



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2022 – 02:07 PM EDT

PDB ID : 7T3V
Title : Metal dependent activation of Plasmodium falciparum M17 aminopeptidase, spacegroup P22121 after crystals soaked with Zn²⁺
Authors : Webb, C.T.; McGowan, S.
Deposited on : 2021-12-08
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

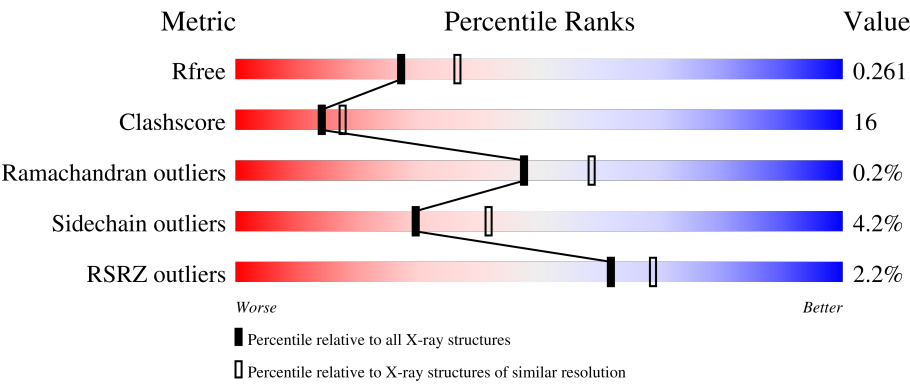
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	527	<div><div>0%</div><div>73%24%..</div></div>
1	B	527	<div><div>4%</div><div>65%33%.</div></div>
1	C	527	<div><div>2%</div><div>68%28%..</div></div>
1	D	527	<div><div>2%</div><div>71%25%..</div></div>
1	E	527	<div><div>2%</div><div>67%29%..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	527	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	B	701	-	-	X	-
2	CO3	C	702	-	-	X	-
2	CO3	F	701	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23536 atoms, of which 28 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3932	2527	635	750	20			
1	B	518	Total	C	N	O	S	0	0	0
			3846	2472	621	733	20			
1	C	518	Total	C	N	O	S	0	0	0
			3921	2524	628	749	20			
1	D	517	Total	C	N	O	S	0	0	0
			3870	2490	623	738	19			
1	E	511	Total	C	N	O	S	0	0	0
			3866	2489	623	735	19			
1	F	509	Total	C	N	O	S	0	0	0
			3732	2399	605	709	19			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	conflict	UNP Q8IL11
A	515	GLN	ASN	conflict	UNP Q8IL11
A	546	GLN	ASN	conflict	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	conflict	UNP Q8IL11
B	515	GLN	ASN	conflict	UNP Q8IL11
B	546	GLN	ASN	conflict	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	conflict	UNP Q8IL11
C	515	GLN	ASN	conflict	UNP Q8IL11
C	546	GLN	ASN	conflict	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	conflict	UNP Q8IL11
D	515	GLN	ASN	conflict	UNP Q8IL11
D	546	GLN	ASN	conflict	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	conflict	UNP Q8IL11
E	515	GLN	ASN	conflict	UNP Q8IL11
E	546	GLN	ASN	conflict	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	conflict	UNP Q8IL11
F	515	GLN	ASN	conflict	UNP Q8IL11
F	546	GLN	ASN	conflict	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		

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

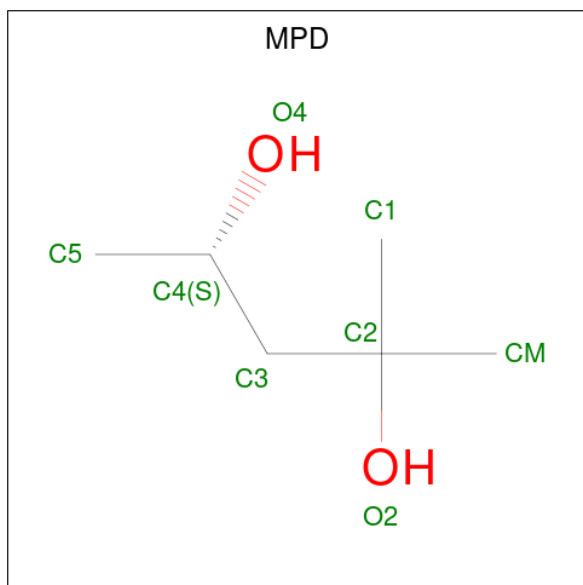
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		

