Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2020 – 06:55 PM BST

PDB ID	:	6Z42
Title	:	The low resolution structure of a zinc-dependent alcohol dehydrogenase from Halomonas elongata.
Authors	:	Gourlay, L.J.
Deposited on	:	2020-05-22
Resolution	:	4.00 Å(reported)

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

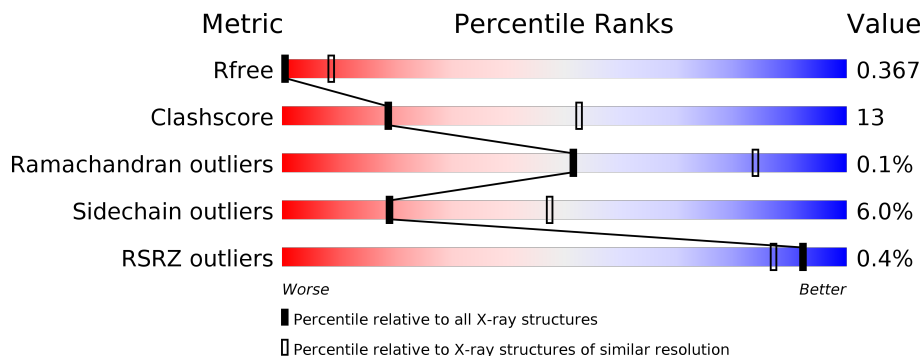|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 4.00 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	Percentile Ranks	Value
Rfree		0.367
Clashscore		13
Ramachandran outliers		0.1%
Sidechain outliers		6.0%
RSRZ outliers		0.4%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 on 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 <=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	363	66% 25% • 7%
1	B	363	64% 26% • 8%
1	C	363	67% 19% • 12%
1	D	363	72% 19% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9733 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 Alcohol dehydrogenase, zinc-containing.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2465	1557	431	464	13			
1	B	334	Total	C	N	O	S	0	0	0
			2469	1563	431	461	14			
1	C	319	Total	C	N	O	S	0	0	0
			2352	1490	415	434	13			
1	D	329	Total	C	N	O	S	0	0	0
			2439	1547	430	448	14			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP E1V3M3
A	-19	GLY	-	expression tag	UNP E1V3M3
A	-18	SER	-	expression tag	UNP E1V3M3
A	-17	SER	-	expression tag	UNP E1V3M3
A	-16	HIS	-	expression tag	UNP E1V3M3
A	-15	HIS	-	expression tag	UNP E1V3M3
A	-14	HIS	-	expression tag	UNP E1V3M3
A	-13	HIS	-	expression tag	UNP E1V3M3
A	-12	HIS	-	expression tag	UNP E1V3M3
A	-11	HIS	-	expression tag	UNP E1V3M3
A	-10	SER	-	expression tag	UNP E1V3M3
A	-9	SER	-	expression tag	UNP E1V3M3
A	-8	GLY	-	expression tag	UNP E1V3M3
A	-7	LEU	-	expression tag	UNP E1V3M3
A	-6	VAL	-	expression tag	UNP E1V3M3
A	-5	PRO	-	expression tag	UNP E1V3M3
A	-4	ARG	-	expression tag	UNP E1V3M3
A	-3	GLY	-	expression tag	UNP E1V3M3
A	-2	SER	-	expression tag	UNP E1V3M3
A	-1	HIS	-	expression tag	UNP E1V3M3
A	1	VAL	-	insertion	UNP E1V3M3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP E1V3M3
B	-19	GLY	-	expression tag	UNP E1V3M3
B	-18	SER	-	expression tag	UNP E1V3M3
B	-17	SER	-	expression tag	UNP E1V3M3
B	-16	HIS	-	expression tag	UNP E1V3M3
B	-15	HIS	-	expression tag	UNP E1V3M3
B	-14	HIS	-	expression tag	UNP E1V3M3
B	-13	HIS	-	expression tag	UNP E1V3M3
B	-12	HIS	-	expression tag	UNP E1V3M3
B	-11	HIS	-	expression tag	UNP E1V3M3
B	-10	SER	-	expression tag	UNP E1V3M3
B	-9	SER	-	expression tag	UNP E1V3M3
B	-8	GLY	-	expression tag	UNP E1V3M3
B	-7	LEU	-	expression tag	UNP E1V3M3
B	-6	VAL	-	expression tag	UNP E1V3M3
B	-5	PRO	-	expression tag	UNP E1V3M3
B	-4	ARG	-	expression tag	UNP E1V3M3
B	-3	GLY	-	expression tag	UNP E1V3M3
B	-2	SER	-	expression tag	UNP E1V3M3
B	-1	HIS	-	expression tag	UNP E1V3M3
B	1	VAL	-	insertion	UNP E1V3M3
C	-20	MET	-	initiating methionine	UNP E1V3M3
C	-19	GLY	-	expression tag	UNP E1V3M3
C	-18	SER	-	expression tag	UNP E1V3M3
C	-17	SER	-	expression tag	UNP E1V3M3
C	-16	HIS	-	expression tag	UNP E1V3M3
C	-15	HIS	-	expression tag	UNP E1V3M3
C	-14	HIS	-	expression tag	UNP E1V3M3
C	-13	HIS	-	expression tag	UNP E1V3M3
C	-12	HIS	-	expression tag	UNP E1V3M3
C	-11	HIS	-	expression tag	UNP E1V3M3
C	-10	SER	-	expression tag	UNP E1V3M3
C	-9	SER	-	expression tag	UNP E1V3M3
C	-8	GLY	-	expression tag	UNP E1V3M3
C	-7	LEU	-	expression tag	UNP E1V3M3
C	-6	VAL	-	expression tag	UNP E1V3M3
C	-5	PRO	-	expression tag	UNP E1V3M3
C	-4	ARG	-	expression tag	UNP E1V3M3
C	-3	GLY	-	expression tag	UNP E1V3M3
C	-2	SER	-	expression tag	UNP E1V3M3
C	-1	HIS	-	expression tag	UNP E1V3M3
C	1	VAL	-	insertion	UNP E1V3M3

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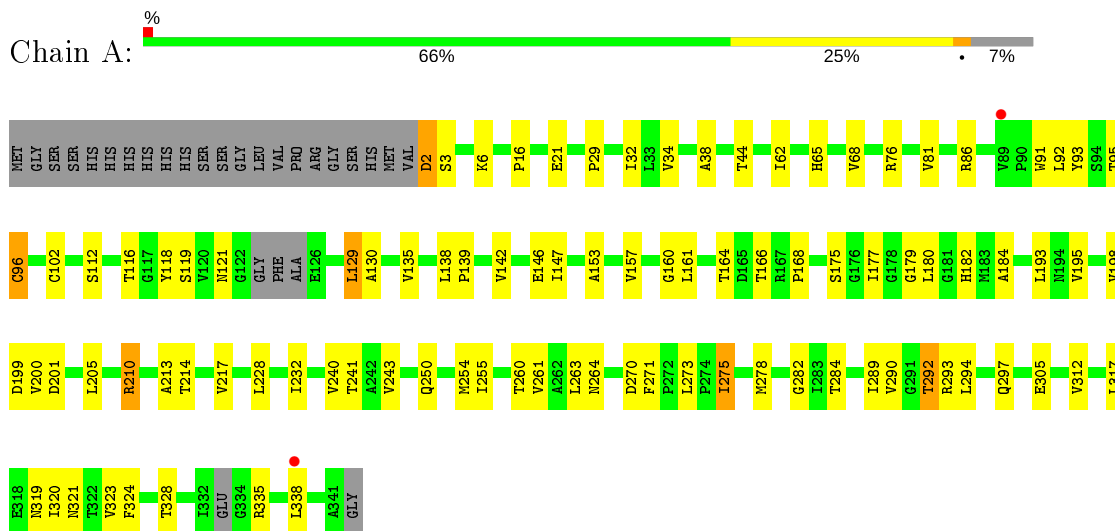| Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP E1V3M3
D	-19	GLY	-	expression tag	UNP E1V3M3
D	-18	SER	-	expression tag	UNP E1V3M3
D	-17	SER	-	expression tag	UNP E1V3M3
D	-16	HIS	-	expression tag	UNP E1V3M3
D	-15	HIS	-	expression tag	UNP E1V3M3
D	-14	HIS	-	expression tag	UNP E1V3M3
D	-13	HIS	-	expression tag	UNP E1V3M3
D	-12	HIS	-	expression tag	UNP E1V3M3
D	-11	HIS	-	expression tag	UNP E1V3M3
D	-10	SER	-	expression tag	UNP E1V3M3
D	-9	SER	-	expression tag	UNP E1V3M3
D	-8	GLY	-	expression tag	UNP E1V3M3
D	-7	LEU	-	expression tag	UNP E1V3M3
D	-6	VAL	-	expression tag	UNP E1V3M3
D	-5	PRO	-	expression tag	UNP E1V3M3
D	-4	ARG	-	expression tag	UNP E1V3M3
D	-3	GLY	-	expression tag	UNP E1V3M3
D	-2	SER	-	expression tag	UNP E1V3M3
D	-1	HIS	-	expression tag	UNP E1V3M3
D	1	VAL	-	insertion	UNP E1V3M3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

