



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 02:04 PM EDT

PDB ID : 7RWM
Title : Structure of Cap5 from Lactococcus lactis
Authors : Huang, R.H.; Fatma, S.; Chakravarti, A.
Deposited on : 2021-08-20
Resolution : 3.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

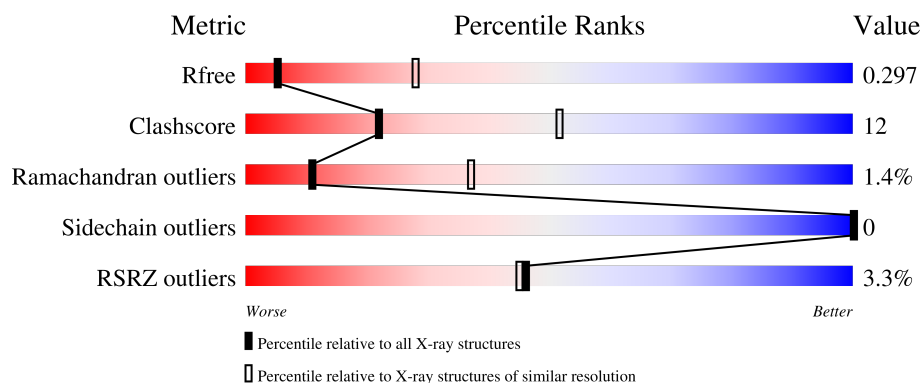
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	385	<div> <div>4%</div> <div>67%</div> <div>24%</div> <div>9%</div> </div>
1	B	385	<div> <div>3%</div> <div>63%</div> <div>28%</div> <div>8%</div> </div>
1	C	385	<div> <div>2%</div> <div>65%</div> <div>25%</div> <div>8%</div> </div>
1	D	385	<div> <div>3%</div> <div>66%</div> <div>24%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11431 atoms, of which 0 are hydrogens and 0 are deuteriums.

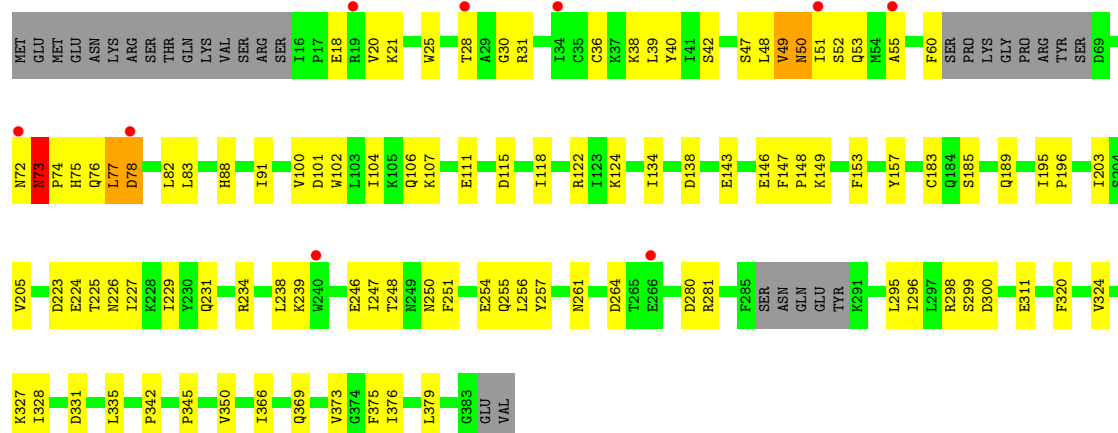
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SAVED domain-containing protein.

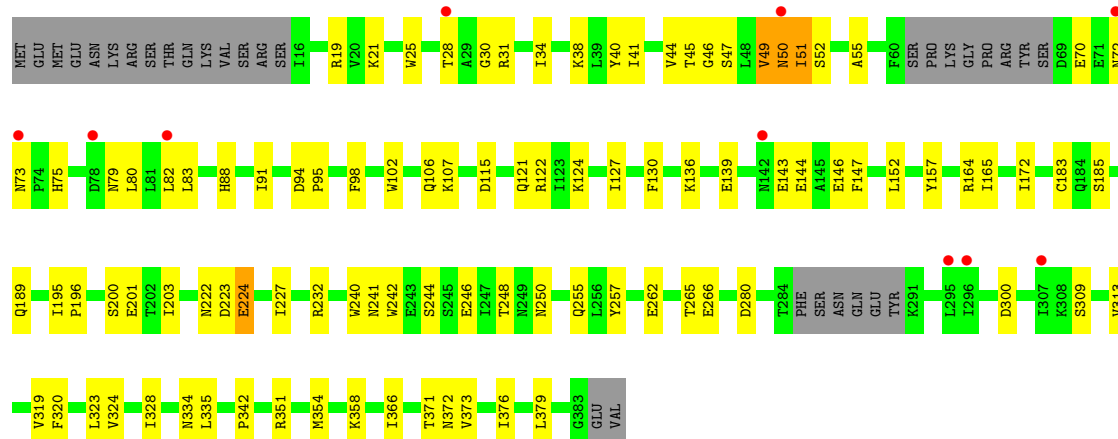
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2843	1818	470	542	13			
1	B	353	Total	C	N	O	S	0	0	0
			2853	1824	472	544	13			
1	C	355	Total	C	N	O	S	0	0	0
			2873	1835	476	549	13			
1	D	354	Total	C	N	O	S	0	0	0
			2858	1826	474	545	13			