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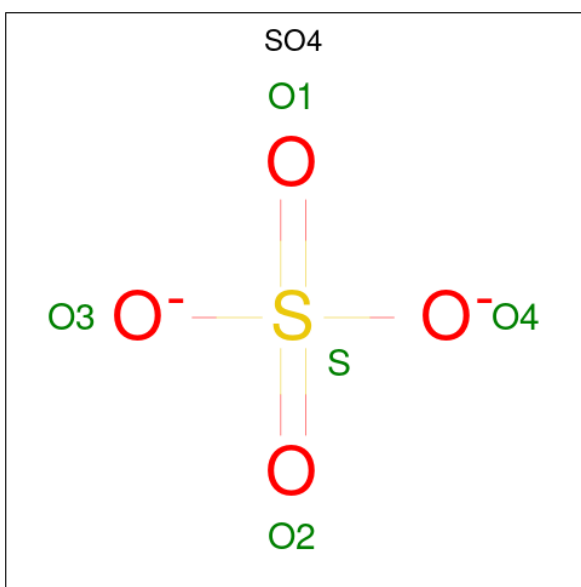
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			22	6	14	2		
4	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

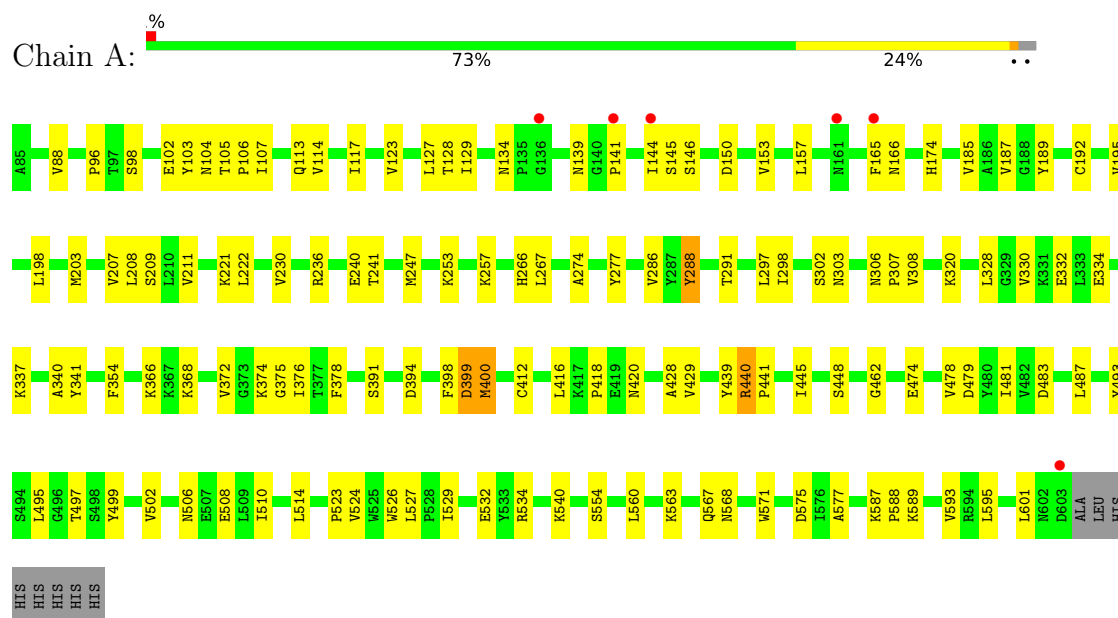
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	B	46	Total	O	0	0
			46	46		
6	C	62	Total	O	0	0
			62	62		
6	D	42	Total	O	0	0
			42	42		
6	E	43	Total	O	0	0
			43	43		
6	F	38	Total	O	0	0
			38	38		