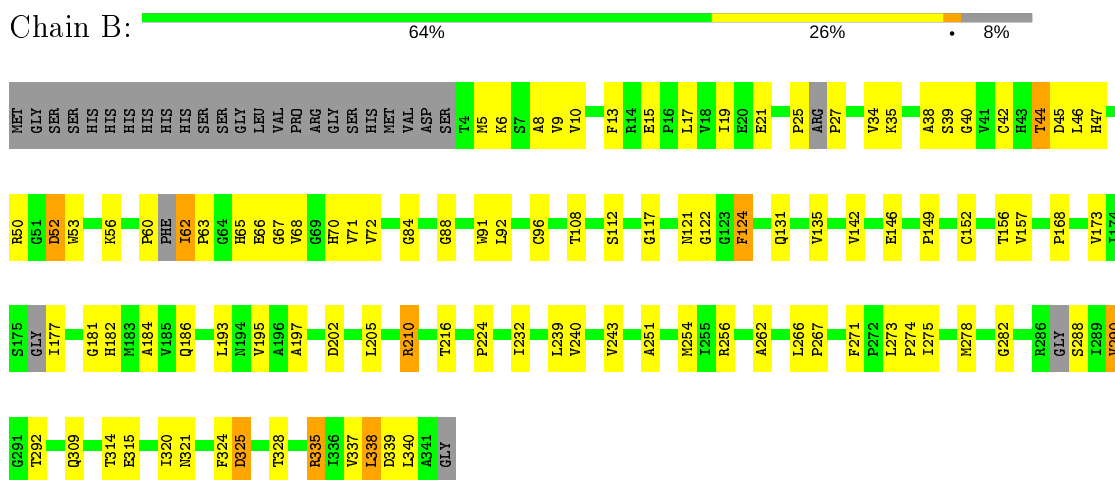| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

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.
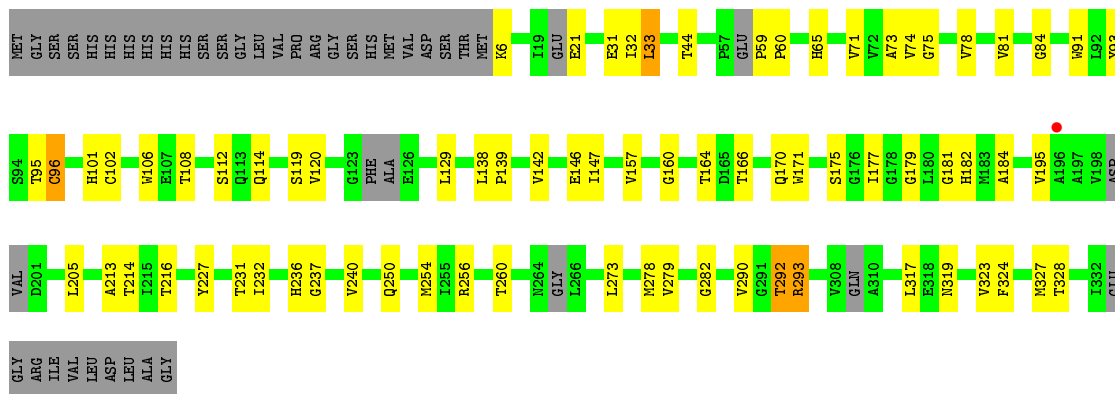
- Molecule 1: Alcohol dehydrogenase, zinc-containing

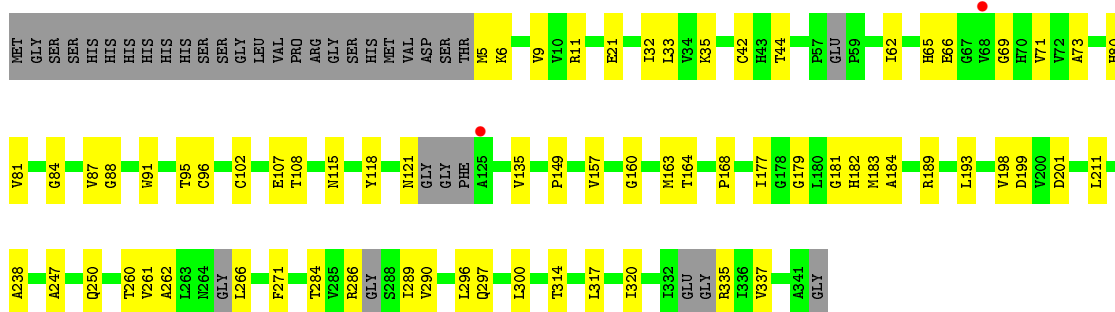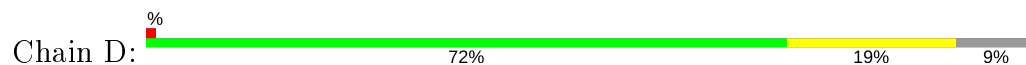- Molecule 1: Alcohol dehydrogenase, zinc-containing

- Molecule 1: Alcohol dehydrogenase, zinc-containing

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET VAL ASP SER THR MET K6 I19 GLU E21 E31 I32 L33 T44 P57 GLU P59 P60 H65 V71 V72 A73 V74 G75 V78 V81 G84 W91 L92 Y93

S94 T95 C96 H101 C102 W106 E107 T108 S112 Q113 Q114 S119 V120 G123 PHE ALA E126 L129 L138 P139 V142 E146 I147 V157 G160 T164 D185 T166 Q170 W171 S175 G176 I177 G178 G179 L180 G181 H182 M183 A184 V195 A196 A197 V198 ASP

VAL D201 L205 A213 T214 I215 T216 Y227 T231 I232 H236 G237 V240 Q250 M254 I255 R256 T260 N264 GLY L266 L273 M278 V279 G282 V290 G291 T292 R293 V308 GLN A310 L317 E318 N319 V323 F324 M327 T328 I332 GLU

GLY ARG ILE VAL LEU ASP LEU ALA GLY

• Molecule 1: Alcohol dehydrogenase, zinc-containing

Chain D:

%

72% 19% 9%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET VAL ASP SER THR M5 K6 V9 V10 R11 E21 I32 L33 V34 K35 C42 H43 T44 P57 GLU P59 I62 H65 E66 G67 V68 G69 H70 V71 V72 A73 H80

V81 G84 V87 G88 W91 T95 C96 C102 E107 T108 N115 Y118 N121 GLY PHE A125 V135 P149 V157 G160 M163 T164 P168 I177 G178 G179 L180 G181 H182 M183 A184 R189 L193 V198 D199 V200 D201 L211

A238 A247 Q250 T260 V261 A262 L263 N264 GLY L266 F271 T284 V285 R286 GLY S288 I289 V290 L296 Q297 L300 T314 L317 I320 I332 GLU GLY R335 I336 V337 A341 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	104.66Å 104.66Å 516.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 4.00 48.50 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.50-4.00) 99.9 (48.50-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.21 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.329 , 0.367 0.329 , 0.367	Depositor DCC
R_{free} test set	1516 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	154.8	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 228.5	EDS
L-test for twinning[2]	$<\lvert L \rvert> = 0.42$, $<L^2> = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9733	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\lvert L \rvert>$, $<L^2>$ 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: 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	0.35	0/2513	0.55	0/3425
1	B	0.34	0/2517	0.59	1/3424 (0.0%)
1	C	0.32	0/2398	0.54	1/3260 (0.0%)
1	D	0.35	0/2486	0.56	0/3382
All	All	0.34	0/9914	0.56	2/13491 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	325	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	33	LEU	CA-CB-CG	5.11	127.05	115.30

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	2465	0	2434	64	0
1	B	2469	0	2452	80	0
1	C	2352	0	2329	37	0
1	D	2439	0	2433	34	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
All	All	9733	0	9648	207	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 13.

