Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 06:38 PM JST

PDB ID	:	8HFD
Title	:	Crystal structure of allantoinase from E. coli BL21
Authors	:	Lin, E.S.; Huang, H.Y.; Yang, P.C.; Liu, H.W.; Huang, C.Y.
Deposited on	:	2022-11-10
Resolution	:	2.07 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 (i) 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 (i)) were used in the production of this report:

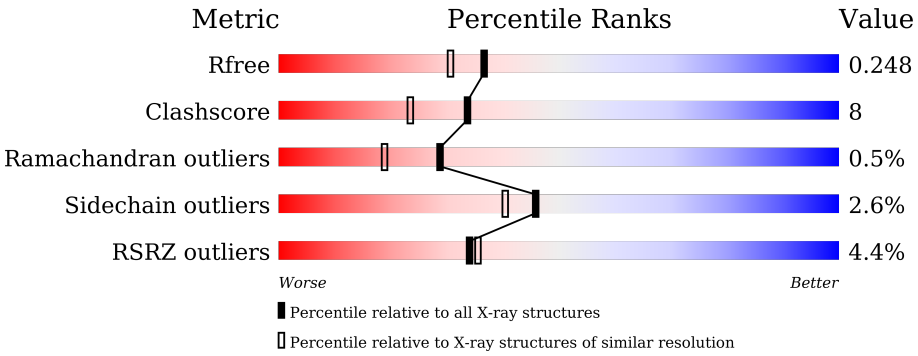
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	459	4% 82% 14%
1	B	459	4% 78% 17%
1	C	459	4% 82% 14%
1	D	459	5% 78% 17%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	C	501	-	-	X	-
2	PEG	D	502	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14819 atoms, of which 60 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 Allantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3473	2179	604	666	24			
1	B	447	Total	C	N	O	S	0	0	0
			3437	2160	596	658	23			
1	C	448	Total	C	N	O	S	0	0	0
			3448	2166	600	659	23			
1	D	445	Total	C	N	O	S	0	0	0
			3425	2152	594	656	23			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	HIS	-	expression tag	UNP A0A1V3VVF3
A	455	HIS	-	expression tag	UNP A0A1V3VVF3
A	456	HIS	-	expression tag	UNP A0A1V3VVF3
A	457	HIS	-	expression tag	UNP A0A1V3VVF3
A	458	HIS	-	expression tag	UNP A0A1V3VVF3
A	459	HIS	-	expression tag	UNP A0A1V3VVF3
B	454	HIS	-	expression tag	UNP A0A1V3VVF3
B	455	HIS	-	expression tag	UNP A0A1V3VVF3
B	456	HIS	-	expression tag	UNP A0A1V3VVF3
B	457	HIS	-	expression tag	UNP A0A1V3VVF3
B	458	HIS	-	expression tag	UNP A0A1V3VVF3
B	459	HIS	-	expression tag	UNP A0A1V3VVF3
C	454	HIS	-	expression tag	UNP A0A1V3VVF3
C	455	HIS	-	expression tag	UNP A0A1V3VVF3
C	456	HIS	-	expression tag	UNP A0A1V3VVF3
C	457	HIS	-	expression tag	UNP A0A1V3VVF3
C	458	HIS	-	expression tag	UNP A0A1V3VVF3
C	459	HIS	-	expression tag	UNP A0A1V3VVF3
D	454	HIS	-	expression tag	UNP A0A1V3VVF3
D	455	HIS	-	expression tag	UNP A0A1V3VVF3
D	456	HIS	-	expression tag	UNP A0A1V3VVF3

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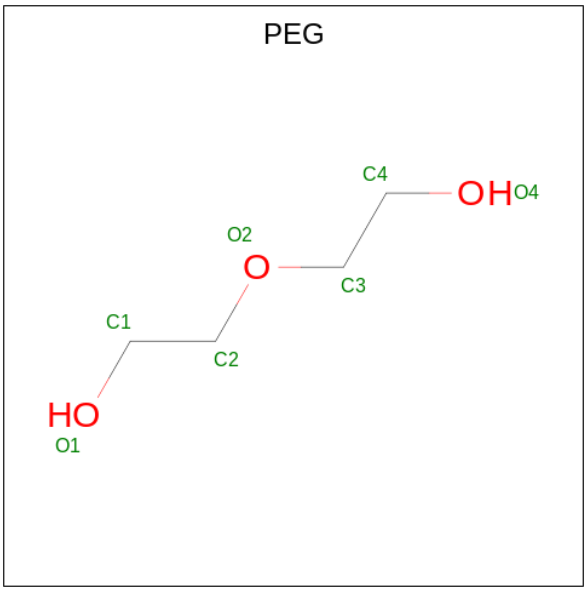
Chain	Residue	Modelled	Actual	Comment	Reference
D	457	HIS	-	expression tag	UNP A0A1V3VVF3
D	458	HIS	-	expression tag	UNP A0A1V3VVF3
D	459	HIS	-	expression tag	UNP A0A1V3VVF3

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		

- 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	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 water.

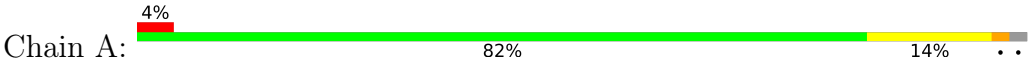
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	264	Total O 264 264	0	0
4	B	245	Total O 245 245	0	0
4	C	222	Total O 222 222	0	0
4	D	195	Total O 195 195	0	0

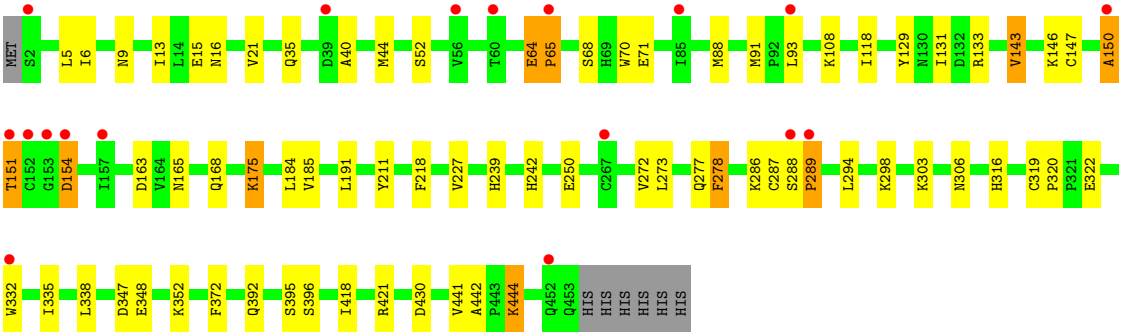
3 Residue-property plots (i)

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: Allantoinase

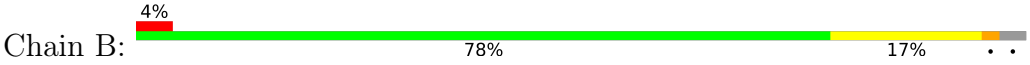
Chain A:

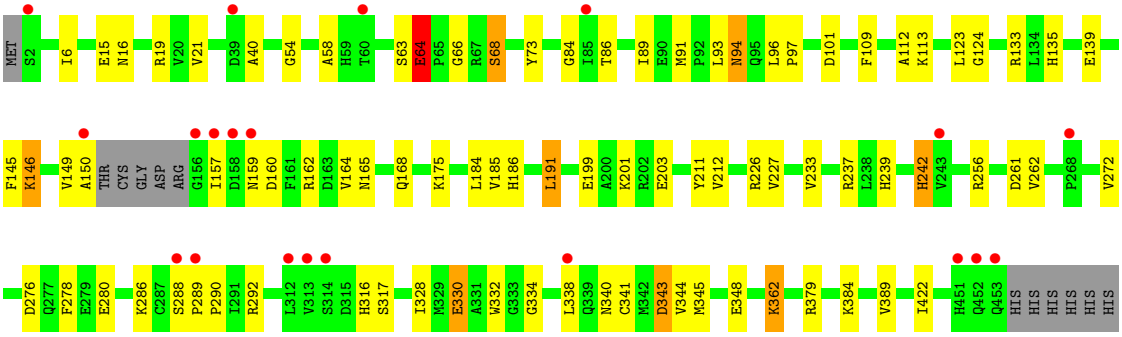




• Molecule 1: Allantoinase

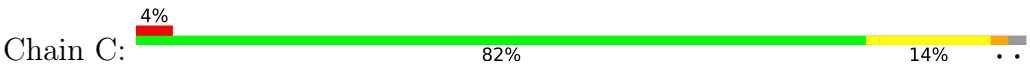
Chain B:

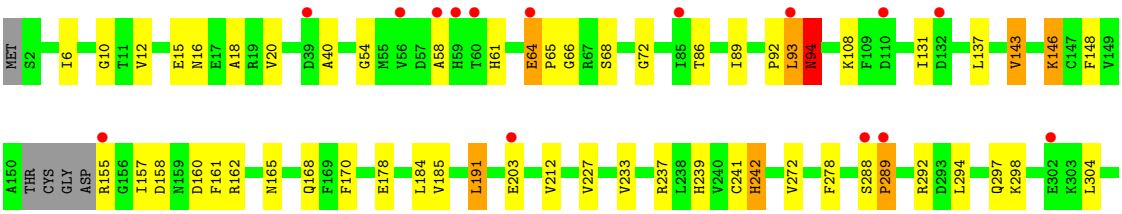


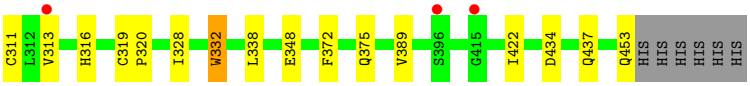


• Molecule 1: Allantoinase

Chain C:

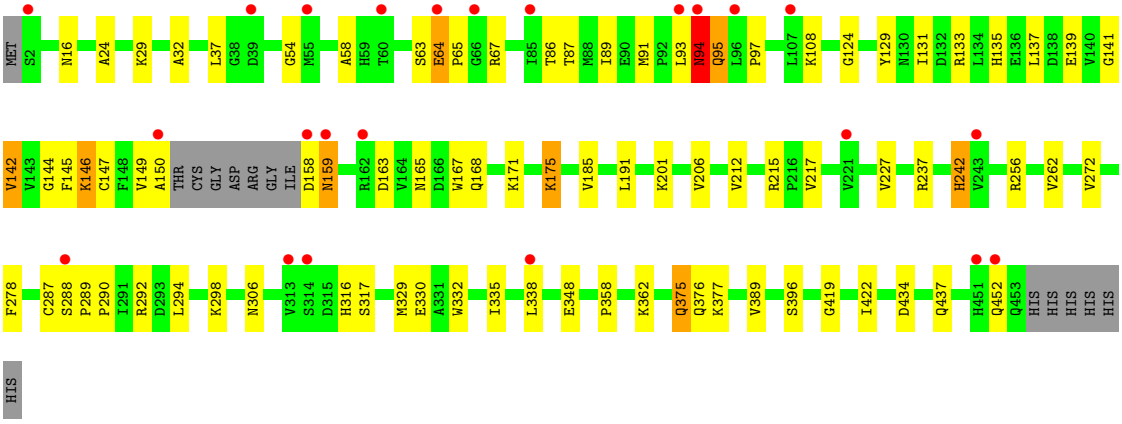






• Molecule 1: Allantoinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.16Å 77.14Å 144.85Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	29.92 – 2.07 29.92 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.92-2.07) 99.1 (29.92-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.92 (at 2.06Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.205 , 0.249 0.208 , 0.248	Depositor DCC
R_{free} test set	1997 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14819	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ZN, KCX

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	0.48	0/3525	0.69	3/4765 (0.1%)
1	B	0.48	0/3488	0.68	3/4714 (0.1%)
1	C	0.42	0/3499	0.65	2/4728 (0.0%)
1	D	0.44	0/3476	0.65	1/4698 (0.0%)
All	All	0.46	0/13988	0.67	9/18905 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	PRO	N-CA-C	-6.60	94.94	112.10
1	C	94	ASN	CB-CA-C	6.26	122.92	110.40
1	B	343	ASP	CB-CG-OD1	5.59	123.34	118.30
1	D	94	ASN	CB-CA-C	5.59	121.58	110.40
1	C	289	PRO	N-CA-C	-5.58	97.60	112.10
1	B	64	GLU	N-CA-C	5.55	125.97	111.00
1	B	94	ASN	CB-CA-C	5.39	121.18	110.40
1	A	65	PRO	N-CA-C	-5.38	98.11	112.10
1	A	150	ALA	CB-CA-C	5.19	117.88	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3473	0	3417	55	0
1	B	3437	0	3384	64	0
1	C	3448	0	3397	60	0
1	D	3425	0	3370	62	0
2	A	14	20	20	4	0
2	B	7	10	10	1	0
2	C	7	10	10	8	0
2	D	14	20	20	8	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	264	0	0	6	0
4	B	245	0	0	4	0
4	C	222	0	0	5	0
4	D	195	0	0	3	0
All	All	14759	60	13628	233	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 8.

