, 27, 48	0
1	D	340/341 (99%)	-0.49	4 (1%) 79 83	10, 14, 26, 47	0
All	All	1352/1364 (99%)	-0.51	14 (1%) 82 85	10, 15, 27, 55	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-5	GLY	4.5
1	A	-2	PRO	4.1
1	C	-1	PHE	3.9
1	A	-1	PHE	3.8
1	D	-4	ILE	3.4
1	D	-5	GLY	3.3
1	A	-4	ILE	2.9
1	C	-4	ILE	2.7
1	D	216	LEU	2.5
1	C	-5	GLY	2.3
1	A	179	GLY	2.3
1	C	1	MET	2.1
1	A	181	GLU	2.1
1	D	119	GLN	2.0

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, 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(\AA^2)	Q<0.9
1	CSO	A	242[A]	7/8	0.97	0.07	10,13,15,15	7
1	CSO	A	242[B]	7/8	0.97	0.07	14,14,17,20	7
1	CSO	C	242[A]	7/8	0.98	0.07	13,14,16,18	7
1	CSO	C	242[B]	7/8	0.98	0.07	10,13,13,14	7
1	CSO	B	242[A]	7/8	0.99	0.05	12,13,15,16	7
1	CSO	B	242[B]	7/8	0.99	0.05	10,11,13,15	7
1	CSO	D	242[A]	7/8	0.99	0.06	11,13,15,16	7
1	CSO	D	242[B]	7/8	0.99	0.06	10,13,15,15	7

6.3 Carbohydrates [i](#)

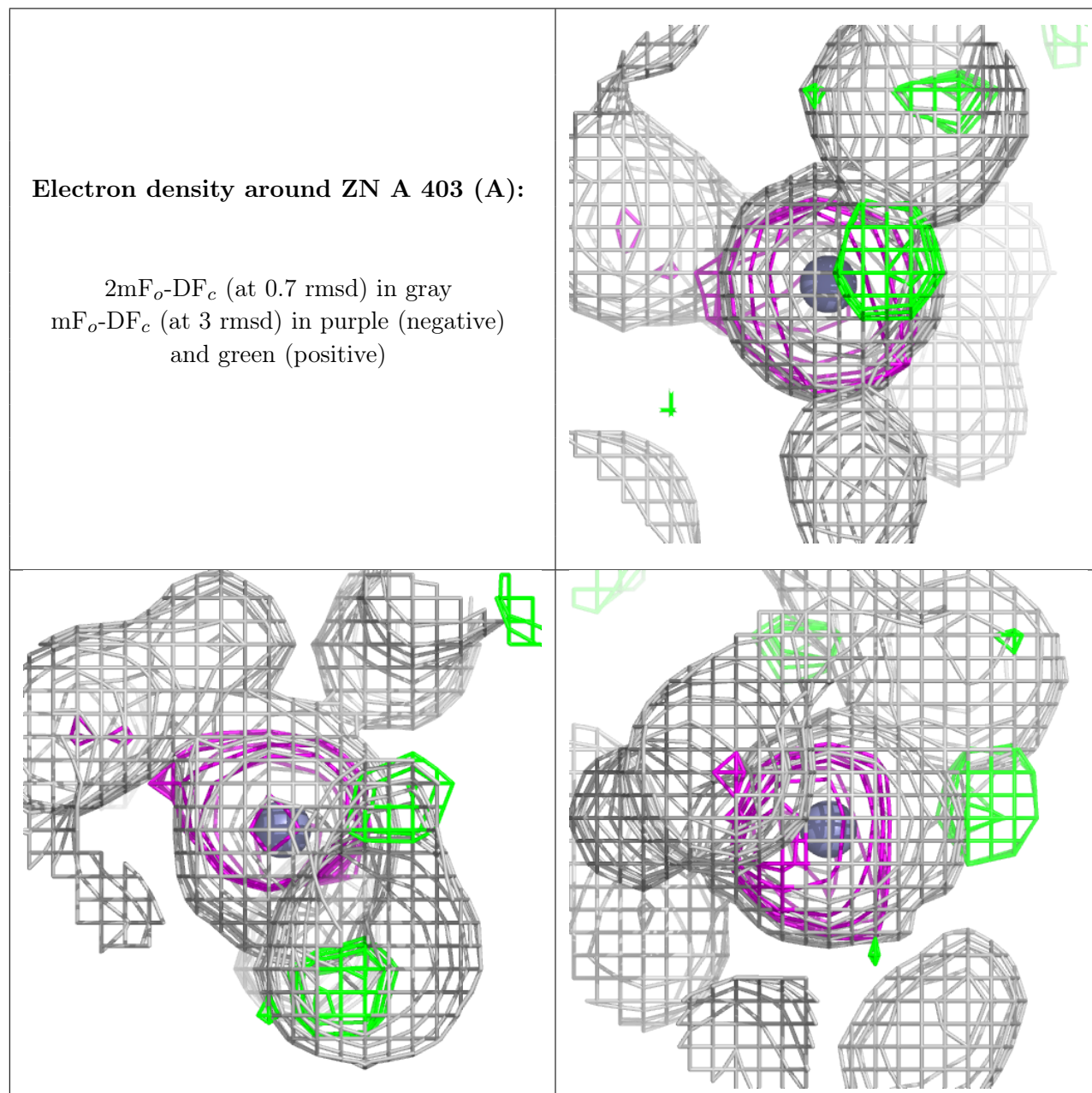
There are no monosaccharides in this entry.