All (207) 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:40:GLY:HA3	1:B:66:GLU:HB2	1.54	0.89
1:B:124:PHE:HZ	1:B:320:ILE:HG12	1.38	0.89
1:B:156:THR:HG22	1:B:290:VAL:H	1.40	0.85
1:B:251:ALA:HA	1:B:254:MET:HE2	1.60	0.81
1:A:16:PRO:HB3	1:A:321:ASN:HD21	1.48	0.78
1:A:175:SER:HA	1:A:198:VAL:HG22	1.65	0.78
1:B:38:ALA:HB2	1:B:68:VAL:HG22	1.63	0.78
1:A:6:LYS:HA	1:A:21:GLU:HA	1.66	0.78
1:D:6:LYS:HA	1:D:21:GLU:HA	1.66	0.75
1:B:177:ILE:HA	1:B:181:GLY:HA3	1.69	0.75
1:A:312:VAL:HG12	1:A:335:ARG:HB3	1.68	0.74
1:B:124:PHE:CZ	1:B:320:ILE:HG12	2.22	0.74
1:D:177:ILE:HA	1:D:181:GLY:HA3	1.70	0.73
1:C:33:LEU:HB3	1:C:73:ALA:HB3	1.72	0.71
1:A:273:LEU:N	1:B:271:PHE:O	2.24	0.71
1:B:5:MET:HG2	1:B:6:LYS:H	1.56	0.70
1:A:2:ASP:OD1	1:A:2:ASP:N	2.27	0.67
1:B:38:ALA:HB3	1:B:68:VAL:H	1.60	0.66
1:B:156:THR:HG22	1:B:290:VAL:N	2.09	0.66
1:A:139:PRO:HD2	1:A:147:ILE:HD13	1.78	0.65
1:A:255:ILE:HD12	1:A:261:VAL:HG22	1.78	0.65
1:B:38:ALA:CB	1:B:68:VAL:HG22	2.27	0.64
1:A:62:ILE:HB	1:A:121:ASN:HB3	1.80	0.64
1:B:157:VAL:HG11	1:B:184:ALA:HA	1.80	0.64
1:D:177:ILE:H	1:D:199:ASP:HB2	1.65	0.62
1:A:157:VAL:HG11	1:A:184:ALA:HA	1.80	0.62
1:B:320:ILE:HG13	1:B:324:PHE:HE1	1.65	0.62
1:A:195:VAL:HG23	1:A:213:ALA:HA	1.82	0.61
1:A:32:ILE:HD11	1:A:81:VAL:HG11	1.81	0.61
1:C:195:VAL:HG23	1:C:213:ALA:HA	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PRO:O	1:B:62:ILE:N	2.34	0.60
1:A:240:VAL:HB	1:A:263:LEU:HD23	1.83	0.60
1:A:175:SER:OG	1:A:240:VAL:HA	2.02	0.59
1:A:324:PHE:O	1:A:328:THR:HG23	2.02	0.59
1:C:278:MET:O	1:C:282:GLY:N	2.36	0.59
1:B:52:ASP:OD1	1:B:52:ASP:N	2.30	0.58
1:B:5:MET:O	1:B:21:GLU:HA	2.03	0.58
1:D:32:ILE:HD11	1:D:81:VAL:HG11	1.86	0.58
1:C:250:GLN:O	1:C:254:MET:HG3	2.04	0.57
1:A:146:GLU:N	1:A:146:GLU:OE2	2.37	0.57
1:A:95:THR:HB	1:A:102:CYS:SG	2.45	0.57
1:B:25:PRO:C	1:B:27:PRO:HD3	2.25	0.57
1:D:296:LEU:O	1:D:300:LEU:HG	2.05	0.57
1:A:275:ILE:HD11	1:B:267:PRO:HG2	1.86	0.57
1:B:62:ILE:HG22	1:B:124:PHE:HB2	1.86	0.56
1:B:62:ILE:HB	1:B:122:GLY:H	1.70	0.56
1:D:317:LEU:O	1:D:320:ILE:HG13	2.05	0.56
1:C:96:CYS:HB3	1:C:112:SER:HB2	1.88	0.56
1:B:96:CYS:HB3	1:B:112:SER:HB2	1.87	0.56
1:B:202:ASP:HA	1:B:205:LEU:HB2	1.88	0.56
1:C:157:VAL:HG11	1:C:184:ALA:HA	1.88	0.55
1:A:65:HIS:HB2	1:A:91:TRP:HA	1.87	0.55
1:A:271:PHE:O	1:B:273:LEU:N	2.28	0.55
1:B:65:HIS:HB2	1:B:91:TRP:HA	1.87	0.55
1:B:8:ALA:HB2	1:B:19:ILE:HG12	1.88	0.55
1:A:210:ARG:HB3	1:A:210:ARG:HH11	1.71	0.55
1:B:320:ILE:HG13	1:B:324:PHE:CE1	2.41	0.54
1:C:138:LEU:HD22	1:C:147:ILE:HG21	1.90	0.54
1:A:93:TYR:CE1	1:A:130:ALA:HA	2.43	0.54
1:A:142:VAL:HB	1:A:147:ILE:HD11	1.89	0.54
1:B:239:LEU:HA	1:B:262:ALA:HB3	1.88	0.54
1:D:42:CYS:HB2	1:D:66:GLU:OE2	2.07	0.54
1:A:320:ILE:HB	1:A:338:LEU:HD21	1.88	0.53
1:A:175:SER:HA	1:A:198:VAL:CG2	2.36	0.53
1:B:9:VAL:HG11	1:B:60:PRO:HB2	1.91	0.53
1:D:157:VAL:HG11	1:D:184:ALA:HA	1.90	0.53
1:B:46:LEU:HA	1:B:324:PHE:HE2	1.72	0.53
1:D:149:PRO:HB3	1:D:335:ARG:HG2	1.89	0.52
1:B:17:LEU:H	1:B:321:ASN:HD21	1.56	0.52
1:D:33:LEU:HB3	1:D:73:ALA:HB3	1.92	0.52
1:D:182:HIS:HB2	1:D:211:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:HIS:CD2	1:B:50:ARG:HD2	2.44	0.52
1:B:168:PRO:HA	1:B:193:LEU:HD23	1.91	0.52
1:B:35:LYS:H	1:B:72:VAL:HG23	1.75	0.51
1:A:179:GLY:O	1:A:182:HIS:ND1	2.44	0.51
1:C:71:VAL:HB	1:C:84:GLY:H	1.75	0.51
1:B:38:ALA:HB3	1:B:68:VAL:N	2.24	0.51
1:C:232:ILE:O	1:C:256:ARG:NH2	2.43	0.51
1:B:46:LEU:HA	1:B:324:PHE:CE2	2.46	0.51
1:A:138:LEU:HD22	1:A:147:ILE:HG21	1.93	0.51
1:A:275:ILE:HD12	1:B:243:VAL:HG11	1.92	0.51
1:C:177:ILE:HA	1:C:181:GLY:HA3	1.94	0.49
1:A:228:LEU:HD22	1:A:232:ILE:HD12	1.95	0.49
1:B:45:ASP:OD1	1:B:65:HIS:CE1	2.66	0.49
1:C:65:HIS:HB2	1:C:91:TRP:HA	1.93	0.49
1:A:93:TYR:HE1	1:A:130:ALA:HA	1.76	0.49
1:D:65:HIS:HB2	1:D:91:TRP:HA	1.95	0.49
1:B:210:ARG:HB3	1:B:210:ARG:HH11	1.78	0.49
1:B:339:ASP:OD1	1:B:340:LEU:N	2.45	0.49
1:C:160:GLY:O	1:C:164:THR:HG23	2.13	0.49
1:C:139:PRO:HD2	1:C:147:ILE:HD13	1.95	0.49
1:D:95:THR:HG21	1:D:107:GLU:HB2	1.94	0.49
1:D:35:LYS:O	1:D:69:GLY:HA3	2.13	0.49
1:B:149:PRO:HB3	1:B:335:ARG:HG2	1.95	0.48
1:B:34:VAL:HG12	1:B:71:VAL:HA	1.95	0.48
1:D:88:GLY:O	1:D:135:VAL:HG13	2.14	0.48
1:B:71:VAL:HB	1:B:84:GLY:H	1.78	0.48
1:A:241:THR:HA	1:A:264:ASN:HB3	1.95	0.48
1:A:292:THR:OG1	1:A:293:ARG:N	2.47	0.48
1:A:317:LEU:O	1:A:320:ILE:HG22	2.13	0.48
1:C:32:ILE:O	1:C:129:LEU:HA	2.14	0.48
1:A:270:ASP:CG	1:B:274:PRO:HG3	2.34	0.47
1:A:177:ILE:HG12	1:A:199:ASP:HB2	1.96	0.47
1:A:32:ILE:HG22	1:A:34:VAL:HG23	1.95	0.47
1:C:95:THR:HB	1:C:102:CYS:SG	2.54	0.47
1:B:38:ALA:O	1:B:67:GLY:HA2	2.14	0.47
1:C:319:ASN:O	1:C:323:VAL:HG23	2.14	0.47
1:D:247:ALA:HA	1:D:250:GLN:HG2	1.96	0.47
1:A:275:ILE:HD11	1:B:267:PRO:CG	2.44	0.47
1:B:47:HIS:HD2	1:B:50:ARG:HD2	1.79	0.47