All (233) 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:63:SER:HA	1:D:95:GLN:HG3	1.52	0.92
1:B:15:GLU:OE1	1:D:16:ASN:HB3	1.70	0.90
1:C:64:GLU:HG3	1:C:72:GLY:HA2	1.56	0.88
1:B:288:SER:HB3	1:B:289:PRO:HD3	1.57	0.86
1:D:306:ASN:HD21	2:D:502:PEG:H21	1.38	0.86
1:D:288:SER:HB3	1:D:289:PRO:HD3	1.60	0.84
1:C:434:ASP:HB3	1:C:437:GLN:HG3	1.60	0.83
1:B:109:PHE:O	1:B:113:LYS:HE3	1.81	0.80
1:C:272:VAL:HG22	1:C:348:GLU:HG3	1.64	0.79
1:A:306:ASN:HD21	2:A:502:PEG:H12	1.47	0.79
1:B:91:MET:SD	1:B:146:KCX:HG2	2.25	0.77
1:B:343:ASP:HB3	1:B:422:ILE:CD1	2.15	0.76
1:A:294:LEU:HG	1:A:298:LYS:HE3	1.68	0.74
1:C:292:ARG:HG2	2:C:501:PEG:H41	1.68	0.73
1:A:288:SER:HB3	1:A:289:PRO:HD3	1.69	0.73
1:A:150:ALA:O	1:A:165:ASN:HA	1.90	0.72
1:C:237:ARG:HD2	4:C:705:HOH:O	1.90	0.71
1:C:131:ILE:HD11	1:C:168:GLN:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ASN:HD21	2:D:502:PEG:H41	1.58	0.68
1:A:91:MET:SD	1:A:146:KCX:HG2	2.35	0.67
1:C:292:ARG:CG	2:C:501:PEG:H41	2.24	0.67
1:C:272:VAL:CG2	1:C:348:GLU:HG3	2.24	0.67
1:B:272:VAL:HG22	1:B:348:GLU:HG3	1.76	0.66
1:C:212:VAL:CG1	2:C:501:PEG:H42	2.25	0.66
1:D:167:TRP:CZ2	1:D:171:LYS:HD3	2.31	0.66
1:B:272:VAL:CG2	1:B:348:GLU:HG3	2.25	0.66
1:D:306:ASN:ND2	2:D:502:PEG:H21	2.09	0.66
1:D:306:ASN:ND2	2:D:502:PEG:H41	2.12	0.65
1:B:15:GLU:HG2	1:B:362:LYS:NZ	2.11	0.65
1:A:430:ASP:HB2	1:A:444:LYS:HE2	1.80	0.64
1:C:64:GLU:HG3	1:C:72:GLY:CA	2.28	0.64
1:A:9:ASN:HB3	4:A:605:HOH:O	1.99	0.63
1:A:306:ASN:ND2	2:A:502:PEG:H31	2.15	0.62
1:B:276:ASP:O	1:B:280:GLU:HG3	2.00	0.61
1:A:65:PRO:HG3	1:A:108:LYS:HG3	1.81	0.61
1:B:54:GLY:HA2	1:B:389:VAL:HG23	1.83	0.61
1:C:158:ASP:HA	1:C:162:ARG:HH12	1.67	0.60
1:B:162:ARG:NH1	4:B:601:HOH:O	2.33	0.60
1:D:272:VAL:HG22	1:D:348:GLU:HG3	1.85	0.59
1:D:294:LEU:O	1:D:298:LYS:HG2	2.02	0.59
1:C:92:PRO:HD2	1:C:93:LEU:HD23	1.85	0.59
1:A:16:ASN:HB3	1:C:15:GLU:OE2	2.03	0.58
1:A:64:GLU:O	1:A:68:SER:HB3	2.03	0.58
1:B:362:LYS:HD2	4:B:765:HOH:O	2.03	0.58
1:C:143:VAL:CG1	1:C:372:PHE:HB3	2.33	0.58
1:C:157:ILE:HB	1:C:160:ASP:HB2	1.86	0.58
1:C:288:SER:HB3	1:C:289:PRO:HD3	1.86	0.58
1:C:292:ARG:HG2	2:C:501:PEG:C4	2.33	0.58
1:D:237:ARG:HD2	4:D:645:HOH:O	2.03	0.58
1:C:170:PHE:HE1	1:C:233:VAL:HG12	1.69	0.57
1:B:288:SER:HB3	1:B:289:PRO:CD	2.31	0.57
1:D:91:MET:SD	1:D:146:KCX:HG2	2.44	0.57
1:A:347:ASP:O	1:A:352:LYS:HG3	2.05	0.56
1:C:143:VAL:HG11	1:C:372:PHE:HB3	1.88	0.56
1:B:343:ASP:HB3	1:B:422:ILE:HD13	1.86	0.56
1:D:64:GLU:O	1:D:65:PRO:C	2.44	0.56
1:D:171:LYS:HE3	1:D:175:LYS:HE2	1.87	0.55
1:B:317:SER:O	1:B:332:TRP:HZ3	1.89	0.55
1:C:64:GLU:O	1:C:65:PRO:C	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:TYR:CE1	1:B:286:LYS:HE3	2.42	0.55
1:B:15:GLU:HG2	1:B:362:LYS:HZ1	1.72	0.55
1:A:133:ARG:HD3	4:A:792:HOH:O	2.06	0.54
1:C:316:HIS:CG	1:C:338:LEU:HB2	2.43	0.54
1:A:316:HIS:CG	1:A:338:LEU:HB2	2.42	0.54
1:D:141:GLY:HA2	4:D:655:HOH:O	2.07	0.54
1:D:185:VAL:HG11	1:D:227:VAL:HG21	1.89	0.54
1:B:237:ARG:HD3	1:B:261:ASP:OD2	2.08	0.53
1:C:58:ALA:HA	1:C:89:ILE:HB	1.90	0.53
1:C:294:LEU:O	1:C:298:LYS:HG2	2.07	0.53
1:B:199:GLU:O	1:B:203:GLU:HG3	2.09	0.53
1:A:146:KCX:HG3	1:A:184:LEU:HB2	1.89	0.53
1:D:201:LYS:HZ1	1:D:330:GLU:CD	2.12	0.53
1:D:64:GLU:HB3	1:D:65:PRO:HD3	1.90	0.53
1:A:131:ILE:HD11	1:A:168:GLN:HB3	1.91	0.53
1:A:5:LEU:HD11	1:A:44:MET:HG3	1.91	0.52
1:A:306:ASN:HD21	2:A:502:PEG:H31	1.72	0.52
1:D:316:HIS:CG	1:D:338:LEU:HB2	2.43	0.52
1:D:288:SER:HB3	1:D:289:PRO:CD	2.36	0.52
1:B:316:HIS:CG	1:B:338:LEU:HB2	2.45	0.52
1:D:29:LYS:HE2	1:D:376:GLN:NE2	2.25	0.52
1:A:191:LEU:HD21	1:B:165:ASN:CG	2.30	0.51
1:D:434:ASP:HB3	1:D:437:GLN:HB2	1.93	0.51
1:B:201:LYS:HE3	1:B:330:GLU:OE2	2.10	0.51
1:D:256:ARG:HG2	1:D:262:VAL:HG13	1.92	0.51
1:D:292:ARG:HG2	2:D:501:PEG:H11	1.92	0.51
1:C:328:ILE:HD13	4:C:652:HOH:O	2.09	0.51
1:A:185:VAL:HG11	1:A:227:VAL:HG21	1.92	0.51
1:A:322:GLU:HB2	4:A:627:HOH:O	2.11	0.51
1:A:151:THR:CG2	1:B:226:ARG:HH12	2.24	0.51
1:D:317:SER:HG	1:D:332:TRP:HH2	1.57	0.51
1:C:157:ILE:HG22	1:C:158:ASP:O	2.12	0.50
1:D:272:VAL:CG2	1:D:348:GLU:HG3	2.40	0.50
1:D:97:PRO:HA	1:D:159:ASN:HB2	1.93	0.50
1:C:158:ASP:HA	1:C:162:ARG:NH1	2.26	0.50
1:B:341:CYS:O	1:B:345:MET:HB2	2.12	0.50
1:A:6:ILE:HG13	1:A:40:ALA:HB2	1.93	0.50
1:A:146:KCX:HD3	1:A:147:CYS:N	2.27	0.50
1:B:149:VAL:O	1:B:150:ALA:C	2.49	0.50
1:C:292:ARG:HB3	2:C:501:PEG:H41	1.93	0.49
1:D:256:ARG:CG	1:D:262:VAL:HG13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HD12	1:A:52:SER:HB2	1.94	0.49
1:B:64:GLU:O	1:B:68:SER:CB	2.61	0.49
1:B:58:ALA:HA	1:B:89:ILE:HB	1.94	0.49
1:B:63:SER:OG	1:B:94:ASN:HB2	2.12	0.49
1:D:129:TYR:O	1:D:133:ARG:NH1	2.43	0.49
1:C:61:HIS:CE1	1:C:93:LEU:HG	2.48	0.49
1:C:54:GLY:HA3	1:C:86:THR:OG1	2.13	0.48
1:C:65:PRO:HG3	1:C:108:LYS:HG3	1.95	0.48
1:D:58:ALA:HA	1:D:89:ILE:HB	1.94	0.48
1:C:292:ARG:CB	2:C:501:PEG:H41	2.42	0.48
1:A:441:VAL:HG23	1:A:442:ALA:O	2.13	0.48
1:D:217:VAL:HG23	2:D:501:PEG:H22	1.95	0.48
1:B:157:ILE:HB	1:B:160:ASP:HB2	1.95	0.48
1:B:84:GLY:O	1:B:389:VAL:HG21	2.14	0.48
1:A:16:ASN:HB2	4:A:631:HOH:O	2.14	0.48
1:B:101:ASP:OD2	1:B:133:ARG:NH1	2.41	0.48
1:C:319:CYS:SG	1:C:332:TRP:CD1	3.07	0.48
1:B:6:ILE:HG13	1:B:40:ALA:HB2	1.95	0.47
1:B:135:HIS:O	1:B:139:GLU:HG3	2.14	0.47
1:A:64:GLU:O	1:A:64:GLU:HG3	2.10	0.47
1:A:184:LEU:HG	1:A:239:HIS:HB3	1.95	0.47
1:A:319:CYS:HB2	1:A:320:PRO:HD2	1.96	0.47
1:B:185:VAL:HG11	1:B:227:VAL:HG11	1.96	0.47
1:A:175:LYS:HA	1:A:175:LYS:HD2	1.70	0.47
1:D:24:ALA:HB2	1:D:37:LEU:HD13	1.97	0.47
1:D:63:SER:OG	1:D:94:ASN:HB2	2.14	0.47
2:A:501:PEG:H11	4:A:655:HOH:O	2.15	0.46
1:B:212:VAL:HG22	1:B:290:PRO:HB2	1.95	0.46
1:D:206:VAL:HG12	1:D:329:MET:HG3	1.97	0.46
1:A:272:VAL:HG22	1:A:348:GLU:HG3	1.97	0.46
1:D:171:LYS:O	1:D:175:LYS:HD2	2.14	0.46
1:D:146:KCX:HD3	1:D:147:CYS:N	2.30	0.46
1:B:184:LEU:HG	1:B:239:HIS:HB3	1.98	0.46
1:C:203:GLU:HB3	4:C:607:HOH:O	2.14	0.46
1:D:317:SER:O	1:D:332:TRP:HZ3	1.98	0.46
1:D:142:VAL:HG13	1:D:144:GLY:H	1.81	0.46
1:B:66:GLY:HA3	1:B:96:LEU:HB2	1.98	0.45
1:D:65:PRO:CG	1:D:108:LYS:HG3	2.47	0.45
1:A:392:GLN:HG2	1:A:395:SER:HB3	1.97	0.45
1:A:88:MET:HG2	1:A:118:ILE:HD11	1.97	0.45
1:A:211:TYR:CE1	1:A:286:LYS:HE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:CYS:HB3	1:D:335:ILE:HG12	1.99	0.45
1:A:218:PHE:CD2	1:B:233:VAL:HG11	2.51	0.45
1:B:292:ARG:HD3	2:B:501:PEG:H21	1.99	0.45
1:D:212:VAL:HG22	1:D:290:PRO:HB2	1.98	0.45
1:A:287:CYS:HB3	1:A:335:ILE:HG12	1.99	0.45
1:B:19:ARG:HG3	1:B:21:VAL:HG13	1.98	0.45
1:A:21:VAL:HA	1:A:35:GLN:HE22	1.83	0.44
1:A:129:TYR:O	1:A:133:ARG:NH1	2.51	0.44
1:C:10:GLY:O	1:C:20:VAL:HA	2.17	0.44
1:C:184:LEU:HG	1:C:239:HIS:HB3	2.00	0.44
2:D:501:PEG:H32	4:D:619:HOH:O	2.16	0.44
1:B:54:GLY:HA3	1:B:86:THR:OG1	2.18	0.44
1:D:67:ARG:HD2	1:D:94:ASN:O	2.18	0.44
1:A:278:PHE:CZ	1:A:286:LYS:HA	2.53	0.44
1:B:97:PRO:HB3	1:B:159:ASN:CG	2.38	0.44
1:B:256:ARG:HG3	1:B:262:VAL:HG13	1.99	0.44
1:D:65:PRO:HG2	1:D:108:LYS:HG3	1.99	0.44
1:D:131:ILE:HD11	1:D:168:GLN:HB3	2.00	0.44
1:C:389:VAL:HG21	1:C:422:ILE:HD12	1.98	0.44
1:D:215:ARG:HB2	1:D:290:PRO:HG3	1.98	0.44
1:A:151:THR:HG21	1:B:226:ARG:HH12	1.83	0.44
1:D:54:GLY:HA3	1:D:86:THR:OG1	2.17	0.44
1:D:389:VAL:HG11	1:D:422:ILE:HD12	2.00	0.44
1:A:143:VAL:CG1	1:A:372:PHE:HB3	2.48	0.43
1:C:212:VAL:HG12	2:C:501:PEG:H42	1.99	0.43
1:B:15:GLU:HG2	1:B:362:LYS:HZ3	1.79	0.43
1:B:272:VAL:O	1:B:272:VAL:CG1	2.67	0.43
1:A:250:GLU:HG3	1:A:303:LYS:HE3	1.99	0.43
1:C:93:LEU:O	1:C:94:ASN:HB2	2.18	0.43
1:D:87:THR:OG1	1:D:377:LYS:HE3	2.18	0.43
1:A:184:LEU:HD12	1:A:184:LEU:N	2.33	0.43
1:C:12:VAL:O	1:C:18:ALA:HA	2.19	0.43
1:D:358:PRO:O	1:D:362:LYS:HG2	2.18	0.43
1:B:124:GLY:O	1:B:145:PHE:HA	2.18	0.43
1:B:242:HIS:O	1:B:242:HIS:ND1	2.49	0.43
1:A:396:SER:HA	1:A:418:ILE:O	2.18	0.43
1:C:58:ALA:HB3	1:C:313:VAL:HG11	2.01	0.43
1:C:64:GLU:O	1:C:66:GLY:N	2.51	0.43
1:B:157:ILE:HG22	1:B:159:ASN:H	1.84	0.43
1:D:306:ASN:HD21	2:D:502:PEG:C4	2.28	0.43
1:A:273:LEU:HA	1:A:277:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:VAL:HG11	2:C:501:PEG:H42	1.98	0.42
1:B:164:VAL:HB	1:B:168:GLN:HB2	2.02	0.42
1:A:288:SER:HB3	1:A:289:PRO:CD	2.45	0.42
1:A:319:CYS:SG	1:A:332:TRP:CD1	3.11	0.42
1:D:242:HIS:O	1:D:242:HIS:ND1	2.51	0.42
1:D:375:GLN:HE21	1:D:375:GLN:HB2	1.48	0.42
1:A:154:ASP:HB2	1:A:163:ASP:OD2	2.20	0.42
1:C:319:CYS:HB2	1:C:320:PRO:HD2	2.01	0.42
1:C:143:VAL:HG13	1:C:372:PHE:HB3	2.01	0.42
1:D:135:HIS:O	1:D:139:GLU:HG3	2.19	0.42
1:A:143:VAL:HG22	1:A:372:PHE:O	2.20	0.42
1:B:73:TYR:CE2	1:B:112:ALA:HB2	2.54	0.42
1:D:396:SER:OG	1:D:419:GLY:HA2	2.20	0.42
1:B:332:TRP:CZ3	1:B:334:GLY:HA3	2.55	0.42
1:C:61:HIS:HB2	1:C:316:HIS:O	2.19	0.42
1:D:65:PRO:CD	1:D:108:LYS:HG3	2.50	0.42
1:D:131:ILE:HD11	1:D:168:GLN:HG2	2.01	0.42
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.92	0.42
1:A:70:TRP:CD1	1:A:320:PRO:HD3	2.55	0.42
1:A:218:PHE:CG	1:B:233:VAL:HG11	2.54	0.42
1:B:64:GLU:O	1:B:68:SER:OG	2.33	0.42
1:B:97:PRO:HB3	1:B:159:ASN:ND2	2.34	0.41
1:A:165:ASN:CG	1:B:191:LEU:HD11	2.41	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.94	0.41
1:C:191:LEU:HD11	1:D:165:ASN:CG	2.41	0.41
1:C:6:ILE:HG13	1:C:40:ALA:HB2	2.02	0.41
1:C:64:GLU:HG2	1:C:68:SER:CB	2.50	0.41
1:C:148:PHE:CD1	1:C:161:PHE:HE2	2.39	0.41
1:B:186:HIS:HE1	1:B:288:SER:HB3	1.86	0.41
1:C:184:LEU:HD11	1:C:372:PHE:HE1	1.85	0.41
1:D:124:GLY:O	1:D:145:PHE:HA	2.20	0.41
1:C:16:ASN:HB2	4:C:693:HOH:O	2.19	0.41
1:B:89:ILE:HG22	1:B:123:LEU:HG	2.02	0.41
1:B:328:ILE:HG13	4:B:723:HOH:O	2.20	0.41
1:D:24:ALA:HB3	1:D:32:ALA:HB3	2.03	0.41
1:B:340:ASN:O	1:B:344:VAL:HB	2.21	0.41
1:B:379:ARG:HG3	1:B:384:LYS:HG3	2.02	0.41
1:C:165:ASN:CG	1:D:191:LEU:HD21	2.41	0.41
1:C:242:HIS:O	1:C:242:HIS:ND1	2.52	0.41
1:A:421:ARG:HD2	4:A:607:HOH:O	2.19	0.40
1:B:422:ILE:N	1:B:422:ILE:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:HIS:HE1	1:C:93:LEU:HG	1.85	0.40
1:C:146:KCX:HZ	1:C:146:KCX:HG2	1.66	0.40
1:C:64:GLU:HG2	1:C:68:SER:HB2	2.03	0.40
1:C:185:VAL:HG11	1:C:227:VAL:HG21	2.03	0.40
1:A:93:LEU:HD23	1:A:93:LEU:H	1.86	0.40
1:C:241:CYS:O	1:C:242:HIS:C	2.59	0.40
1:B:113:LYS:HE2	1:B:113:LYS:HA	2.02	0.40
1:B:16:ASN:HB2	4:B:686:HOH:O	2.21	0.40
1:C:297:GLN:HB2	4:C:634:HOH:O	2.21	0.40
1:D:149:VAL:HG12	1:D:150:ALA:H	1.86	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	449/459 (98%)	435 (97%)	12 (3%)	2 (0%)	34	25
1	B	442/459 (96%)	429 (97%)	12 (3%)	1 (0%)	47	39
1	C	443/459 (96%)	428 (97%)	13 (3%)	2 (0%)	29	19
1	D	440/459 (96%)	427 (97%)	10 (2%)	3 (1%)	22	11
All	All	1774/1836 (97%)	1719 (97%)	47 (3%)	8 (0%)	29	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	B	242	HIS
1	C	94	ASN
1	C	242	HIS
1	D	242	HIS