- Molecule 2 is ZINC ION (three-letter code: 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		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		



• Molecule 1: SAVED domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	180.77Å 180.77Å 93.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.19 – 3.40 45.19 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.19-3.40) 98.6 (45.19-3.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.95 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.249 , 0.295 0.249 , 0.297	Depositor DCC
R_{free} test set	1999 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	85.3	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11431	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.22 % 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 5.9639e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/2898	0.52	1/3924 (0.0%)
1	B	0.29	0/2909	0.55	1/3941 (0.0%)
1	C	0.26	0/2929	0.52	1/3967 (0.0%)
1	D	0.26	0/2914	0.50	0/3947
All	All	0.27	0/11650	0.52	3/15779 (0.0%)

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	C	0	1

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	48	LEU	CA-CB-CG	6.42	130.07	115.30
1	B	48	LEU	CA-CB-CG	6.35	129.91	115.30
1	C	234	ARG	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	73	ASN	Peptide

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	2843	0	2825	69	0
1	B	2853	0	2830	86	0
1	C	2873	0	2839	74	0
1	D	2858	0	2820	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	11431	0	11314	268	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 12.

All (268) 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:80:LEU:O	1:B:107:LYS:NZ	2.02	0.93
1:C:31:ARG:NH2	1:D:115:ASP:OD1	2.06	0.86
1:C:28:THR:HG21	1:C:82:LEU:HD12	1.57	0.84
1:C:49:VAL:HA	1:D:19:ARG:HG2	1.65	0.78
1:B:266:GLU:HG2	1:B:337:CYS:HB3	1.66	0.77
1:B:91:ILE:HD11	1:B:103:LEU:HD21	1.66	0.76
1:B:48:LEU:HB3	1:B:50:ASN:H	1.51	0.76
1:D:262:GLU:O	1:D:334:ASN:ND2	2.15	0.76
1:A:48:LEU:HB3	1:A:50:ASN:H	1.52	0.74
1:A:118:ILE:HG23	1:B:31:ARG:NH1	2.02	0.74
1:A:321:ARG:NH2	1:A:361:ASP:OD2	2.18	0.74
1:C:73:ASN:HB3	1:C:74:PRO:HD2	1.69	0.74
1:A:169:LEU:HD23	1:A:172:ILE:HD11	1.68	0.73
1:D:342:PRO:HG3	1:D:366:ILE:HD11	1.69	0.72
1:D:250:ASN:HB3	1:D:300:ASP:OD2	1.90	0.72
1:B:31:ARG:HH21	1:B:38:LYS:HE3	1.54	0.71
1:B:91:ILE:HA	1:B:98:PHE:HD2	1.56	0.71
1:A:31:ARG:HH21	1:A:38:LYS:HE3	1.56	0.70
1:B:60:PHE:HE1	1:B:104:ILE:HD11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:VAL:HG13	1:C:76:GLN:HE21	1.55	0.70
1:C:342:PRO:HG3	1:C:366:ILE:HD11	1.72	0.70
1:A:27:ILE:HD11	1:A:77:LEU:HD13	1.74	0.69
1:D:143:GLU:OE2	1:D:232:ARG:NE	2.22	0.69
1:C:83:LEU:HD11	1:C:91:ILE:HD11	1.75	0.69
1:B:27:ILE:HD11	1:B:77:LEU:HD13	1.75	0.69
1:C:254:GLU:OE1	1:C:298:ARG:NH2	2.15	0.68
1:D:122:ARG:NH1	1:D:152:LEU:O	2.28	0.67
1:C:373:VAL:HG12	1:C:376:ILE:HD11	1.77	0.66
1:C:118:ILE:HD11	1:D:31:ARG:NH2	2.10	0.66
1:C:83:LEU:HD13	1:C:88:HIS:HA	1.77	0.66
1:B:91:ILE:HD11	1:B:103:LEU:CD2	2.25	0.65
1:A:342:PRO:HG3	1:A:366:ILE:HD11	1.77	0.65
1:D:203:ILE:HB	1:D:227:ILE:HG12	1.78	0.65
1:B:319:VAL:HG13	1:B:323:LEU:HD12	1.79	0.65
1:B:83:LEU:HD13	1:B:88:HIS:HA	1.79	0.64
1:B:321:ARG:NH2	1:B:361:ASP:OD2	2.22	0.64
1:D:124:LYS:HB2	1:D:201:GLU:HG3	1.78	0.64
1:A:266:GLU:HG2	1:A:337:CYS:HB3	1.79	0.64
1:A:31:ARG:HH12	1:B:118:ILE:HG12	1.63	0.64