1:B:68:VAL:HG12	1:B:88:GLY:HA3	1.96	0.47
1:C:175:SER:OG	1:C:240:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:CYS:HB2	1:B:66:GLU:OE2	2.15	0.46
1:A:86:ARG:NH1	1:A:139:PRO:O	2.48	0.46
1:B:152:CYS:O	1:B:156:THR:HG23	2.15	0.46
1:A:38:ALA:HA	1:A:338:LEU:O	2.16	0.46
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.77	0.46
1:A:93:TYR:HB2	1:A:116:THR:HG23	1.97	0.46
1:C:142:VAL:HG12	1:C:146:GLU:HB2	1.97	0.46
1:B:142:VAL:HG12	1:B:146:GLU:HB2	1.98	0.45
1:D:179:GLY:O	1:D:183:MET:HG2	2.16	0.45
1:B:314:THR:HA	1:B:337:VAL:O	2.16	0.45
1:A:289:ILE:HG13	1:A:290:VAL:HG22	1.99	0.45
1:B:13:PHE:O	1:B:15:GLU:HG2	2.17	0.45
1:B:5:MET:HG2	1:B:6:LYS:N	2.27	0.45
1:A:198:VAL:HA	1:A:217:VAL:HG13	1.99	0.45
1:A:210:ARG:HB3	1:A:210:ARG:NH1	2.32	0.45
1:A:32:ILE:O	1:A:129:LEU:HA	2.16	0.45
1:C:227:TYR:O	1:C:231:THR:OG1	2.27	0.45
1:B:197:ALA:HB3	1:B:216:THR:HG22	1.99	0.44
1:B:62:ILE:HD12	1:B:121:ASN:HB3	1.98	0.44
1:C:205:LEU:HD22	1:C:216:THR:HB	1.99	0.44
1:A:65:HIS:CD2	1:A:91:TRP:HB2	2.52	0.44
1:A:153:ALA:HB1	1:A:180:LEU:HG	2.00	0.44
1:B:62:ILE:HG22	1:B:124:PHE:CB	2.47	0.44
1:D:66:GLU:OE1	1:D:335:ARG:NH2	2.50	0.44
1:C:237:GLY:HA2	1:C:260:THR:O	2.17	0.44
1:D:87:VAL:HB	1:D:135:VAL:CG1	2.47	0.44
1:A:195:VAL:CG2	1:A:213:ALA:HA	2.46	0.44
1:B:243:VAL:HG12	1:B:271:PHE:HE2	1.83	0.44
1:D:314:THR:HA	1:D:337:VAL:O	2.16	0.44
1:A:240:VAL:HG12	1:A:243:VAL:HG22	1.99	0.44
1:D:160:GLY:O	1:D:164:THR:HG23	2.18	0.44
1:C:31:GLU:O	1:C:75:GLY:N	2.51	0.44
1:B:278:MET:O	1:B:282:GLY:N	2.51	0.43
1:B:34:VAL:HB	1:B:70:HIS:O	2.17	0.43
1:C:324:PHE:O	1:C:328:THR:HG23	2.17	0.43
1:D:71:VAL:HB	1:D:84:GLY:H	1.84	0.43
1:D:95:THR:HB	1:D:102:CYS:SG	2.58	0.43
1:A:96:CYS:HB3	1:A:112:SER:HB2	2.00	0.43
1:D:238:ALA:O	1:D:262:ALA:N	2.44	0.43
1:A:160:GLY:O	1:A:164:THR:HG23	2.18	0.43
1:B:35:LYS:H	1:B:72:VAL:CG2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HG22	1:B:62:ILE:HG23	2.01	0.43
1:C:179:GLY:HA2	1:C:182:HIS:HD1	1.84	0.43
1:D:260:THR:HG22	1:D:284:THR:OG1	2.18	0.43
1:A:250:GLN:O	1:A:254:MET:HG3	2.18	0.43
1:C:195:VAL:CG2	1:C:213:ALA:HA	2.48	0.43
1:A:29:PRO:HA	1:A:76:ARG:H	1.82	0.43
1:A:157:VAL:CG1	1:A:184:ALA:HA	2.49	0.43
1:A:199:ASP:HB3	1:A:205:LEU:HG	2.00	0.43
1:B:232:ILE:O	1:B:256:ARG:NH2	2.52	0.42
1:A:62:ILE:H	1:A:121:ASN:CG	2.22	0.42
1:B:9:VAL:HG12	1:B:10:VAL:H	1.83	0.42
1:A:68:VAL:HB	1:A:138:LEU:HD11	2.00	0.42
1:C:279:VAL:HB	1:D:266:LEU:HD21	2.01	0.42
1:A:177:ILE:CG1	1:A:199:ASP:HB2	2.49	0.42
1:B:173:VAL:HG11	1:B:254:MET:CE	2.49	0.42
1:C:292:THR:OG1	1:C:293:ARG:N	2.53	0.42
1:C:59:PRO:HA	1:C:60:PRO:HD3	1.86	0.42
1:C:74:VAL:HB	1:C:78:VAL:HG11	2.01	0.42
1:D:62:ILE:HB	1:D:121:ASN:HB3	2.02	0.42
1:A:278:MET:O	1:A:282:GLY:N	2.52	0.42
1:C:101:HIS:HB3	1:C:106:TRP:O	2.19	0.42
1:B:186:GLN:OE1	1:B:309:GLN:N	2.44	0.42
1:B:17:LEU:N	1:B:321:ASN:HD21	2.17	0.42
1:D:168:PRO:HA	1:D:193:LEU:HD23	2.00	0.42
1:D:266:LEU:HD11	1:D:289:ILE:HD13	2.00	0.42
1:A:168:PRO:HA	1:A:193:LEU:HD23	2.01	0.42
1:A:319:ASN:O	1:A:323:VAL:HG23	2.20	0.42
1:B:25:PRO:O	1:B:27:PRO:HD3	2.20	0.42
1:D:163:MET:O	1:D:286:ARG:HD2	2.19	0.42
1:B:224:PRO:HB2	1:B:254:MET:SD	2.60	0.41
1:D:115:ASN:HB2	1:D:118:TYR:HB3	2.02	0.41
1:A:142:VAL:HG12	1:A:146:GLU:HB2	2.02	0.41
1:B:40:GLY:CA	1:B:66:GLU:HB2	2.37	0.41
1:A:164:THR:O	1:A:166:THR:HG23	2.20	0.41
1:B:240:VAL:HG12	1:B:243:VAL:HG22	2.02	0.41
1:C:6:LYS:HA	1:C:21:GLU:HA	2.03	0.41
1:B:62:ILE:HA	1:B:63:PRO:HD3	1.93	0.41
1:C:164:THR:O	1:C:166:THR:HG23	2.20	0.41
1:C:171:TRP:H	1:C:236:HIS:CE1	2.39	0.41
1:C:93:TYR:HB3	1:C:114:GLN:O	2.20	0.41
1:D:198:VAL:HG12	1:D:198:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LEU:N	1:D:271:PHE:O	2.51	0.41
1:B:45:ASP:OD1	1:B:65:HIS:ND1	2.54	0.41
1:B:9:VAL:HG12	1:B:10:VAL:N	2.35	0.41
1:A:161:LEU:O	1:A:164:THR:OG1	2.29	0.41
1:B:39:SER:OG	1:B:338:LEU:N	2.54	0.41
1:B:320:ILE:CG1	1:B:324:PHE:HE1	2.34	0.41
1:B:44:THR:HG23	1:B:53:TRP:HH2	1.85	0.41
1:C:170:GLN:HB3	1:C:236:HIS:CG	2.56	0.41
1:B:315:GLU:O	1:B:338:LEU:HA	2.21	0.40
1:B:5:MET:CG	1:B:6:LYS:H	2.29	0.40
1:A:260:THR:HA	1:A:284:THR:O	2.22	0.40
1:B:62:ILE:O	1:B:117:GLY:HA2	2.21	0.40
1:D:80:HIS:CE1	1:D:81:VAL:HG12	2.56	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	330/363 (91%)	310 (94%)	20 (6%)	0	100	100
1	B	324/363 (89%)	312 (96%)	11 (3%)	1 (0%)	41	75
1	C	305/363 (84%)	290 (95%)	15 (5%)	0	100	100
1	D	317/363 (87%)	305 (96%)	12 (4%)	0	100	100
All	All	1276/1452 (88%)	1217 (95%)	58 (4%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	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	254/284 (89%)	236 (93%)	18 (7%)	14	42
1	B	258/284 (91%)	238 (92%)	20 (8%)	12	39
1	C	244/284 (86%)	232 (95%)	12 (5%)	25	52
1	D	254/284 (89%)	243 (96%)	11 (4%)	29	56
All	All	1010/1136 (89%)	949 (94%)	61 (6%)	19	47