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Mol	Chain	Res	Type
1	D	94	ASN
1	A	71	GLU
1	D	64	GLU

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	369/376 (98%)	361 (98%)	8 (2%)	52	46
1	B	365/376 (97%)	357 (98%)	8 (2%)	52	46
1	C	366/376 (97%)	354 (97%)	12 (3%)	38	31
1	D	364/376 (97%)	354 (97%)	10 (3%)	44	39
All	All	1464/1504 (97%)	1426 (97%)	38 (3%)	46	40

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	64	GLU
1	A	143	VAL
1	A	151	THR
1	A	154	ASP
1	A	175	LYS
1	A	278	PHE
1	A	444	LYS
1	B	64	GLU
1	B	68	SER
1	B	93	LEU
1	B	175	LYS
1	B	191	LEU
1	B	278	PHE
1	B	330	GLU
1	B	362	LYS
1	C	64	GLU
1	C	93	LEU

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Mol	Chain	Res	Type
1	C	143	VAL
1	C	155	ARG
1	C	178	GLU
1	C	191	LEU
1	C	278	PHE
1	C	304	LEU
1	C	311	CYS
1	C	332	TRP
1	C	375	GLN
1	C	453	GLN
1	D	93	LEU
1	D	95	GLN
1	D	142	VAL
1	D	158	ASP
1	D	159	ASN
1	D	163	ASP
1	D	175	LYS
1	D	278	PHE
1	D	375	GLN
1	D	452	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	174	GLN
1	A	306	ASN
1	A	375	GLN
1	B	437	GLN
1	B	452	GLN
1	C	9	ASN
1	C	35	GLN
1	D	159	ASN
1	D	306	ASN
1	D	375	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	KCX	D	146	3,1	9,11,12	2.22	1 (11%)	5,12,14	3.24	1 (20%)
1	KCX	C	146	3,1	9,11,12	1.08	1 (11%)	5,12,14	1.18	1 (20%)
1	KCX	B	146	3,1	9,11,12	1.04	1 (11%)	5,12,14	1.76	1 (20%)
1	KCX	A	146	3,1	9,11,12	0.47	0	5,12,14	0.34	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
1	KCX	D	146	3,1	-	6/9/10/12	-
1	KCX	C	146	3,1	-	4/9/10/12	-
1	KCX	B	146	3,1	-	2/9/10/12	-
1	KCX	A	146	3,1	-	5/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	KCX	OQ1-CX	6.49	1.33	1.21
1	B	146	KCX	CE-NZ	2.31	1.51	1.46
1	C	146	KCX	CE-NZ	2.17	1.51	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	146	KCX	OQ1-CX-NZ	-7.24	113.74	124.96
1	B	146	KCX	OQ1-CX-NZ	-3.84	119.01	124.96
1	C	146	KCX	OQ1-CX-NZ	-2.39	121.25	124.96