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, 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.

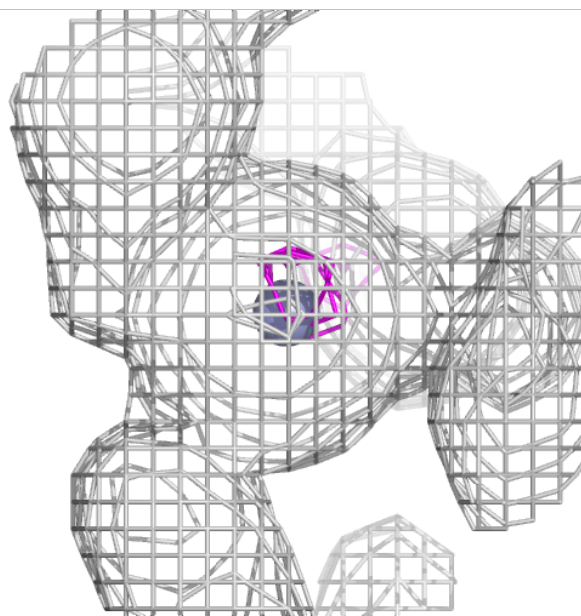
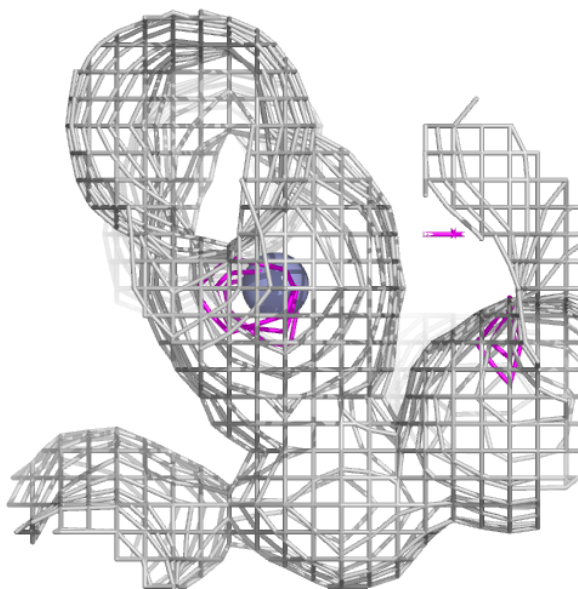
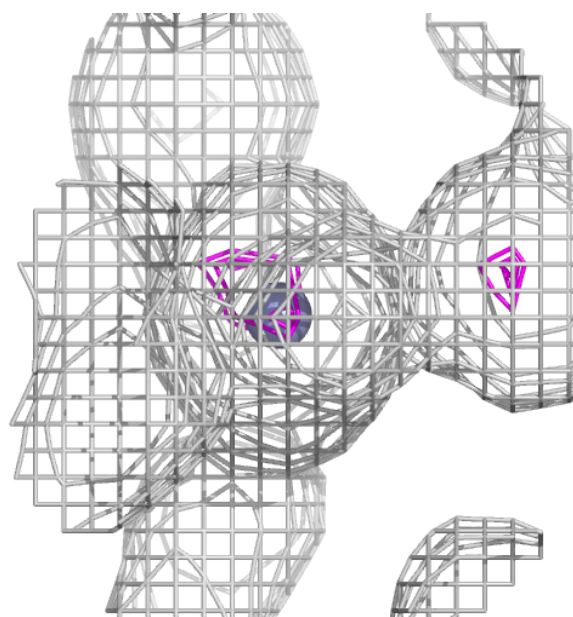
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PGE	D	401	10/10	0.79	0.15	53,63,66,67	0
5	PEG	B	701	7/7	0.82	0.10	51,52,55,58	0
2	EDO	A	402	4/4	0.86	0.17	42,45,47,54	0
2	EDO	B	702	4/4	0.92	0.14	29,35,40,41	0
2	EDO	C	401	4/4	0.93	0.08	36,37,41,45	0
2	EDO	A	401	4/4	0.97	0.14	27,34,38,38	0
6	MG	C	406	1/1	0.98	0.12	29,29,29,29	0
4	CL	D	405	1/1	0.98	0.06	51,51,51,51	0
3	ZN	A	403[A]	1/1	0.99	0.05	17,17,17,17	1
4	CL	C	404	1/1	0.99	0.04	37,37,37,37	0
4	CL	B	704	1/1	1.00	0.04	13,13,13,13	0
4	CL	B	705	1/1	1.00	0.04	22,22,22,22	0
4	CL	C	403	1/1	1.00	0.05	23,23,23,23	0
3	ZN	B	703[A]	1/1	1.00	0.04	14,14,14,14	1
4	CL	C	405	1/1	1.00	0.07	30,30,30,30	0
4	CL	D	403	1/1	1.00	0.04	28,28,28,28	0
4	CL	D	404	1/1	1.00	0.04	14,14,14,14	0
3	ZN	C	402	1/1	1.00	0.05	16,16,16,16	1
3	ZN	D	402[A]	1/1	1.00	0.03	15,15,15,15	1
4	CL	A	404	1/1	1.00	0.03	25,25,25,25	0
4	CL	A	405	1/1	1.00	0.07	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.