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	SER
1	A	44	THR
1	A	92	LEU
1	A	96	CYS
1	A	118	TYR
1	A	119	SER
1	A	129	LEU
1	A	135	VAL
1	A	200	VAL
1	A	201	ASP
1	A	210	ARG
1	A	214	THR
1	A	275	ILE
1	A	292	THR
1	A	294	LEU
1	A	297	GLN
1	A	305	GLU
1	B	44	THR
1	B	52	ASP
1	B	56	LYS
1	B	62	ILE
1	B	92	LEU
1	B	108	THR

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Mol	Chain	Res	Type
1	B	124	PHE
1	B	131	GLN
1	B	135	VAL
1	B	182	HIS
1	B	195	VAL
1	B	210	ARG
1	B	266	LEU
1	B	275	ILE
1	B	288	SER
1	B	292	THR
1	B	325	ASP
1	B	328	THR
1	B	335	ARG
1	B	338	LEU
1	C	44	THR
1	C	81	VAL
1	C	96	CYS
1	C	108	THR
1	C	119	SER
1	C	120	VAL
1	C	214	THR
1	C	290	VAL
1	C	292	THR
1	C	293	ARG
1	C	317	LEU
1	C	327	MET
1	D	5	MET
1	D	9	VAL
1	D	11	ARG
1	D	44	THR
1	D	96	CYS
1	D	108	THR
1	D	189	ARG
1	D	201	ASP
1	D	261	VAL
1	D	290	VAL
1	D	297	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	115	ASN
1	A	297	GLN
1	A	321	ASN
1	B	47	HIS
1	B	131	GLN
1	B	321	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 8 ligands modelled in this entry, 8 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 (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	336/363 (92%)	-0.34	2 (0%)	89	84	72, 109, 167, 196	58 (17%)
1	B	334/363 (92%)	-0.41	0	100	100	63, 98, 123, 181	114 (34%)
1	C	319/363 (87%)	-0.31	1 (0%)	94	90	88, 131, 190, 216	110 (34%)
1	D	329/363 (90%)	-0.32	2 (0%)	89	84	81, 113, 150, 169	98 (29%)
All	All	1318/1452 (90%)	-0.35	5 (0%)	92	87	63, 111, 174, 216	380 (28%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	VAL	2.3