1:B:73:ASN:H	1:B:74:PRO:HD2	1.62	0.64
1:C:146:GLU:OE2	1:C:239:LYS:N	2.31	0.64
1:D:83:LEU:HD13	1:D:88:HIS:HA	1.80	0.64
1:D:80:LEU:O	1:D:107:LYS:NZ	2.21	0.63
1:A:44:VAL:HG23	1:A:45:THR:HG23	1.80	0.63
1:B:44:VAL:HG23	1:B:45:THR:HG23	1.80	0.63
1:D:328:ILE:HG22	1:D:335:LEU:HD22	1.81	0.62
1:C:328:ILE:HG22	1:C:335:LEU:HD22	1.82	0.62
1:B:73:ASN:H	1:B:74:PRO:CD	2.12	0.62
1:C:250:ASN:HB3	1:C:300:ASP:OD2	2.00	0.61
1:A:141:LYS:HA	1:A:144:GLU:HG2	1.82	0.61
1:B:60:PHE:CE1	1:B:104:ILE:HD11	2.36	0.60
1:D:28:THR:HG21	1:D:82:LEU:HD12	1.83	0.60
1:D:28:THR:HG23	1:D:30:GLY:H	1.66	0.60
1:B:342:PRO:HG3	1:B:366:ILE:HD11	1.84	0.60
1:A:48:LEU:CB	1:A:50:ASN:H	2.15	0.59
1:C:74:PRO:HA	1:C:77:LEU:HB2	1.82	0.59
1:B:250:ASN:HB3	1:B:300:ASP:OD2	2.02	0.59
1:A:17:PRO:HB2	1:A:19:ARG:HD3	1.83	0.59
1:A:31:ARG:HH12	1:B:118:ILE:CG1	2.15	0.59
1:B:48:LEU:CB	1:B:50:ASN:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:HG23	1:D:45:THR:HG23	1.84	0.59
1:A:31:ARG:HH22	1:B:118:ILE:HD11	1.68	0.59
1:D:255:GLN:NE2	1:D:257:TYR:O	2.26	0.59
1:D:319:VAL:HG13	1:D:323:LEU:HD12	1.84	0.58
1:A:83:LEU:HD13	1:A:88:HIS:HA	1.84	0.58
1:B:265:THR:HB	1:B:336:LYS:HB2	1.85	0.58
1:A:18:GLU:HG2	1:A:21:LYS:HD2	1.85	0.58
1:B:73:ASN:N	1:B:74:PRO:HD2	2.19	0.58
1:D:222:ASN:HD22	1:D:358:LYS:HE3	1.69	0.58
1:B:91:ILE:HA	1:B:98:PHE:CD2	2.39	0.58
1:B:60:PHE:HE2	1:B:81:LEU:HD22	1.68	0.58
1:D:373:VAL:HG12	1:D:376:ILE:HD11	1.86	0.57
1:B:172:ILE:HG22	1:B:175:ASP:HB3	1.85	0.57
1:D:55:ALA:HB1	1:D:82:LEU:HD22	1.85	0.57
1:C:60:PHE:HE1	1:C:104:ILE:HG22	1.70	0.57
1:C:100:VAL:O	1:C:104:ILE:HG23	2.05	0.57
1:C:72:ASN:HB2	1:D:47:SER:HB2	1.86	0.57
1:B:313:VAL:HG11	1:B:351:ARG:HG3	1.87	0.57
1:A:319:VAL:HG13	1:A:323:LEU:HD12	1.88	0.56
1:A:94:ASP:OD1	1:B:149:LYS:NZ	2.36	0.56
1:C:255:GLN:NE2	1:C:257:TYR:O	2.36	0.56
1:D:49:VAL:HG12	1:D:52:SER:HB2	1.86	0.56
1:C:247:ILE:HG12	1:C:311:GLU:HB3	1.87	0.56
1:D:196:PRO:O	1:D:200:SER:OG	2.20	0.56
1:A:153:PHE:HE1	1:B:98:PHE:HE1	1.53	0.56
1:C:115:ASP:HB2	1:D:31:ARG:HH22	1.71	0.56
1:D:223:ASP:O	1:D:224:GLU:HB2	2.05	0.56
1:C:281:ARG:NH2	1:C:369:GLN:OE1	2.39	0.55
1:B:373:VAL:HG12	1:B:376:ILE:HD11	1.89	0.55
1:C:115:ASP:O	1:C:118:ILE:HD12	2.07	0.55
1:C:118:ILE:HD11	1:D:31:ARG:HH22	1.71	0.55
1:B:124:LYS:HB2	1:B:201:GLU:HG3	1.89	0.54
1:B:72:ASN:HB3	1:B:74:PRO:HD2	1.88	0.54
1:B:88:HIS:O	1:B:92:ASP:OD2	2.26	0.54
1:B:133:ILE:HD12	1:B:208:ILE:HG12	1.89	0.54
1:A:305:ASP:HB2	1:A:308:LYS:HD3	1.90	0.53
1:A:118:ILE:HG23	1:B:31:ARG:HH12	1.71	0.53
1:C:256:LEU:HD11	1:C:296:ILE:HD11	1.90	0.53
1:C:73:ASN:HB3	1:C:74:PRO:CD	2.39	0.53
1:D:91:ILE:HA	1:D:98:PHE:CD2	2.44	0.53
1:A:313:VAL:HG11	1:A:351:ARG:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HD21	1:A:327:LYS:HE3	1.91	0.52
1:A:117:VAL:O	1:A:121:GLN:HG2	2.09	0.52
1:B:141:LYS:HA	1:B:144:GLU:HG2	1.92	0.52
1:C:229:ILE:HD12	1:C:350:VAL:HG11	1.91	0.52
1:A:124:LYS:HB2	1:A:201:GLU:HG3	1.91	0.52
1:B:369:GLN:HE22	1:B:374:GLY:H	1.58	0.52
1:A:121:GLN:OE1	1:B:113:LYS:HE3	2.10	0.52
1:D:79:ASN:HB3	1:D:80:LEU:HD12	1.91	0.52
1:D:102:TRP:O	1:D:106:GLN:HG2	2.10	0.52
1:B:355:ASN:OD1	1:B:355:ASN:O	2.27	0.51
1:D:94:ASP:N	1:D:95:PRO:HD3	2.26	0.51
1:A:195:ILE:HB	1:A:196:PRO:HD3	1.93	0.51
1:C:146:GLU:HG3	1:C:238:LEU:HD22	1.91	0.51
1:A:121:GLN:NE2	1:B:110:PHE:HD1	2.08	0.51
1:B:90:MET:HG2	1:B:98:PHE:HE2	1.76	0.50
1:C:73:ASN:C	1:C:75:HIS:H	2.13	0.50