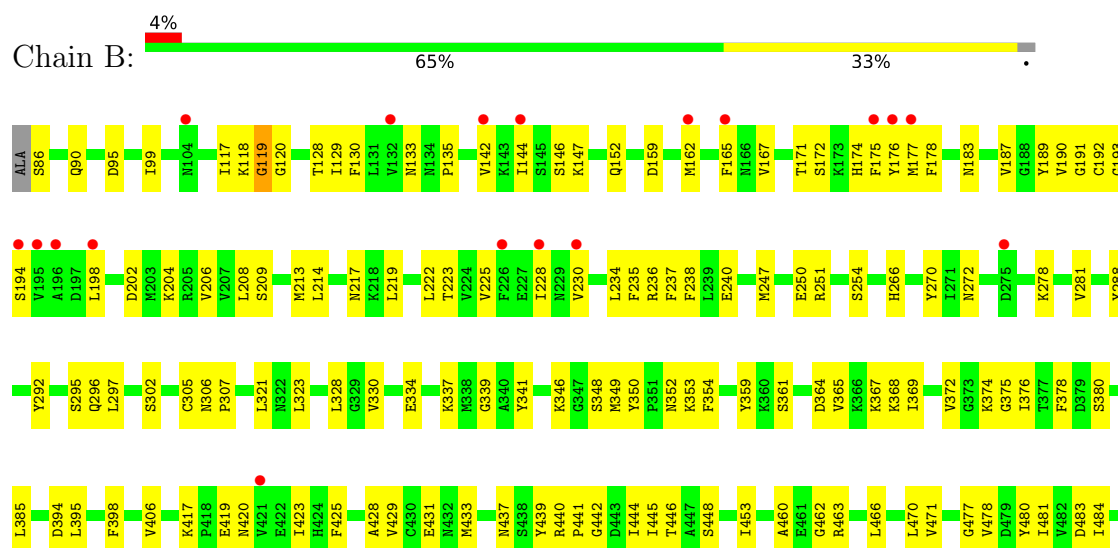
3 Residue-property plots

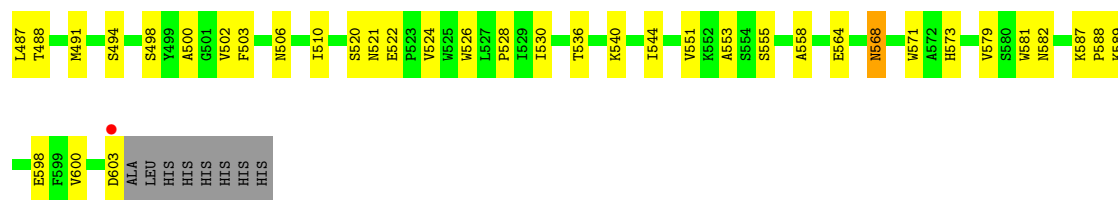
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: M17 leucyl aminopeptidase