1	A	338	LEU	2.2
1	D	125	ALA	2.2
1	C	196	ALA	2.1
1	D	68	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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(Å^2)	Q<0.9
2	ZN	C	402	1/1	0.81	0.22	86,86,86,86	1
2	ZN	B	402	1/1	0.83	0.19	72,72,72,72	1
2	ZN	D	401	1/1	0.83	0.13	124,124,124,124	0
2	ZN	A	401	1/1	0.84	0.18	85,85,85,85	1
2	ZN	B	401	1/1	0.85	0.14	83,83,83,83	0
2	ZN	D	402	1/1	0.89	0.09	78,78,78,78	1
2	ZN	C	401	1/1	0.97	0.09	118,118,118,118	0
2	ZN	A	402	1/1	0.98	0.08	87,87,87,87	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 C 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
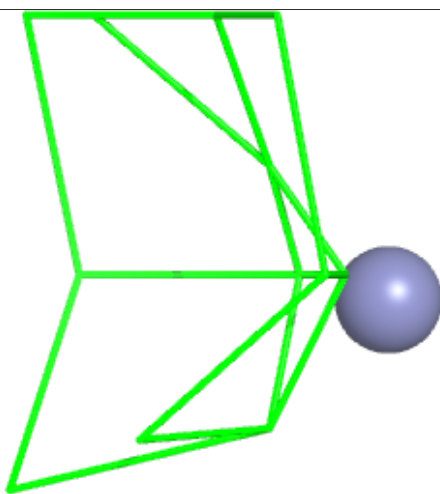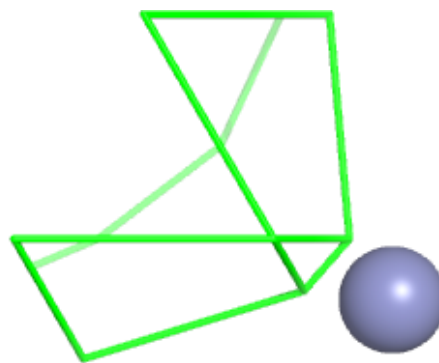and green (positive)
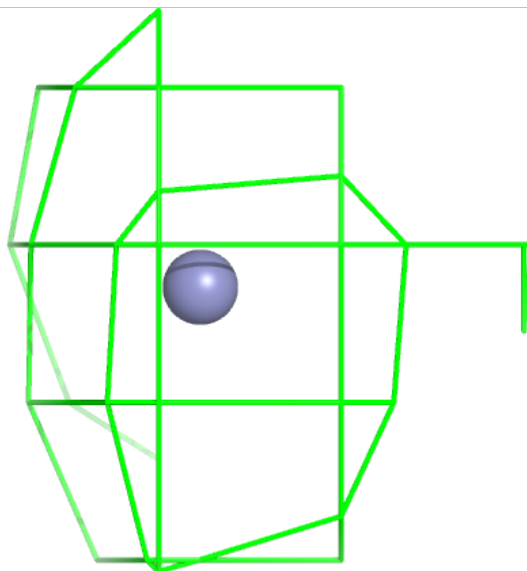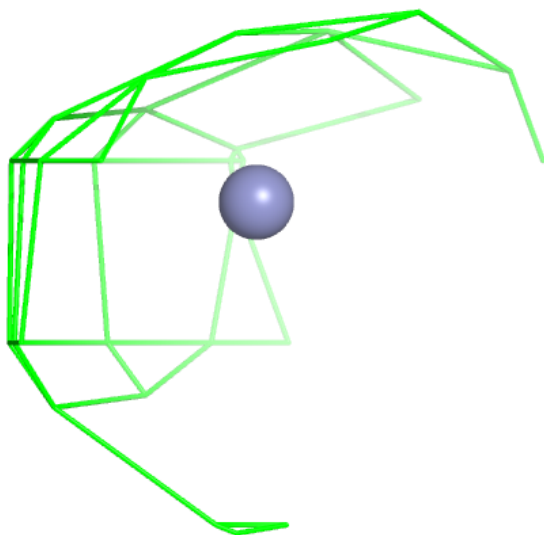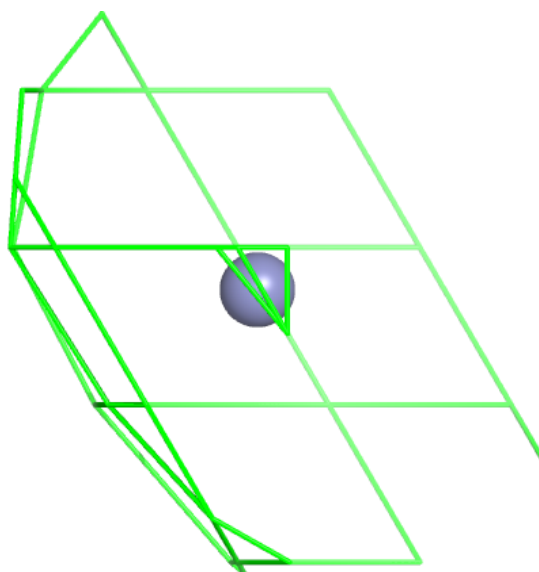
Electron density around ZN B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
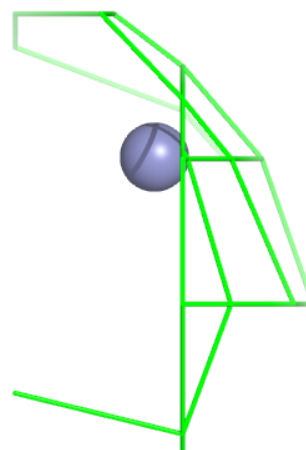mF_o-DF_c (at 3 rmsd) in purple (negative)
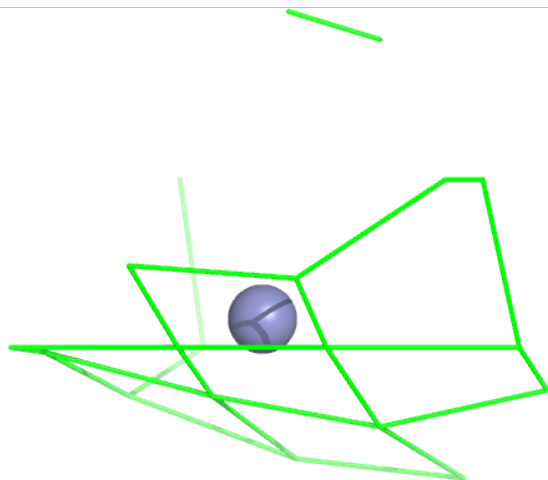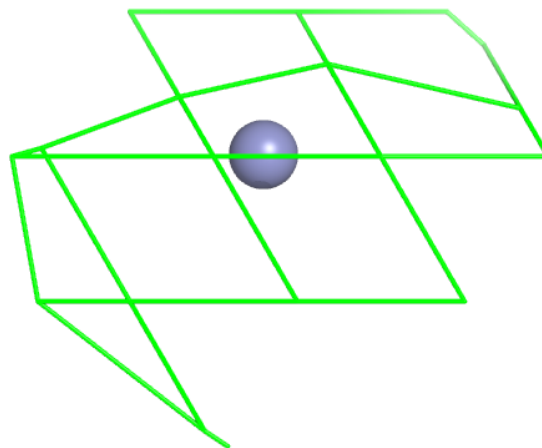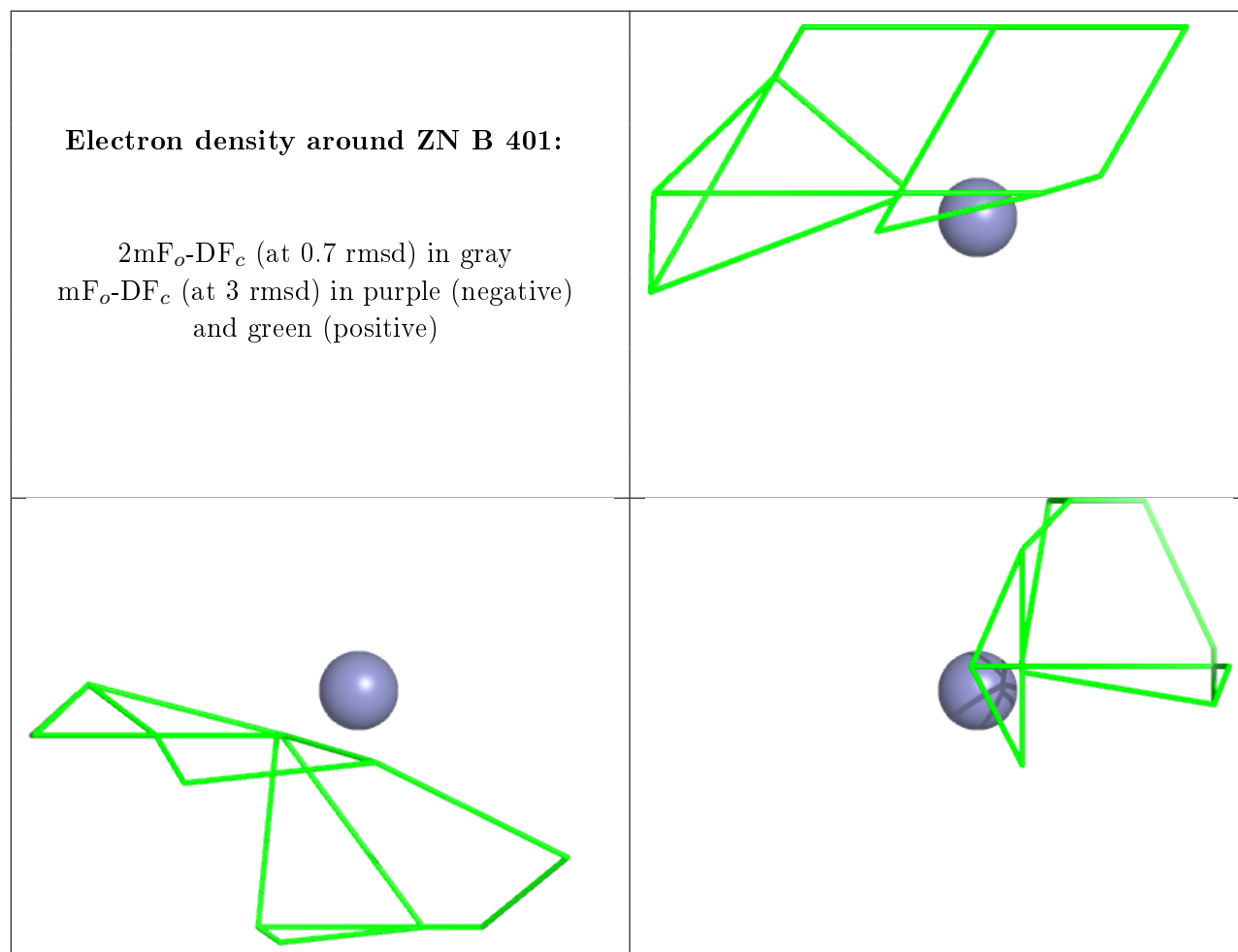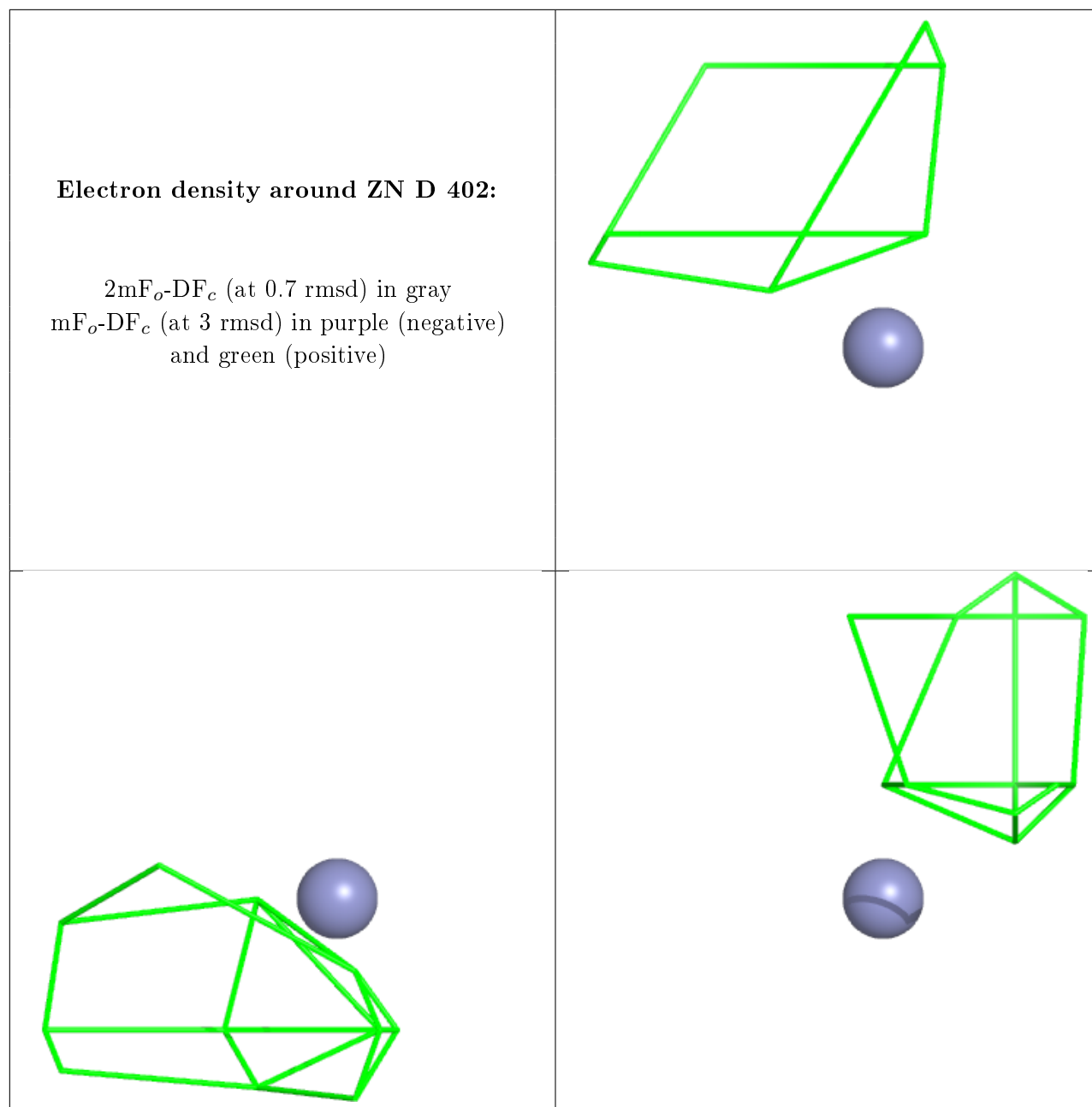and green (positive)
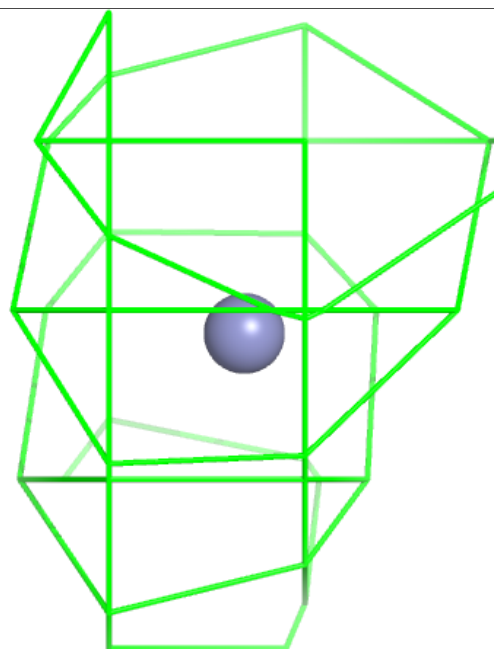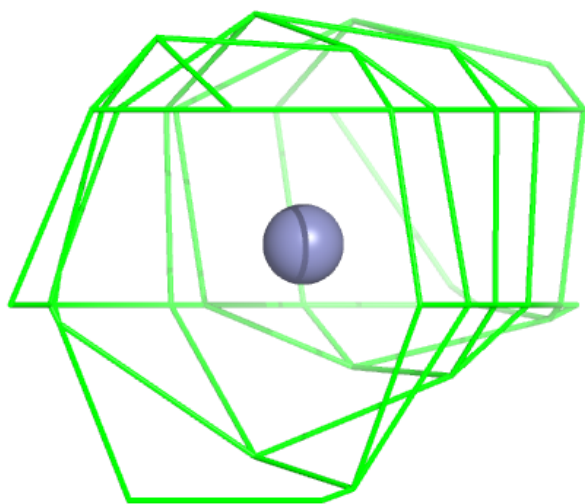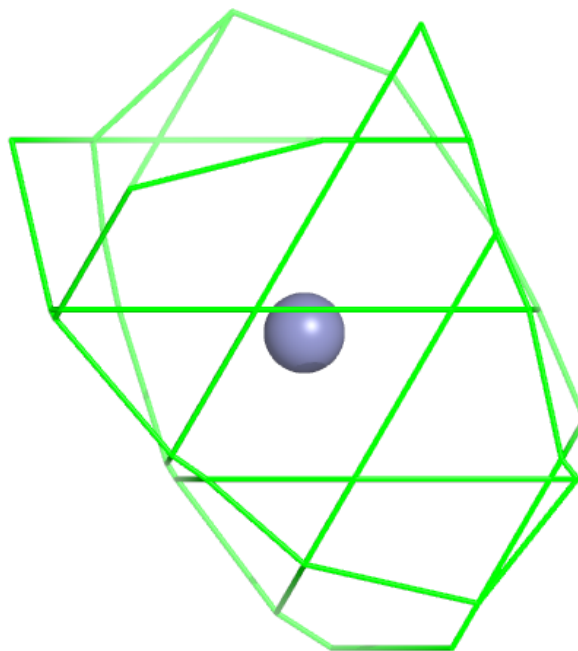
Electron density around ZN D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
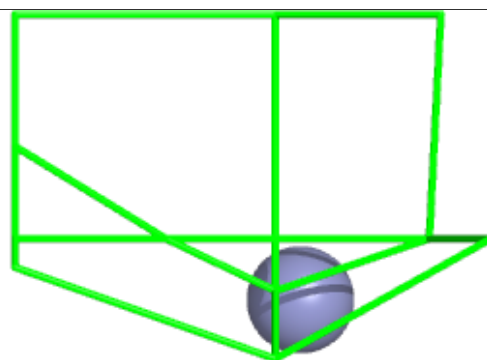
Electron density around ZN A 401:

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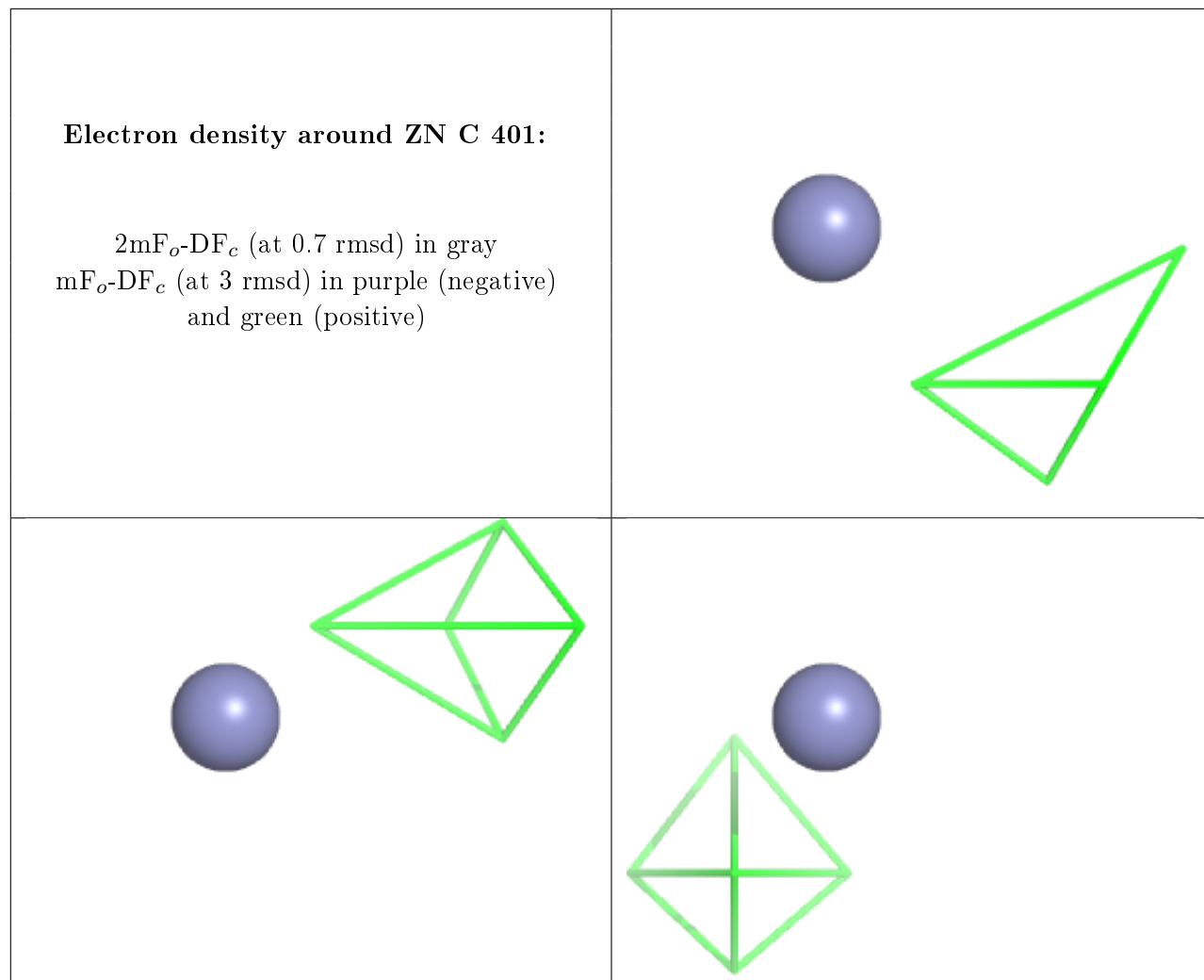$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