1:D:146:GLU:OE2	1:D:240:TRP:HD1	1.93	0.50
1:A:183:CYS:SG	1:A:379:LEU:HD22	2.51	0.50
1:A:49:VAL:HA	1:B:19:ARG:HG3	1.94	0.50
1:C:205:VAL:HB	1:C:229:ILE:HD13	1.94	0.49
1:D:280:ASP:OD1	1:D:280:ASP:N	2.44	0.49
1:B:73:ASN:N	1:B:74:PRO:CD	2.74	0.49
1:A:83:LEU:HD11	1:A:91:ILE:HD11	1.94	0.49
1:C:28:THR:HG23	1:C:30:GLY:H	1.77	0.49
1:C:102:TRP:O	1:C:106:GLN:HG2	2.12	0.49
1:D:265:THR:HG23	1:D:266:GLU:HG3	1.95	0.49
1:C:18:GLU:HG2	1:C:21:LYS:HD2	1.95	0.49
1:C:224:GLU:O	1:C:226:ASN:N	2.45	0.49
1:D:28:THR:HG21	1:D:82:LEU:CD1	2.43	0.49
1:B:270:ILE:HD11	1:B:282:ILE:HG13	1.95	0.48
1:D:185:SER:O	1:D:189:GLN:HG3	2.13	0.48
1:C:124:LYS:HG2	1:C:157:TYR:CE1	2.48	0.48
1:C:203:ILE:HB	1:C:227:ILE:HG12	1.95	0.48
1:B:183:CYS:SG	1:B:379:LEU:HD22	2.54	0.48
1:B:141:LYS:HD3	1:B:144:GLU:OE2	2.13	0.48
1:B:16:ILE:N	1:B:17:PRO:HD3	2.29	0.48
1:D:172:ILE:HG22	1:D:172:ILE:O	2.14	0.48
1:B:272:SER:HB3	1:B:276:GLU:HA	1.96	0.48
1:A:91:ILE:HA	1:A:98:PHE:CD2	2.48	0.48
1:B:87:HIS:O	1:B:91:ILE:HG22	2.13	0.47
1:A:23:ALA:O	1:A:27:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLN:OE1	1:C:345:PRO:HB2	2.14	0.47
1:D:222:ASN:ND2	1:D:358:LYS:HE3	2.29	0.47
1:D:28:THR:HG23	1:D:30:GLY:N	2.29	0.47
1:D:224:GLU:HA	1:D:354:MET:HE3	1.96	0.47
1:C:47:SER:HB2	1:D:72:ASN:HB2	1.95	0.47
1:A:18:GLU:HA	1:A:21:LYS:HD2	1.97	0.47
1:A:113:LYS:HD3	1:B:121:GLN:OE1	2.13	0.47
1:C:295:LEU:HD13	1:C:328:ILE:HD11	1.96	0.47
1:A:20:VAL:HG21	1:A:76:GLN:NE2	2.29	0.47
1:A:56:HIS:CE1	1:A:85:ALA:HA	2.50	0.47
1:B:28:THR:HG23	1:B:30:GLY:H	1.79	0.47
1:B:35:CYS:HB3	1:B:87:HIS:CE1	2.50	0.47
1:D:144:GLU:OE2	1:D:164:ARG:NE	2.47	0.47
1:A:122:ARG:NH1	1:A:152:LEU:O	2.48	0.47
1:D:320:PHE:O	1:D:324:VAL:HB	2.15	0.47
1:B:117:VAL:O	1:B:121:GLN:HG2	2.15	0.47
1:A:28:THR:HG23	1:A:30:GLY:H	1.80	0.46
1:C:149:LYS:O	1:C:153:PHE:HD1	1.99	0.46
1:A:373:VAL:HG12	1:A:376:ILE:HD11	1.96	0.46
1:D:241:ASN:OD1	1:D:242:TRP:N	2.49	0.46
1:A:109:GLU:O	1:A:113:LYS:HB2	2.16	0.46
1:C:21:LYS:O	1:C:25:TRP:CD1	2.69	0.46
1:C:50:ASN:O	1:C:52:SER:N	2.49	0.46
1:B:56:HIS:CE1	1:B:85:ALA:HA	2.51	0.46
1:A:121:GLN:HG3	1:B:36:CYS:SG	2.56	0.45
1:D:144:GLU:OE2	1:D:164:ARG:NH2	2.49	0.45
1:B:358:LYS:O	1:B:360:ILE:HD12	2.17	0.45
1:C:51:ILE:HD12	1:C:51:ILE:H	1.82	0.45
1:C:246:GLU:O	1:C:248:THR:HG23	2.17	0.45
1:D:136:LYS:HE2	1:D:139:GLU:OE2	2.16	0.45
1:C:76:GLN:C	1:C:78:ASP:H	2.20	0.45
1:C:143:GLU:O	1:C:146:GLU:HB3	2.17	0.45
1:C:20:VAL:HG22	1:C:72:ASN:OD1	2.17	0.45
1:C:36:CYS:SG	1:D:121:GLN:HG3	2.56	0.45
1:A:31:ARG:NH1	1:B:118:ILE:HG12	2.28	0.45
1:B:233:PHE:O	1:B:239:LYS:HB3	2.17	0.45
1:B:346:VAL:O	1:B:349:PRO:HD2	2.17	0.45
1:B:172:ILE:CG2	1:B:175:ASP:HB3	2.45	0.44
1:C:147:PHE:HB2	1:C:148:PRO:HD3	1.99	0.44
1:B:319:VAL:O	1:B:324:VAL:HG23	2.18	0.44
1:C:223:ASP:OD2	1:C:226:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:O	1:A:114:VAL:HG23	2.17	0.44
1:B:251:PHE:HD2	1:B:315:GLU:HG3	1.83	0.44
1:C:183:CYS:SG	1:C:379:LEU:HD22	2.58	0.44
1:C:40:TYR:HA	1:C:50:ASN:HB2	2.00	0.44
1:D:25:TRP:CD1	1:D:51:ILE:HG21	2.53	0.44
1:A:373:VAL:CG1	1:A:376:ILE:HD11	2.48	0.44
1:B:369:GLN:NE2	1:B:370:GLN:O	2.46	0.44
1:A:24:LEU:HG	1:A:82:LEU:CD2	2.48	0.44
1:B:75:HIS:HA	1:B:78:ASP:HB2	2.00	0.43
1:B:102:TRP:O	1:B:106:GLN:HG2	2.17	0.43
1:B:143:GLU:O	1:B:146:GLU:HG2	2.18	0.43
1:C:369:GLN:HA	1:C:375:PHE:HA	1.99	0.43
1:B:21:LYS:O	1:B:25:TRP:CD1	2.71	0.43