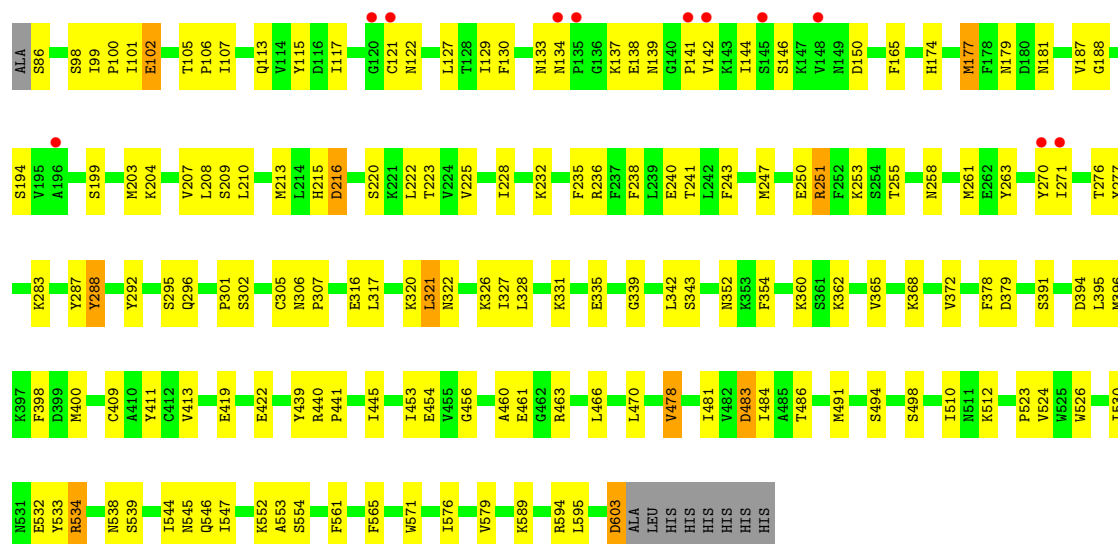


• Molecule 1: M17 leucyl aminopeptidase

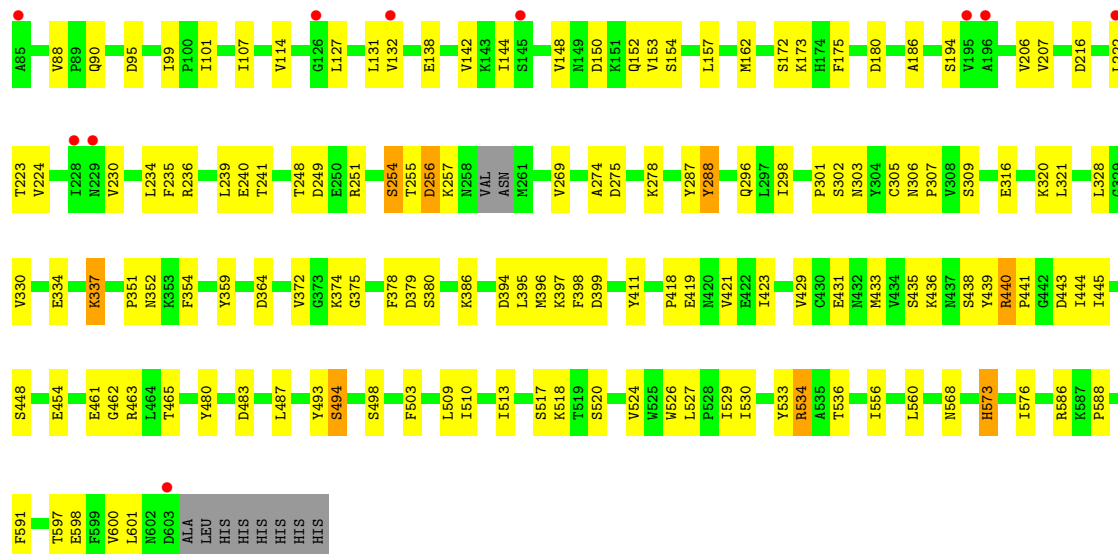




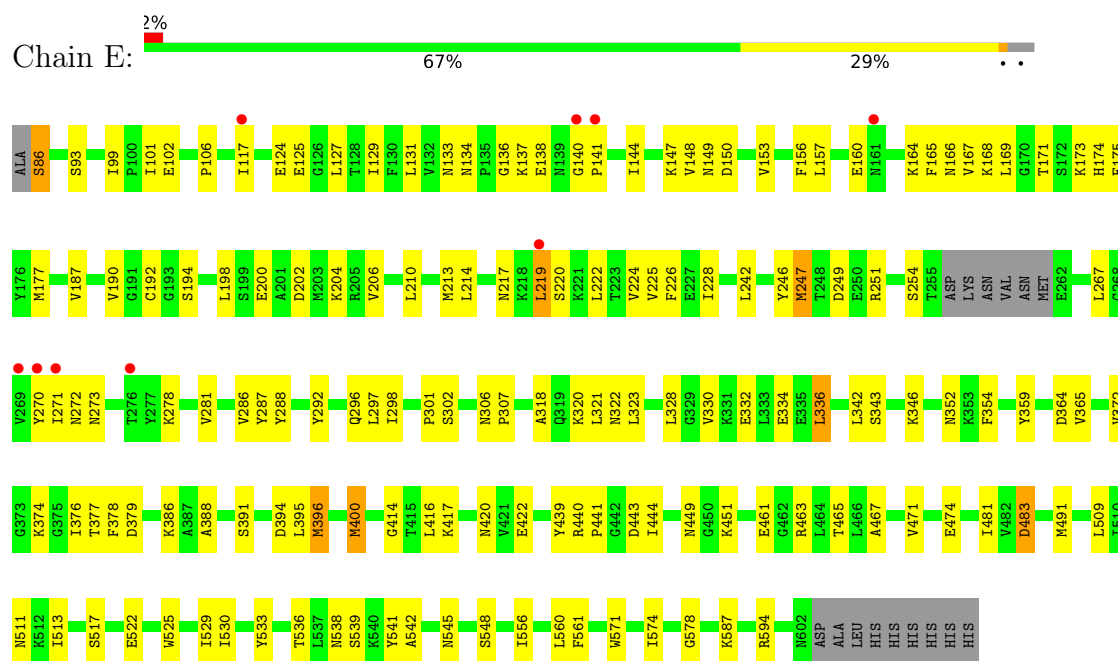
• Molecule 1: M17 leucyl aminopeptidase



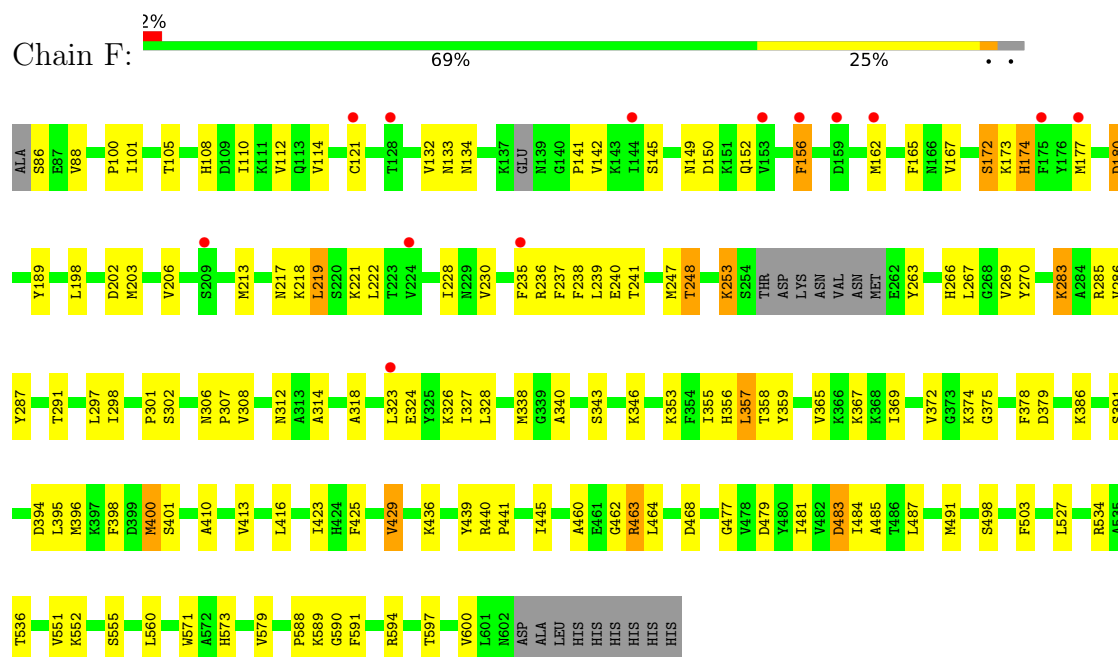
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.76Å 172.76Å 176.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 2.30 47.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.24-2.30) 95.5 (47.24-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.264 0.219 , 0.261	Depositor DCC
R_{free} test set	1994 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23536	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, MPD, SO4, 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	0.28	0/4010	0.47	0/5450
1	B	0.28	0/3922	0.47	0/5342
1	C	0.31	0/3999	0.49	0/5433
1	D	0.29	0/3947	0.47	0/5368
1	E	0.29	0/3943	0.48	0/5357
1	F	0.28	0/3807	0.48	0/5189
All	All	0.29	0/23628	0.48	0/32139