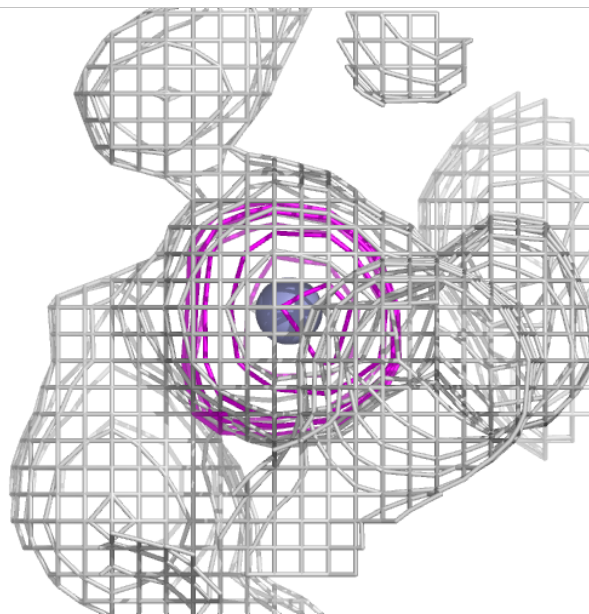
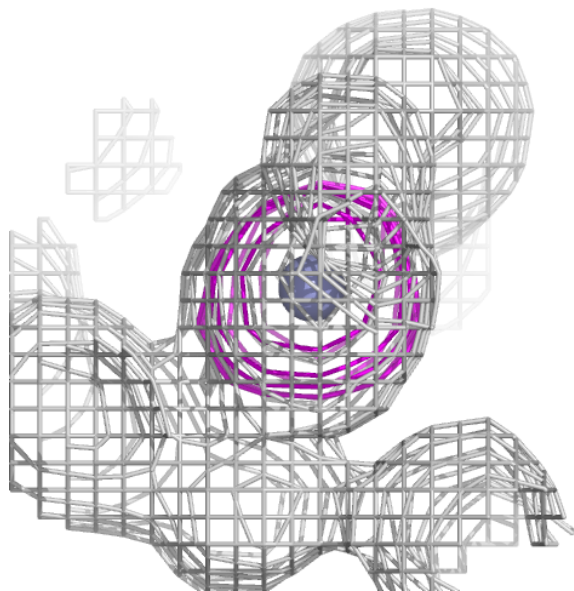
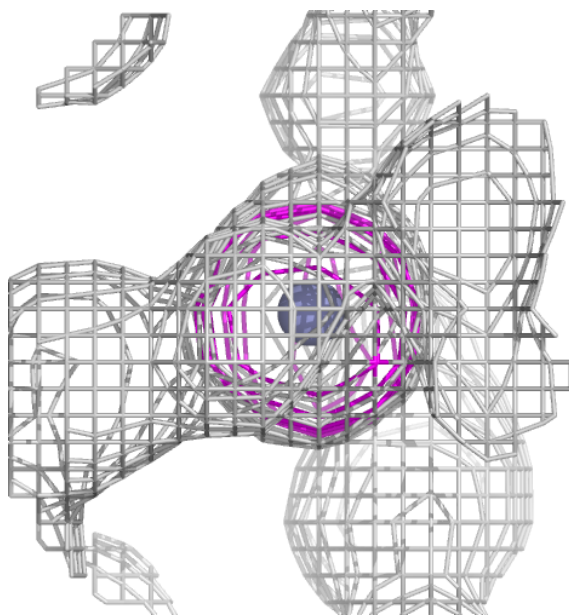
Electron density around ZN B 703 (A):