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	146	KCX	N-CA-CB-CG
1	A	146	KCX	C-CA-CB-CG
1	A	146	KCX	OQ1-CX-NZ-CE
1	A	146	KCX	OQ2-CX-NZ-CE
1	B	146	KCX	N-CA-CB-CG
1	B	146	KCX	C-CA-CB-CG
1	C	146	KCX	C-CA-CB-CG
1	D	146	KCX	N-CA-CB-CG
1	D	146	KCX	C-CA-CB-CG
1	D	146	KCX	OQ1-CX-NZ-CE
1	D	146	KCX	OQ2-CX-NZ-CE
1	C	146	KCX	CA-CB-CG-CD
1	C	146	KCX	CG-CD-CE-NZ
1	D	146	KCX	CE-CD-CG-CB
1	D	146	KCX	CA-CB-CG-CD
1	A	146	KCX	CE-CD-CG-CB
1	C	146	KCX	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	146	KCX	2	0
1	C	146	KCX	1	0
1	B	146	KCX	1	0
1	A	146	KCX	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
2	PEG	A	502	-	6,6,6	0.10	0	5,5,5	0.10	0
2	PEG	D	502	-	6,6,6	0.12	0	5,5,5	0.08	0
2	PEG	C	501	-	6,6,6	0.36	0	5,5,5	0.64	0
2	PEG	A	501	-	6,6,6	0.26	0	5,5,5	0.23	0
2	PEG	D	501	-	6,6,6	0.14	0	5,5,5	0.17	0
2	PEG	B	501	-	6,6,6	0.18	0	5,5,5	0.13	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	PEG	A	502	-	-	1/4/4/4	-
2	PEG	D	502	-	-	3/4/4/4	-
2	PEG	C	501	-	-	3/4/4/4	-
2	PEG	A	501	-	-	3/4/4/4	-
2	PEG	D	501	-	-	2/4/4/4	-
2	PEG	B	501	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PEG	O1-C1-C2-O2
2	C	501	PEG	O2-C3-C4-O4
2	D	502	PEG	O2-C3-C4-O4
2	A	502	PEG	O2-C3-C4-O4
2	A	501	PEG	O2-C3-C4-O4
2	C	501	PEG	O1-C1-C2-O2
2	D	502	PEG	O1-C1-C2-O2
2	D	502	PEG	C4-C3-O2-C2
2	B	501	PEG	O2-C3-C4-O4
2	D	501	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
2	D	501	PEG	O2-C3-C4-O4
2	A	501	PEG	C4-C3-O2-C2
2	C	501	PEG	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	PEG	3	0
2	D	502	PEG	5	0
2	C	501	PEG	8	0
2	A	501	PEG	1	0
2	D	501	PEG	3	0
2	B	501	PEG	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

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, 95^{th} 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	451/459 (98%)	0.12	18 (3%)	38	40	21, 28, 41, 68	0
1	B	446/459 (97%)	0.20	20 (4%)	33	34	19, 27, 41, 76	0
1	C	447/459 (97%)	0.20	18 (4%)	38	40	23, 31, 44, 61	0
1	D	444/459 (96%)	0.25	23 (5%)	27	27	23, 31, 45, 68	0
All	All	1788/1836 (97%)	0.19	79 (4%)	34	35	19, 30, 44, 76	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	GLY	6.2
1	B	150	ALA	6.0
1	A	288	SER	5.1
1	B	156	GLY	5.1
1	B	157	ILE	4.8
1	A	151	THR	4.7
1	C	288	SER	4.2
1	D	150	ALA	4.1
1	B	158	ASP	3.9
1	A	152	CYS	3.9
1	B	288	SER	3.7
1	D	288	SER	3.6
1	D	2	SER	3.5
1	B	313	VAL	3.5
1	A	154	ASP	3.5
1	C	93	LEU	3.4
1	B	338	LEU	3.3
1	B	60	THR	3.3
1	D	39	ASP	3.2
1	B	314	SER	3.2
1	C	313	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	452	GLN	3.1
1	C	289	PRO	3.1
1	D	85	ILE	3.1
1	D	159	ASN	3.0
1	B	85	ILE	3.0
1	D	96	LEU	3.0
1	C	39	ASP	3.0
1	C	60	THR	2.9
1	B	2	SER	2.9
1	B	159	ASN	2.9
1	D	314	SER	2.9
1	C	58	ALA	2.8
1	D	158	ASP	2.8
1	C	85	ILE	2.8
1	B	451	HIS	2.8
1	A	39	ASP	2.8
1	D	107	LEU	2.8
1	C	132	ASP	2.7
1	A	150	ALA	2.7
1	D	64	GLU	2.6
1	D	338	LEU	2.6
1	B	452	GLN	2.6
1	D	313	VAL	2.5
1	A	93	LEU	2.5
1	C	64	GLU	2.5
1	C	415	GLY	2.5
1	A	65	PRO	2.5
1	A	332	TRP	2.5
1	C	203	GLU	2.5
1	C	56	VAL	2.4
1	B	243	VAL	2.4
1	A	289	PRO	2.4
1	C	396	SER	2.4
1	B	453	GLN	2.4
1	A	60	THR	2.3
1	D	60	THR	2.3
1	B	268	PRO	2.3
1	B	312	LEU	2.3
1	C	302	GLU	2.3
1	A	2	SER	2.3
1	A	452	GLN	2.3
1	A	157	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	39	ASP	2.2
1	A	85	ILE	2.2
1	D	94	ASN	2.2
1	C	110	ASP	2.2
1	D	243	VAL	2.2
1	D	93	LEU	2.1
1	A	56	VAL	2.1
1	D	221	VAL	2.1
1	C	155	ARG	2.1
1	A	267	CYS	2.1
1	D	451	HIS	2.1
1	D	55	MET	2.0
1	B	289	PRO	2.0
1	C	59	HIS	2.0
1	D	162	ARG	2.0
1	D	66	GLY	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, 95^{th} 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
1	KCX	A	146	12/13	0.83	0.24	18,24,30,34	0
1	KCX	D	146	12/13	0.86	0.23	26,32,40,40	0
1	KCX	B	146	12/13	0.95	0.15	22,27,30,35	0
1	KCX	C	146	12/13	0.96	0.15	21,29,33,33	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

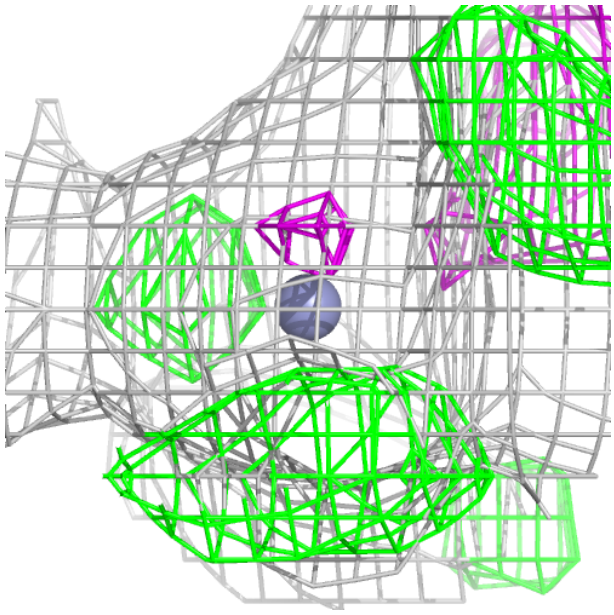
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

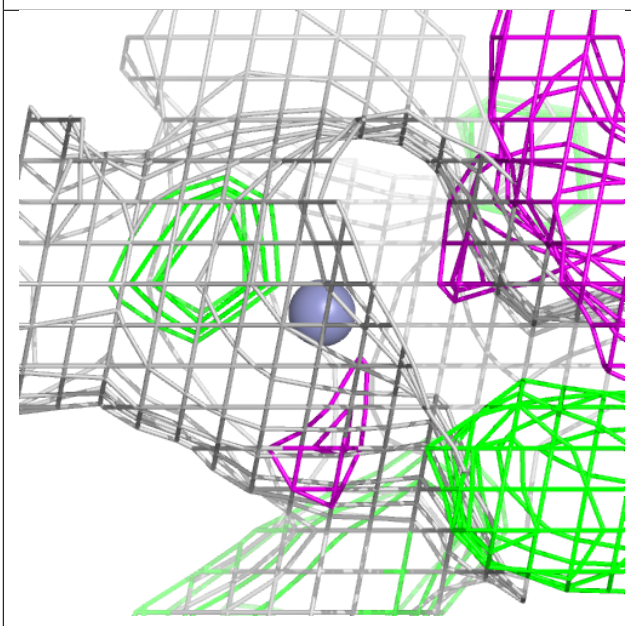
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	A	501	7/7	0.76	0.25	19,45,56,67	0
2	PEG	B	501	7/7	0.79	0.21	24,37,46,51	0
2	PEG	D	501	7/7	0.79	0.20	19,42,51,53	0
2	PEG	C	501	7/7	0.82	0.18	28,40,53,58	0
2	PEG	D	502	7/7	0.88	0.38	20,20,20,20	0
2	PEG	A	502	7/7	0.90	0.34	20,20,20,20	0
3	ZN	D	503	1/1	0.91	0.12	36,36,36,36	0
3	ZN	D	504	1/1	0.93	0.13	36,36,36,36	0
3	ZN	C	502	1/1	0.98	0.14	31,31,31,31	0
3	ZN	B	503	1/1	0.99	0.09	30,30,30,30	0
3	ZN	A	503	1/1	0.99	0.14	25,25,25,25	0
3	ZN	C	503	1/1	0.99	0.11	35,35,35,35	0
3	ZN	A	504	1/1	0.99	0.09	30,30,30,30	0
3	ZN	B	502	1/1	0.99	0.11	26,26,26,26	0