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3932	0	3820	98	0
1	B	3846	0	3674	141	0
1	C	3921	0	3809	113	2
1	D	3870	0	3706	110	0
1	E	3866	0	3761	142	1
1	F	3732	0	3496	148	1
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	2	0
2	C	4	0	0	2	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	5	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
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	C	8	14	14	0	0
4	D	8	14	14	5	0
5	C	5	0	0	0	0
5	E	5	0	0	1	0
6	A	48	0	0	10	0
6	B	46	0	0	10	0
6	C	62	0	0	9	0
6	D	42	0	0	8	0
6	E	43	0	0	14	0
6	F	38	0	0	10	0
All	All	23508	28	22294	708	2

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 16.

All (708) 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:230:VAL:HG23	1:B:234:LEU:HD23	1.35	1.07
1:B:133:ASN:HA	1:B:167:VAL:HG11	1.34	1.03
1:A:495:LEU:HD11	1:A:527:LEU:HD21	1.46	0.98
1:F:463:ARG:HD2	2:F:701:CO3:O3	1.63	0.97
1:C:456:GLY:O	6:C:801:HOH:O	1.84	0.96
1:F:133:ASN:HA	1:F:167:VAL:HG11	1.48	0.95
1:B:117:ILE:HD11	1:B:146:SER:HB3	1.50	0.94
1:E:298:ILE:HA	1:E:400:MET:HE3	1.50	0.93
1:F:105:THR:N	6:F:801:HOH:O	2.01	0.92
1:A:529:ILE:HG23	1:A:560:LEU:HD12	1.51	0.91
1:E:388:ALA:N	6:E:805:HOH:O	2.02	0.91
1:B:175:PHE:HB2	1:B:187:VAL:HG23	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:ASN:HB3	1:E:219:LEU:HD11	1.54	0.90
1:E:214:LEU:HD21	1:E:222:LEU:HD12	1.54	0.90
1:E:202:ASP:OD1	6:E:801:HOH:O	1.91	0.87
1:A:144:ILE:HG13	1:A:157:LEU:HD22	1.57	0.86
1:E:321:LEU:HD12	1:E:414:GLY:HA3	1.58	0.86
1:A:418:PRO:HG3	1:A:601:LEU:HD21	1.56	0.85
1:F:463:ARG:HD2	2:F:701:CO3:C	2.06	0.85
1:E:440:ARG:NH2	6:E:802:HOH:O	1.95	0.84
1:D:533:TYR:O	1:D:536:THR:HG22	1.78	0.84
1:F:110:ILE:O	1:F:285:ARG:NH2	2.07	0.84
1:D:493:TYR:O	6:D:802:HOH:O	1.96	0.83
1:B:579:VAL:O	1:B:589:LYS:HE2	1.78	0.82
1:F:132:VAL:HG21	1:F:142:VAL:HG23	1.61	0.81
1:F:108:HIS:HB2	6:F:801:HOH:O	1.78	0.81
1:E:86:SER:OG	6:E:804:HOH:O	1.99	0.81
1:A:575:ASP:OD2	6:A:801:HOH:O	1.98	0.80
1:E:298:ILE:HA	1:E:400:MET:CE	2.11	0.80
1:E:533:TYR:O	1:E:536:THR:HG22	1.82	0.80
1:E:190:VAL:HG11	1:E:206:VAL:HG13	1.62	0.80