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 D 402:

$2mF_o$-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 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
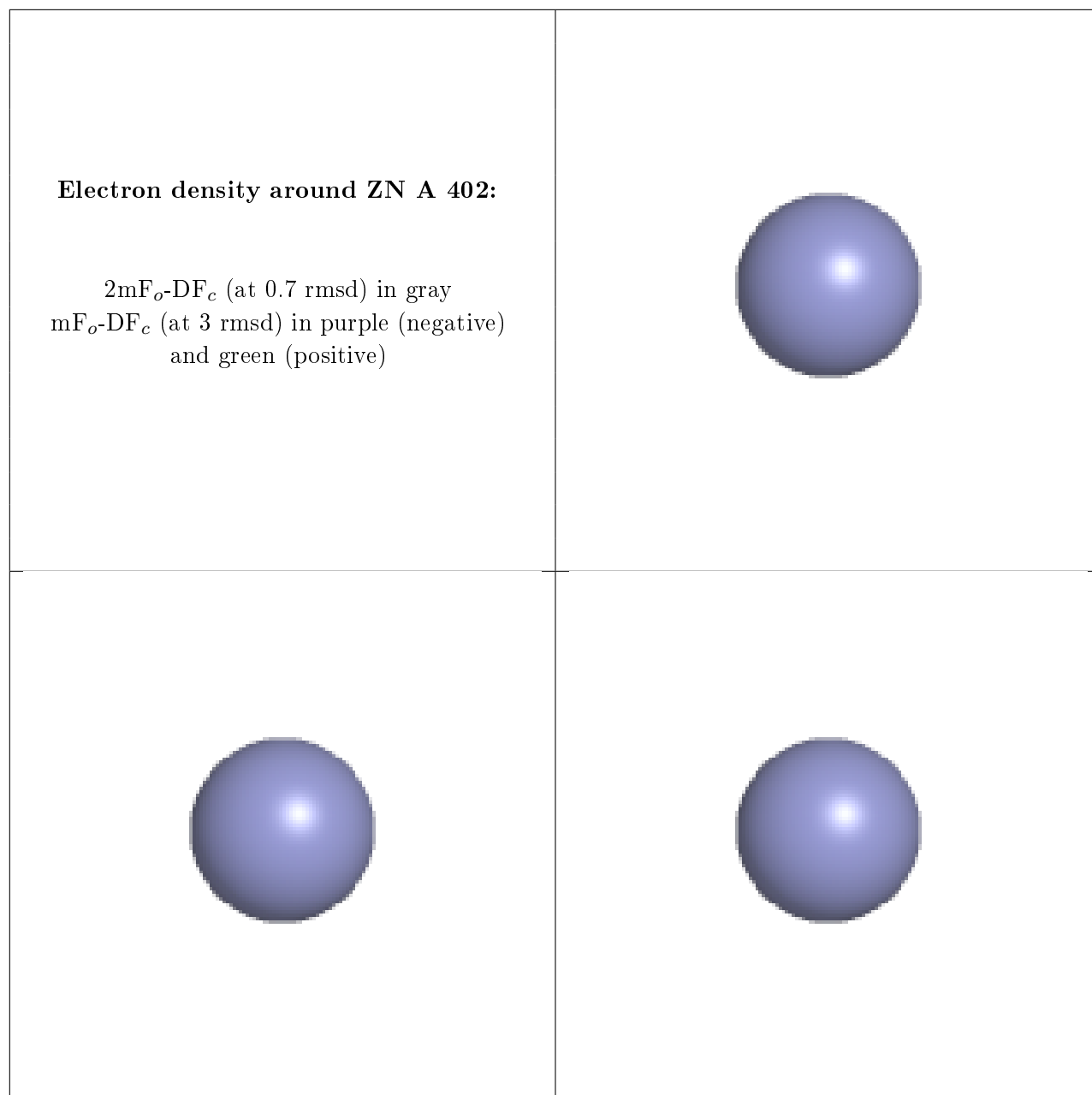
Electron density around ZN A 402:

$2mF_o$-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 (i)

There are no such residues in this entry.