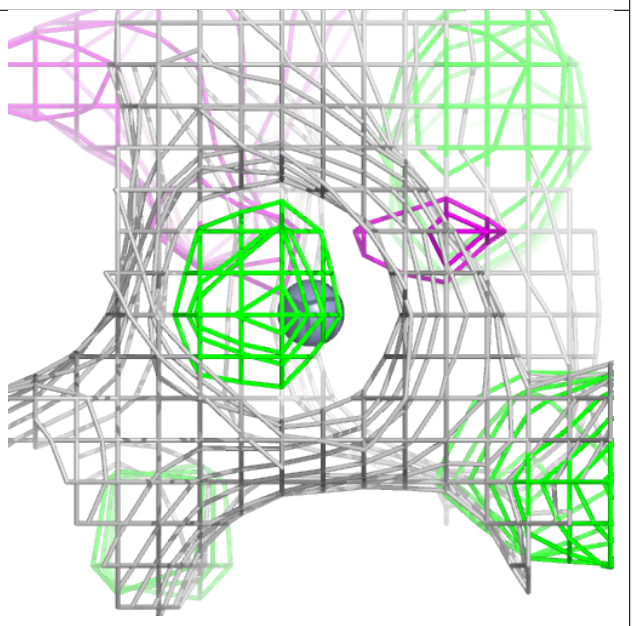
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZN D 503:

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

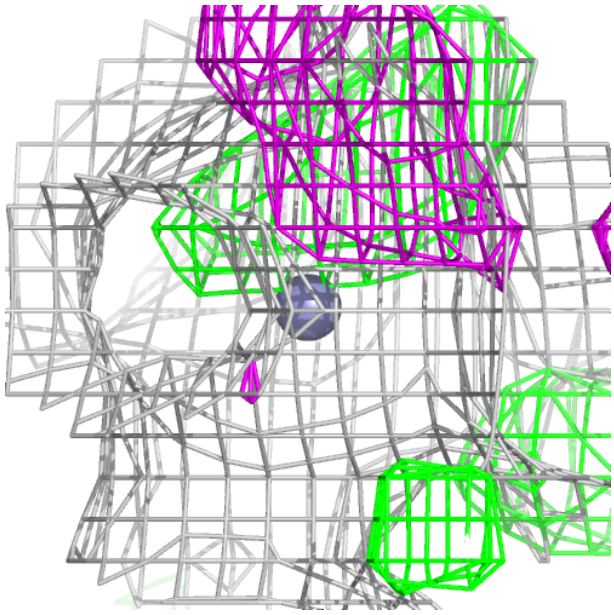


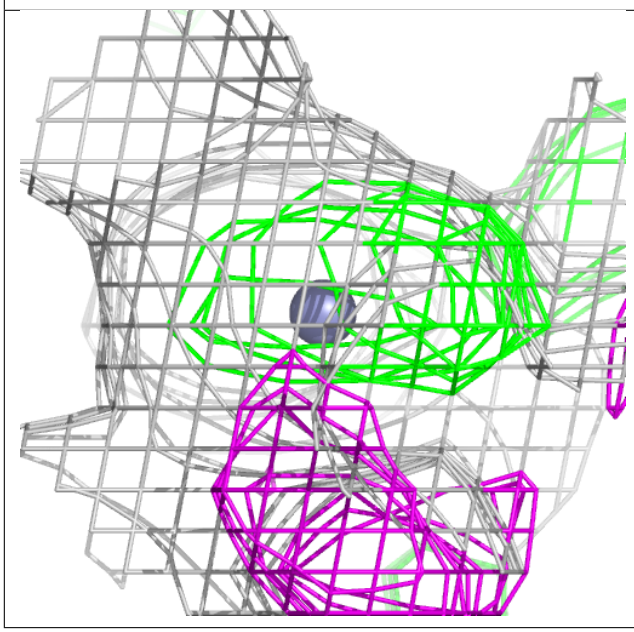


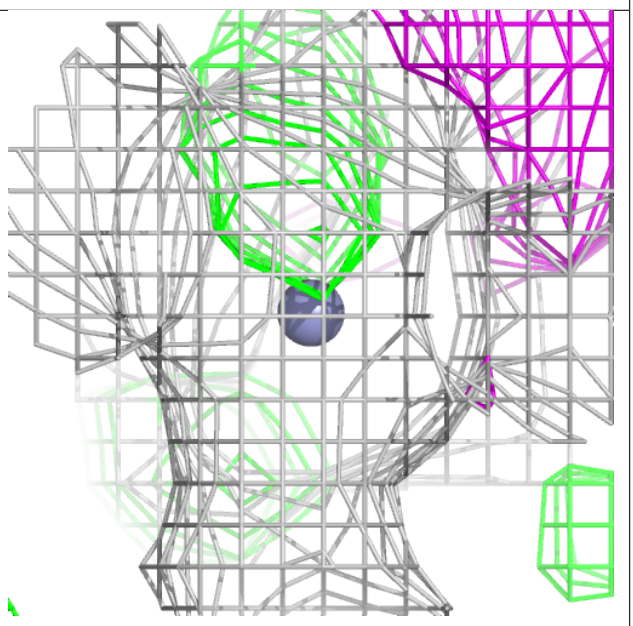


Electron density around ZN D 504:

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

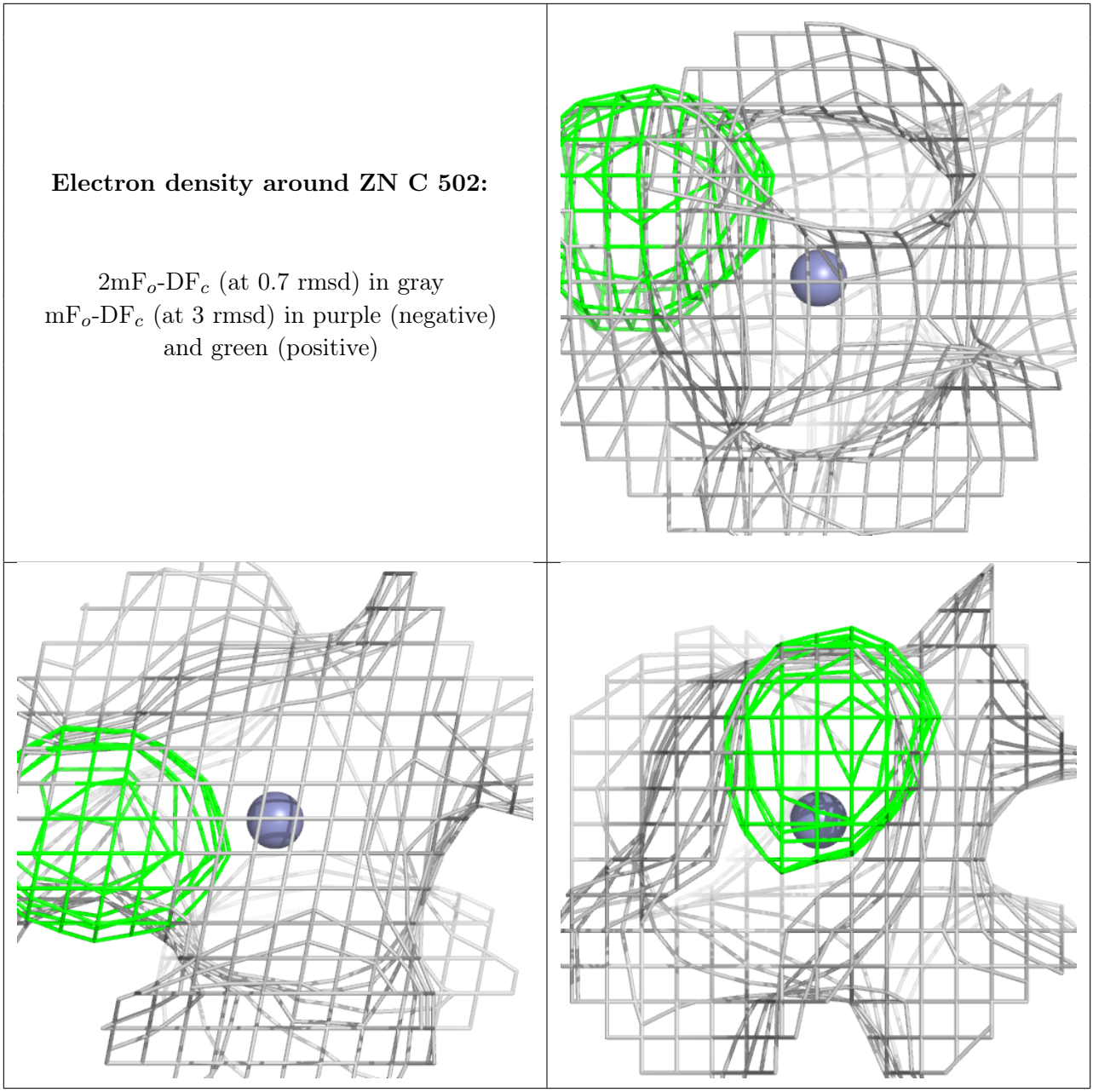






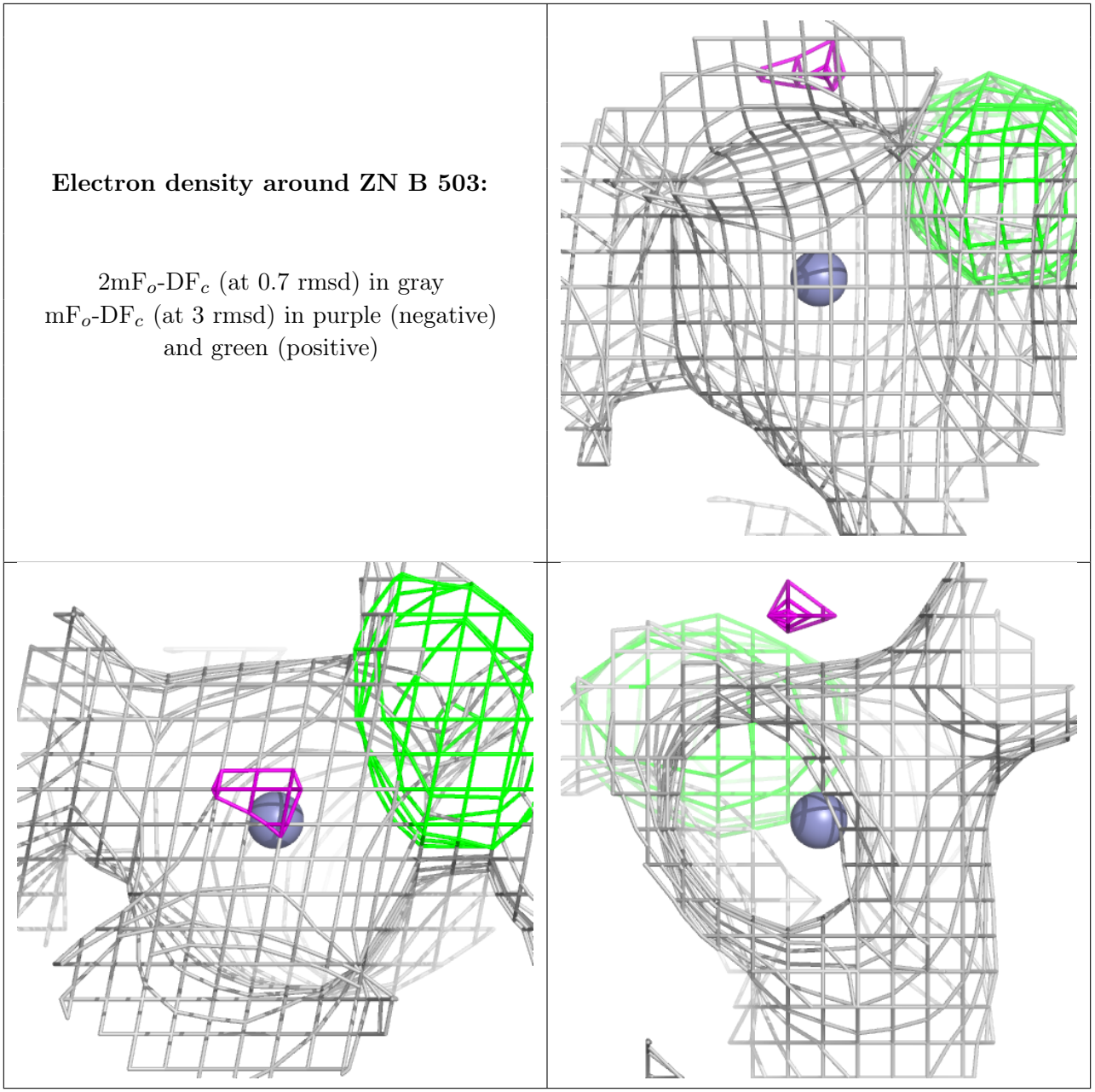
Electron density around ZN C 502:

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



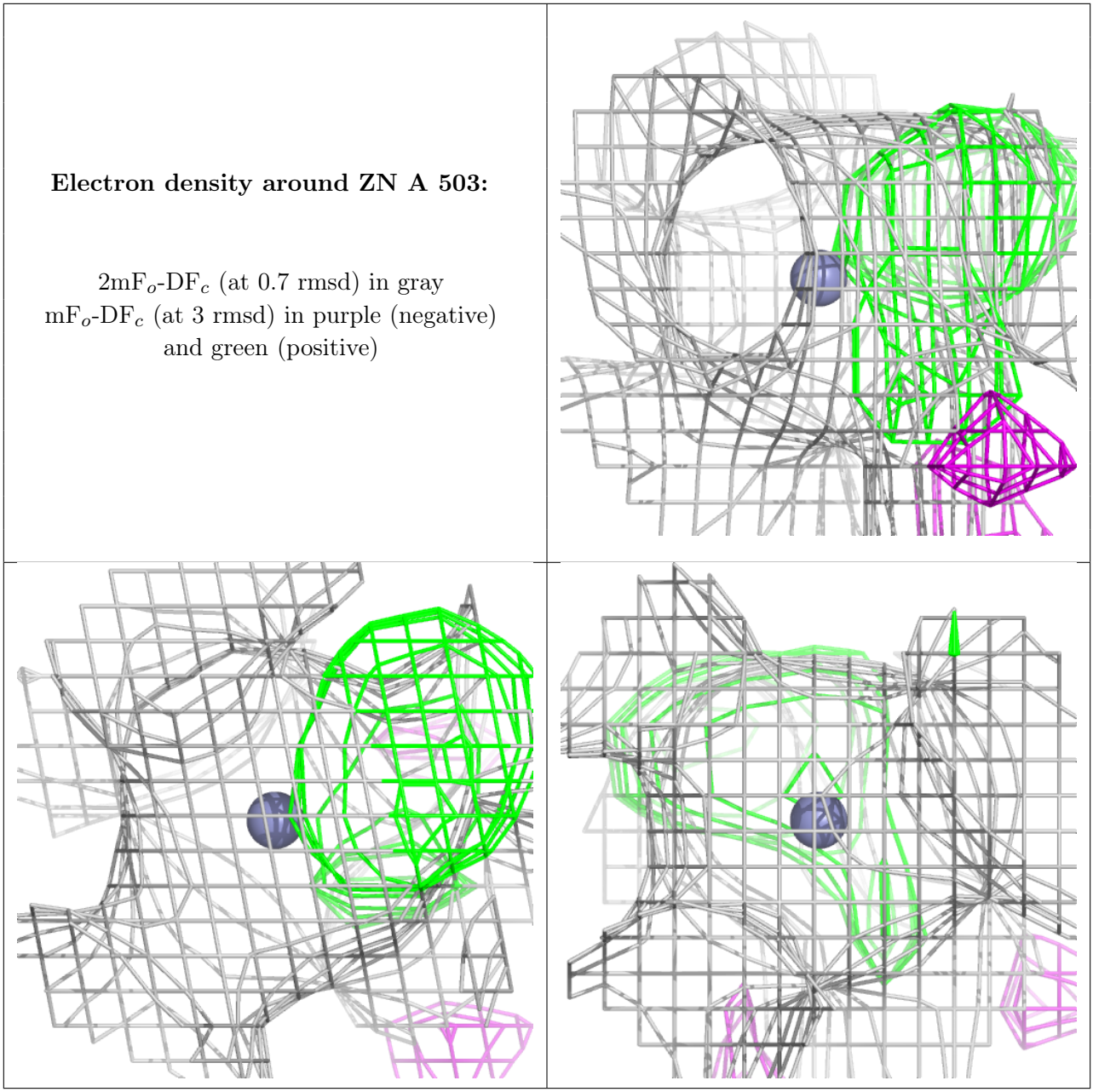
Electron density around ZN B 503:

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



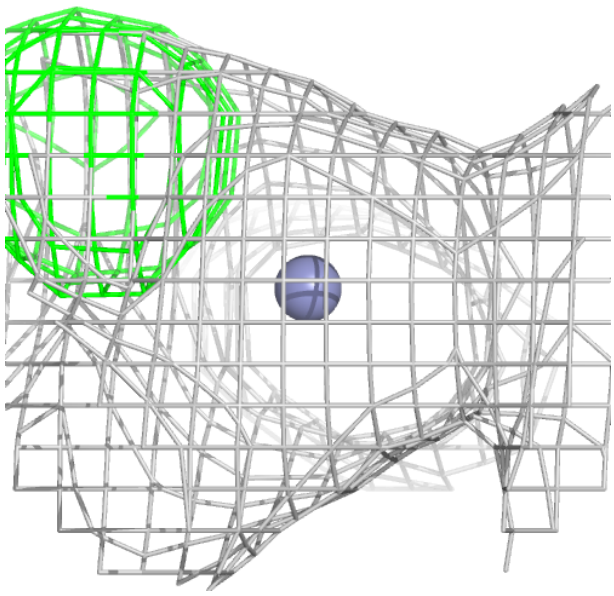
Electron density around ZN A 503:

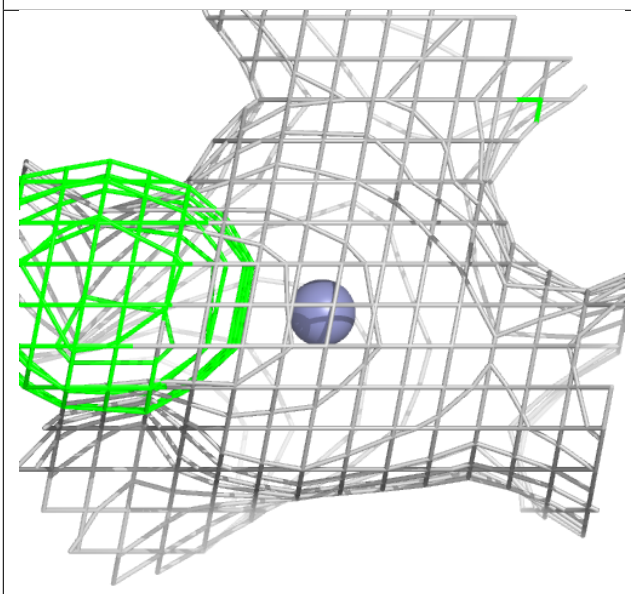
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