1:E:222:LEU:HD21	1:E:224:VAL:HG23	1.64	0.80
1:B:162:MET:HE2	1:B:162:MET:HA	1.64	0.78
1:B:174:HIS:CE1	1:B:213:MET:HG2	2.19	0.78
1:C:362:LYS:O	6:C:802:HOH:O	2.00	0.78
1:E:379:ASP:O	1:E:396:MET:HG2	1.83	0.78
1:D:364:ASP:N	6:D:804:HOH:O	2.17	0.78
1:B:99:ILE:HD11	1:B:305:CYS:HA	1.64	0.77
1:D:431:GLU:CD	1:D:433:MET:HE3	2.05	0.77
1:C:331:LYS:O	1:C:335:GLU:HG3	1.84	0.77
1:F:297:LEU:O	1:F:400:MET:HE1	1.84	0.77
1:A:236:ARG:O	1:A:240:GLU:HG3	1.85	0.76
1:D:440:ARG:HD3	1:D:443:ASP:OD1	1.86	0.76
1:B:128:THR:OG1	1:B:187:VAL:HG12	1.85	0.76
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.67	0.76
1:E:138:GLU:HA	1:E:194:SER:OG	1.86	0.75
1:E:117:ILE:HG22	1:E:272:ASN:HA	1.68	0.75
1:E:148:VAL:HG11	1:E:153:VAL:HG21	1.69	0.75
1:E:286:VAL:HG11	1:E:416:LEU:CD2	2.17	0.75
1:B:506:ASN:O	1:B:510:ILE:HG13	1.87	0.74
1:C:204:LYS:O	1:C:208:LEU:HD12	1.87	0.74
1:A:567:GLN:O	1:A:568:ASN:ND2	2.20	0.74
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:SER:O	6:B:801:HOH:O	2.05	0.74
1:F:198:LEU:HD22	1:F:202:ASP:HB3	1.68	0.74
1:B:142:VAL:HG12	1:B:167:VAL:HG22	1.67	0.74
1:A:88:VAL:HG22	1:A:308:VAL:HG12	1.68	0.73
1:E:226:PHE:HB2	1:E:271:ILE:HG13	1.68	0.73
1:E:153:VAL:HG12	1:E:177:MET:CE	2.18	0.73
1:A:127:LEU:HD21	1:A:129:ILE:HD11	1.70	0.73
1:A:374:LYS:HE3	1:A:462:GLY:HA3	1.70	0.73
1:D:114:VAL:HG12	1:D:274:ALA:HB1	1.70	0.73
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.69	0.73
1:A:479:ASP:OD2	6:A:802:HOH:O	2.07	0.73
1:B:99:ILE:CD1	1:B:305:CYS:HA	2.18	0.73
1:C:258:ASN:ND2	1:C:261:MET:HB2	2.04	0.72
1:C:532:GLU:OE2	1:D:498:SER:OG	2.07	0.72
1:F:174:HIS:HB3	1:F:213:MET:HE1	1.70	0.72
1:C:102:GLU:OE2	1:C:105:THR:HG22	1.89	0.72
1:E:541:TYR:O	1:F:253:LYS:HD2	1.90	0.72
1:F:318:ALA:HB2	1:F:357:LEU:CD2	2.20	0.72
1:F:353:LYS:O	1:F:429:VAL:HG13	1.90	0.72
1:E:153:VAL:HG12	1:E:177:MET:HE2	1.70	0.71
1:B:202:ASP:O	1:B:206:VAL:HG23	1.90	0.71
1:A:554:SER:OG	6:A:803:HOH:O	2.08	0.71
1:C:460:ALA:HA	2:C:702:CO3:O2	1.89	0.71
1:A:104:ASN:O	6:A:804:HOH:O	2.09	0.71
1:F:237:PHE:O	1:F:241:THR:HG23	1.90	0.71
1:F:88:VAL:HG22	1:F:308:VAL:HG12	1.72	0.71