1:B:25:TRP:CD1	1:B:51:ILE:HG21	2.53	0.43
1:C:42:SER:HB3	1:C:48:LEU:HG	1.99	0.43
1:A:72:ASN:C	1:A:74:PRO:HD2	2.39	0.43
1:A:133:ILE:HD12	1:A:208:ILE:HG12	1.99	0.43
1:B:24:LEU:HG	1:B:82:LEU:CD2	2.49	0.43
1:A:194:LYS:HA	1:A:197:LEU:HD12	1.99	0.43
1:D:41:ILE:HG23	1:D:46:GLY:O	2.17	0.43
1:C:185:SER:O	1:C:189:GLN:HG3	2.19	0.43
1:D:21:LYS:O	1:D:25:TRP:CD1	2.72	0.43
1:A:25:TRP:CD1	1:A:51:ILE:HG21	2.54	0.43
1:C:280:ASP:N	1:C:280:ASP:OD1	2.51	0.43
1:A:270:ILE:HD11	1:A:282:ILE:HG13	2.00	0.43
1:D:124:LYS:HG2	1:D:157:TYR:CE1	2.54	0.43
1:A:87:HIS:HA	1:A:90:MET:HB3	2.01	0.42
1:A:280:ASP:OD1	1:A:280:ASP:N	2.50	0.42
1:C:39:LEU:HD13	1:C:55:ALA:HB2	2.01	0.42
1:C:122:ARG:HE	1:D:34:ILE:HG23	1.83	0.42
1:A:91:ILE:HA	1:A:98:PHE:HD2	1.83	0.42
1:C:51:ILE:HG23	1:C:55:ALA:CB	2.49	0.42
1:B:105:LYS:HE2	1:B:109:GLU:OE2	2.19	0.42
1:C:40:TYR:HA	1:C:50:ASN:CB	2.50	0.42
1:C:327:LYS:NZ	1:C:331:ASP:OD2	2.50	0.42
1:C:107:LYS:HE3	1:C:111:GLU:OE2	2.19	0.42
1:D:130:PHE:CD1	1:D:165:ILE:HB	2.55	0.42
1:A:21:LYS:O	1:A:25:TRP:CD1	2.73	0.42
1:A:324:VAL:O	1:A:328:ILE:HG13	2.19	0.42
1:D:31:ARG:HH21	1:D:38:LYS:NZ	2.18	0.42
1:D:195:ILE:HB	1:D:196:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:TRP:O	1:A:106:GLN:HG2	2.20	0.42
1:A:118:ILE:HA	1:A:121:GLN:CG	2.50	0.42
1:D:313:VAL:HG11	1:D:351:ARG:HG3	2.02	0.42
1:A:321:ARG:O	1:A:326:GLU:HG2	2.20	0.41
1:C:25:TRP:CD1	1:C:51:ILE:HG21	2.55	0.41
1:C:118:ILE:HD11	1:D:31:ARG:CZ	2.49	0.41
1:C:320:PHE:O	1:C:324:VAL:HB	2.20	0.41
1:D:183:CYS:SG	1:D:379:LEU:HD22	2.59	0.41
1:A:33:GLU:HG2	1:A:110:PHE:CD2	2.55	0.41
1:B:109:GLU:O	1:B:113:LYS:HE2	2.20	0.41
1:C:101:ASP:O	1:C:104:ILE:HG12	2.20	0.41
1:A:18:GLU:HA	1:A:21:LYS:HB2	2.02	0.41
1:B:172:ILE:HG21	1:B:172:ILE:HD13	1.72	0.41
1:C:261:ASN:HD21	1:C:264:ASP:HB2	1.84	0.41
1:D:246:GLU:O	1:D:248:THR:HG23	2.21	0.41
1:D:40:TYR:HA	1:D:50:ASN:HA	2.03	0.41
1:D:371:THR:O	1:D:372:ASN:HB2	2.21	0.41
1:A:291:LYS:HB3	1:A:291:LYS:HE2	1.86	0.41
1:B:33:GLU:OE1	1:B:81:LEU:HB2	2.20	0.41
1:B:110:PHE:O	1:B:114:VAL:HG23	2.21	0.41
1:C:28:THR:HG23	1:C:30:GLY:N	2.35	0.41
1:C:138:ASP:N	1:C:138:ASP:OD1	2.54	0.41
1:B:102:TRP:CE3	1:B:103:LEU:HD23	2.55	0.41
1:C:31:ARG:HH21	1:C:38:LYS:NZ	2.19	0.41
1:D:127:ILE:HD13	1:D:147:PHE:HB3	2.02	0.41
1:A:121:GLN:HB3	1:A:122:ARG:H	1.47	0.41
1:C:195:ILE:HB	1:C:196:PRO:HD3	2.03	0.41
1:A:73:ASN:O	1:A:75:HIS:N	2.54	0.40
1:A:272:SER:HB3	1:A:276:GLU:HA	2.02	0.40
1:B:124:LYS:CB	1:B:201:GLU:HG3	2.50	0.40
1:B:185:SER:O	1:B:189:GLN:HG3	2.20	0.40
1:B:382:LYS:HB3	1:B:383:GLY:H	1.56	0.40
1:A:120:THR:HG23	1:B:113:LYS:HD2	2.02	0.40
1:B:104:ILE:HA	1:B:104:ILE:HD13	1.89	0.40
1:A:134:ILE:HG22	1:A:140:ILE:HG13	2.03	0.40
1:B:295:LEU:HD21	1:B:327:LYS:HE3	2.03	0.40
1:B:324:VAL:O	1:B:328:ILE:HG13	2.22	0.40
1:C:134:ILE:HD13	1:C:134:ILE:HA	1.95	0.40
1:B:47:SER:O	1:B:48:LEU:HD22	2.22	0.40
1:B:216:TYR:O	1:B:220:LEU:HG	2.21	0.40
1:C:251:PHE:CD1	1:C:299:SER:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:NE2	1:A:370:GLN:O	2.54	0.40
1:C:49:VAL:O	1:C:53:GLN:HB2	2.21	0.40
1:D:244:SER:HB3	1:D:309:SER:HB3	2.04	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	343/385 (89%)	311 (91%)	30 (9%)	2 (1%)	25	57
1	B	347/385 (90%)	310 (89%)	33 (10%)	4 (1%)	13	41
1	C	349/385 (91%)	307 (88%)	36 (10%)	6 (2%)	9	34
1	D	348/385 (90%)	312 (90%)	29 (8%)	7 (2%)	7	30
All	All	1387/1540 (90%)	1240 (89%)	128 (9%)	19 (1%)	11	37