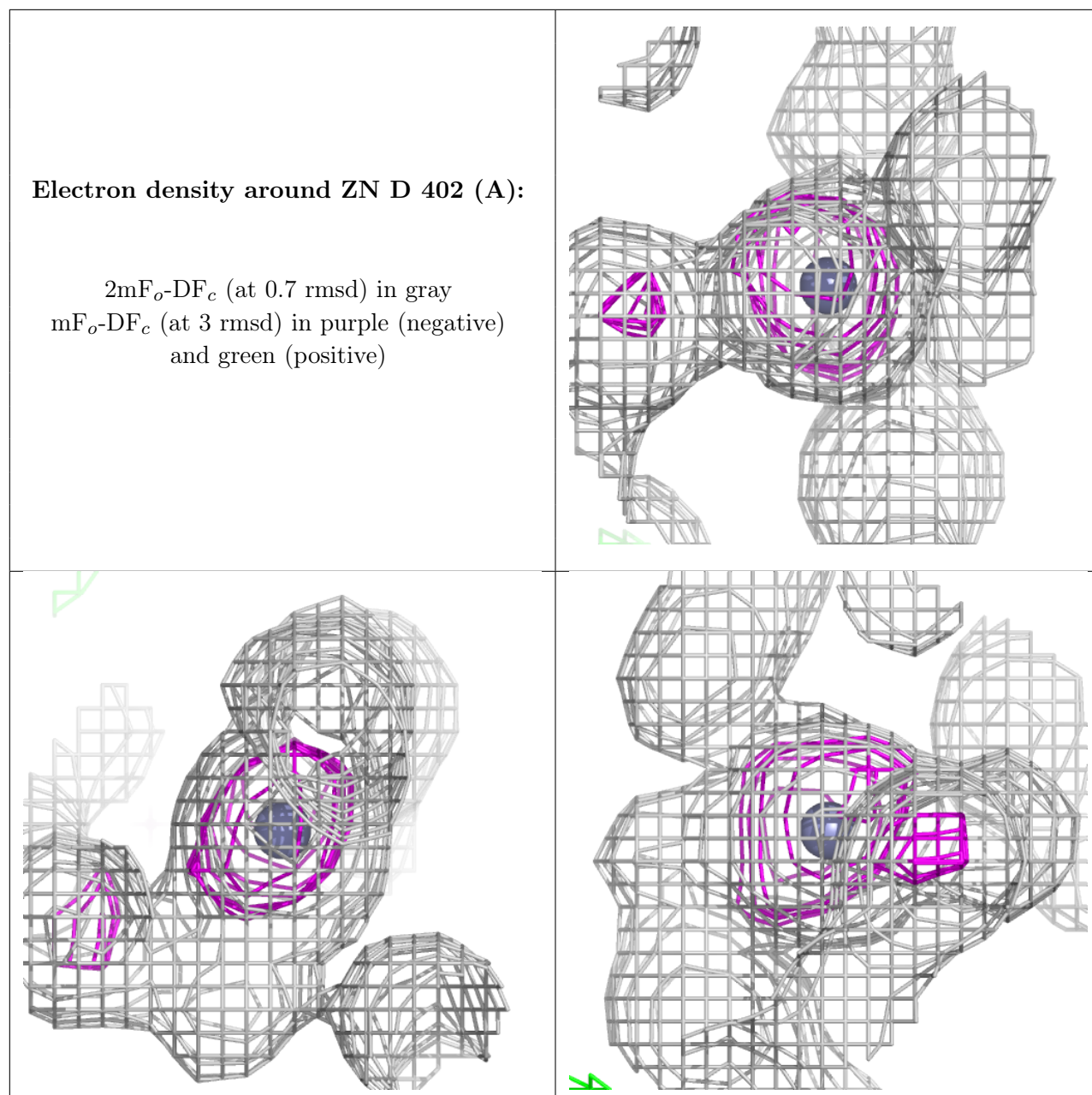
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN C 402:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.