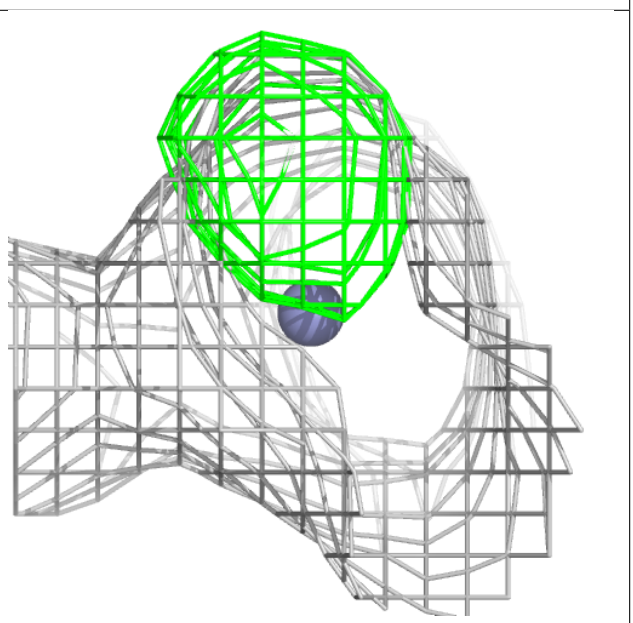


Electron density around ZN C 503:

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

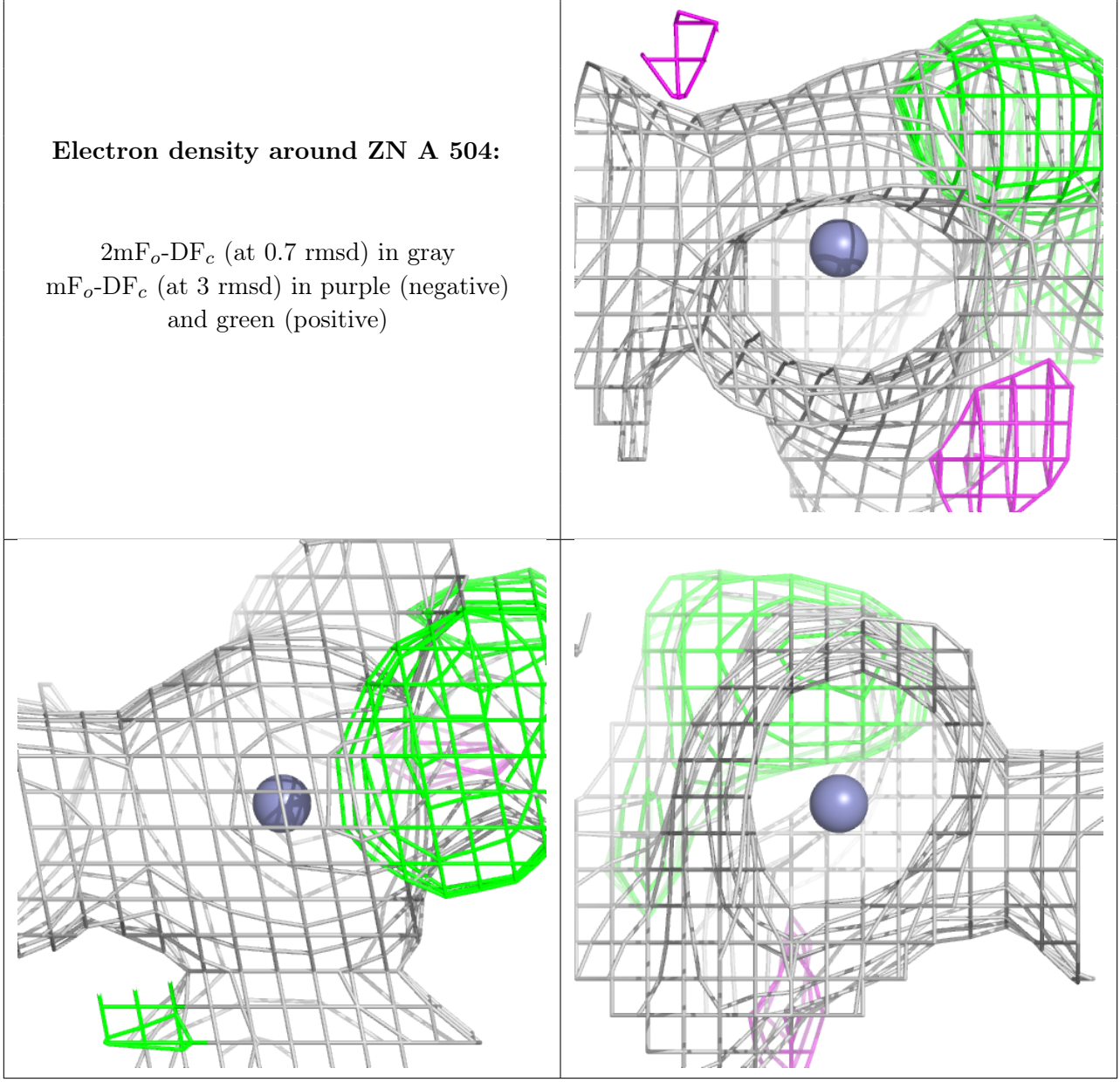






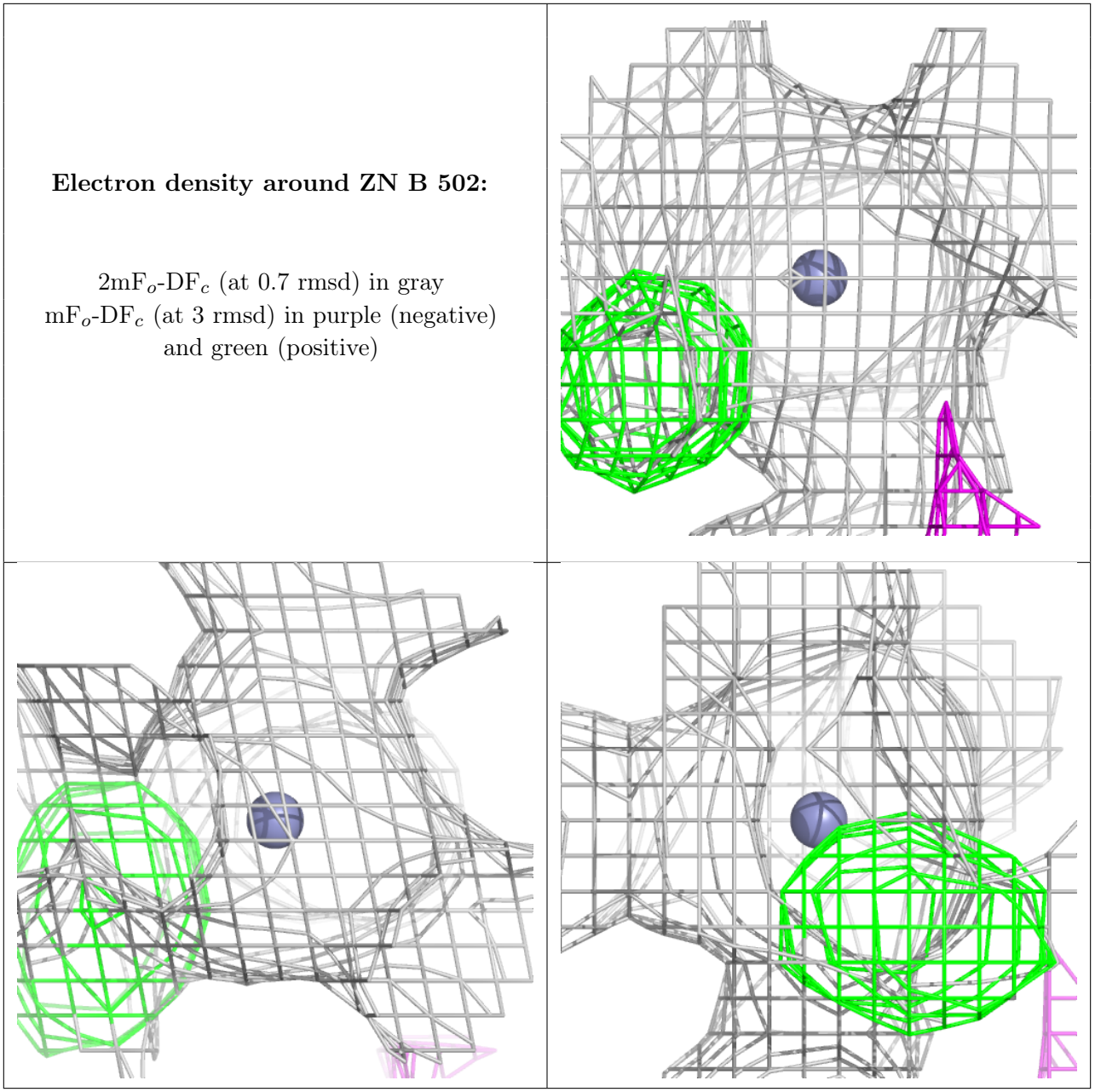
Electron density around ZN A 504:

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



Electron density around ZN B 502:

$2mF_o$-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.