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	73	ASN
1	C	78	ASP
1	D	50	ASN
1	D	51	ILE
1	D	75	HIS
1	D	224	GLU
1	C	50	ASN
1	D	70	GLU
1	A	170	SER
1	C	49	VAL
1	B	17	PRO
1	B	73	ASN

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Mol	Chain	Res	Type
1	B	170	SER
1	B	225	THR
1	C	77	LEU
1	C	225	THR
1	D	73	ASN
1	A	73	ASN
1	D	49	VAL

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	325/360 (90%)	325 (100%)	0	100	100
1	B	325/360 (90%)	325 (100%)	0	100	100
1	C	326/360 (91%)	326 (100%)	0	100	100
1	D	323/360 (90%)	323 (100%)	0	100	100
All	All	1299/1440 (90%)	1299 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	ASN
1	D	222	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	351/385 (91%)	0.50	16 (4%) 32 32	58, 90, 135, 170	0
1	B	353/385 (91%)	0.50	12 (3%) 45 44	64, 93, 143, 171	0
1	C	355/385 (92%)	0.55	9 (2%) 57 55	43, 72, 126, 180	0
1	D	354/385 (91%)	0.47	10 (2%) 53 51	45, 74, 132, 179	0
All	All	1413/1540 (91%)	0.50	47 (3%) 46 45	43, 84, 136, 180	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	ASN	5.8
1	D	72	ASN	4.4
1	D	73	ASN	4.3
1	C	72	ASN	4.0
1	B	77	LEU	4.0
1	A	203	ILE	3.5
1	B	295	LEU	3.4
1	A	291	LYS	3.2
1	C	78	ASP	3.0
1	D	295	LEU	2.7
1	D	296	ILE	2.7
1	D	142	ASN	2.6
1	C	19	ARG	2.6
1	B	51	ILE	2.6
1	A	110	PHE	2.6
1	A	128	LEU	2.6
1	B	262	GLU	2.5
1	A	43	ASP	2.5
1	B	60	PHE	2.5
1	B	31	ARG	2.5
1	B	307	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	362	VAL	2.4
1	D	82	LEU	2.4
1	D	78	ASP	2.3
1	A	122	ARG	2.3
1	C	34	ILE	2.3
1	A	77	LEU	2.3
1	A	197	LEU	2.3
1	B	80	LEU	2.3
1	C	51	ILE	2.3
1	D	307	ILE	2.2
1	C	240	TRP	2.2
1	A	60	PHE	2.2
1	B	162	ILE	2.2
1	B	43	ASP	2.2
1	A	34	ILE	2.2
1	B	172	ILE	2.2
1	C	28	THR	2.2
1	D	28	THR	2.2
1	A	184	GLN	2.1
1	A	22	SER	2.1
1	A	91	ILE	2.1
1	C	55	ALA	2.0
1	A	358	LYS	2.0
1	A	277	ILE	2.0
1	B	338	ILE	2.0
1	C	266	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](#)

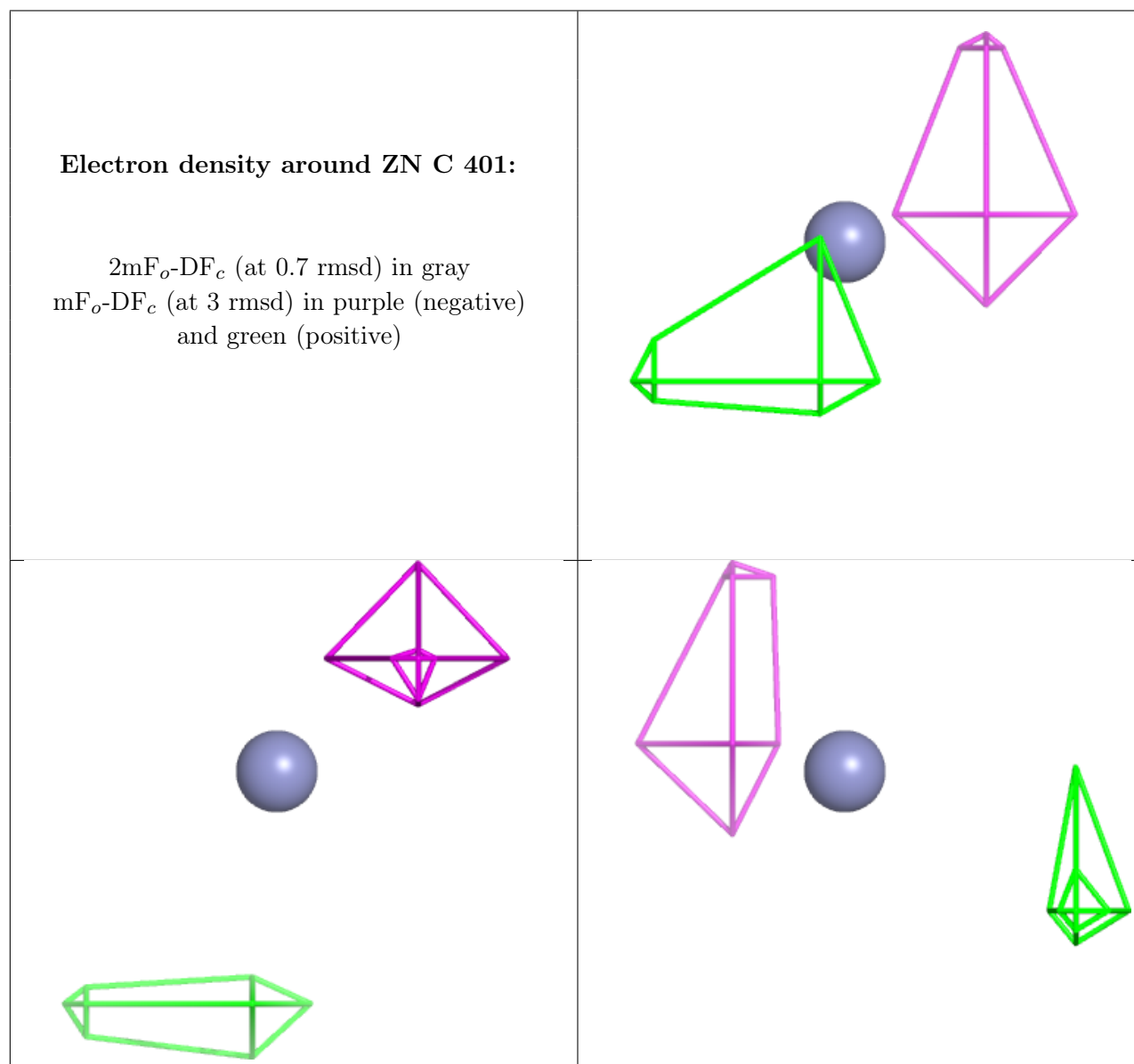
There are no monosaccharides in this entry.

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.

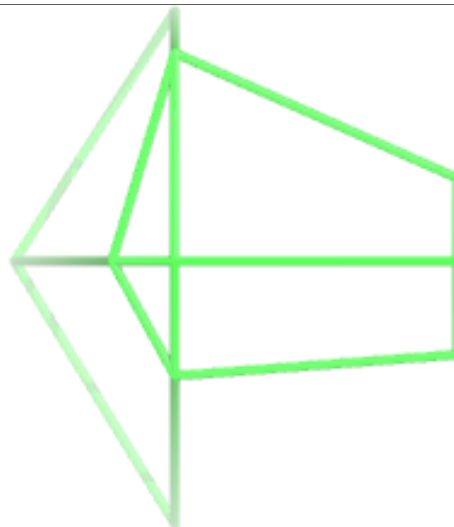
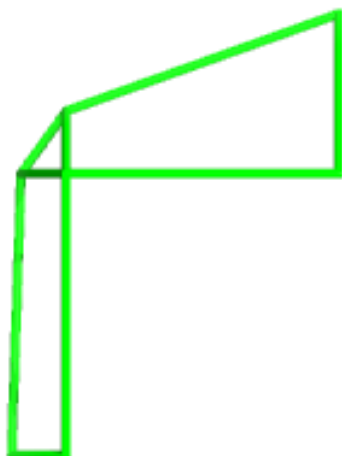
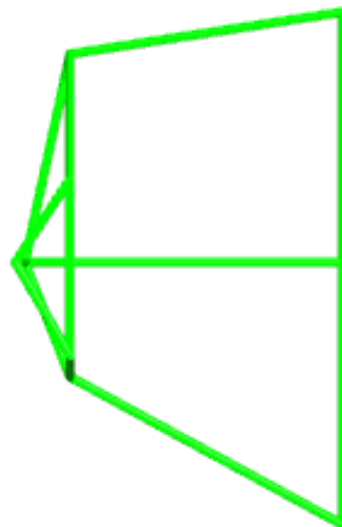
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	C	401	1/1	0.80	0.19	77,77,77,77	0
2	ZN	B	401	1/1	0.94	0.19	85,85,85,85	0
2	ZN	A	401	1/1	0.97	0.13	92,92,92,92	0
2	ZN	D	401	1/1	0.98	0.20	79,79,79,79	0

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.



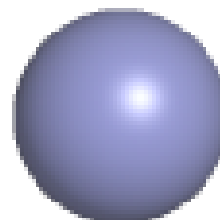
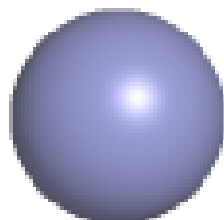
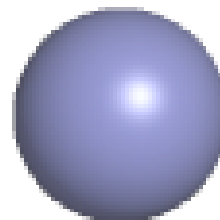
Electron density around ZN B 401:

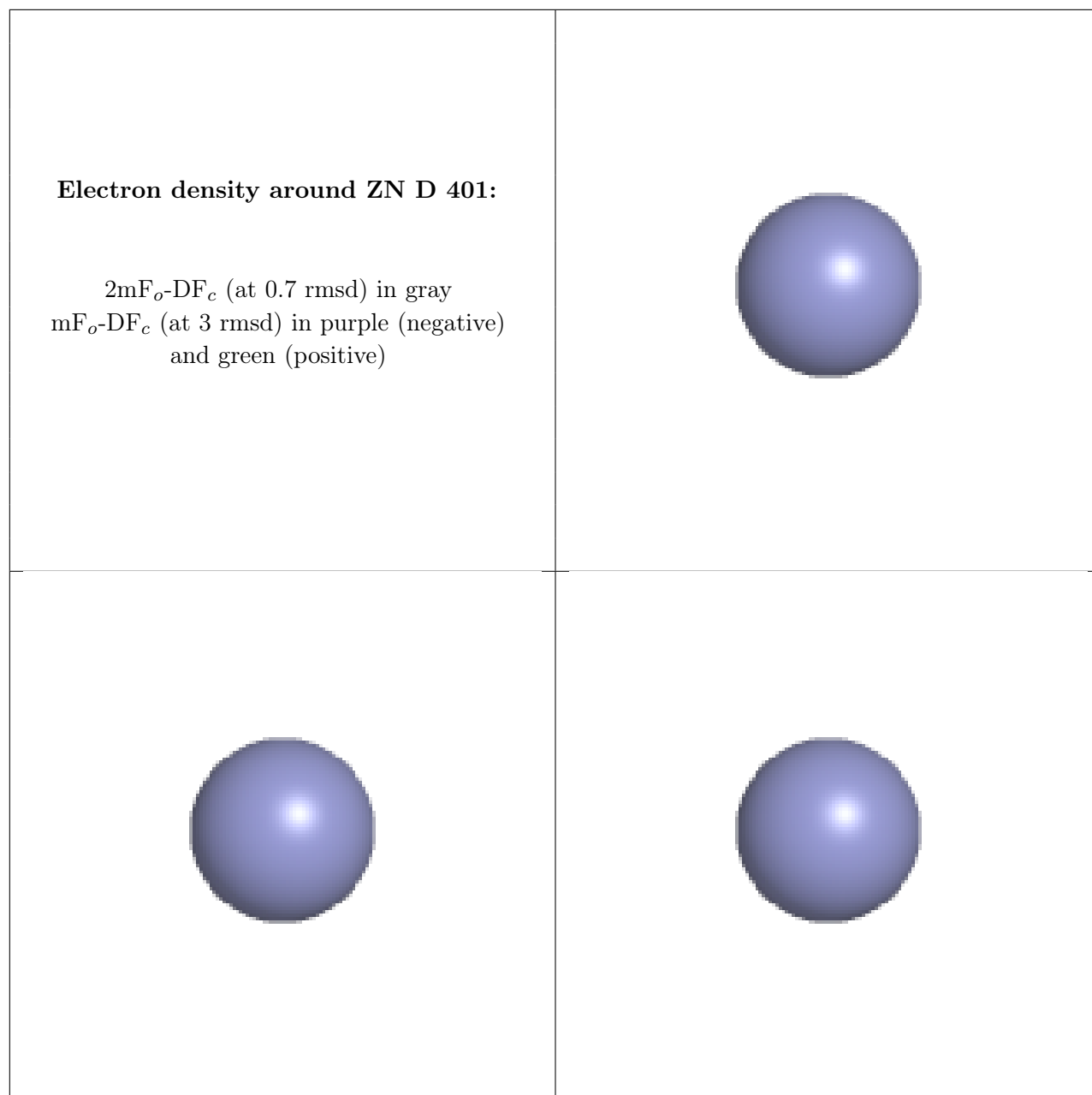
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 401:

$2mF_o-DF_c$ (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.