1:F:152:GLN:OE1	1:F:152:GLN:HA	1.90	0.70
1:B:230:VAL:HG23	1:B:234:LEU:CD2	2.18	0.70
1:D:586:ARG:HD2	6:D:801:HOH:O	1.92	0.70
1:F:298:ILE:HA	1:F:400:MET:CE	2.21	0.70
1:E:440:ARG:HD2	1:F:302:SER:HB2	1.73	0.70
1:E:214:LEU:HD21	1:E:222:LEU:CD1	2.21	0.70
1:E:133:ASN:HA	1:E:167:VAL:HG21	1.72	0.69
1:D:302:SER:OG	1:D:378:PHE:HB2	1.91	0.69
1:A:577:ALA:O	6:A:805:HOH:O	2.11	0.68
1:B:500:ALA:HB3	1:B:524:VAL:HG22	1.75	0.68
1:D:138:GLU:HA	1:D:194:SER:OG	1.93	0.68
1:F:222:LEU:O	1:F:267:LEU:HD12	1.93	0.68
1:A:508:GLU:CD	1:A:508:GLU:H	1.97	0.68
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.74	0.68
1:C:287:TYR:CD2	1:C:594:ARG:HG2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ASP:HA	1:D:278:LYS:HD2	1.76	0.68
1:B:117:ILE:HD11	1:B:146:SER:CB	2.23	0.67
1:E:148:VAL:HG11	1:E:153:VAL:CG2	2.25	0.67
1:D:568:ASN:O	1:D:568:ASN:ND2	2.27	0.67
1:E:167:VAL:HG22	1:E:167:VAL:O	1.94	0.67
1:F:323:LEU:HD11	1:F:359:TYR:HB2	1.76	0.67
1:E:444:ILE:HD13	1:E:542:ALA:HB2	1.77	0.67
1:F:86:SER:HB2	1:F:312:ASN:OD1	1.95	0.67
1:B:395:LEU:O	1:B:395:LEU:HG	1.94	0.67
1:E:391:SER:OG	6:E:806:HOH:O	2.13	0.67
1:C:317:LEU:HD11	1:C:321:LEU:HD22	1.77	0.67
1:F:379:ASP:O	1:F:396:MET:HG3	1.94	0.67
1:E:217:ASN:HB3	1:E:219:LEU:CD1	2.25	0.66
1:F:217:ASN:CB	1:F:219:LEU:HD11	2.24	0.66
1:E:474:GLU:OE1	6:E:807:HOH:O	2.13	0.66
1:A:96:PRO:O	6:A:806:HOH:O	2.12	0.66
1:E:249:ASP:OD1	1:E:251:ARG:HD3	1.95	0.66
1:B:142:VAL:HG12	1:B:167:VAL:CG2	2.24	0.66
1:F:167:VAL:HG12	1:F:167:VAL:O	1.96	0.66
1:B:167:VAL:HG12	1:B:167:VAL:O	1.94	0.65
1:F:228:ILE:CD1	1:F:230:VAL:HG13	2.26	0.65
1:F:314:ALA:HB1	1:F:357:LEU:HD11	1.77	0.65
1:F:114:VAL:HG23	1:F:269:VAL:HG12	1.78	0.65
1:F:100:PRO:O	1:F:101:ILE:HD13	1.96	0.65
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.77	0.65
1:F:463:ARG:N	2:F:701:CO3:O3	2.24	0.65
1:E:200:GLU:OE2	6:E:808:HOH:O	2.14	0.65
1:E:542:ALA:O	1:F:253:LYS:HE2	1.97	0.65
1:B:353:LYS:NZ	6:B:809:HOH:O	2.25	0.65
1:A:286:VAL:HG11	1:A:416:LEU:CD2	2.27	0.64
1:A:563:LYS:O	6:A:808:HOH:O	2.15	0.64
1:B:528:PRO:HG3	1:E:525:TRP:CD2	2.32	0.64
1:B:478:VAL:N	6:B:811:HOH:O	2.26	0.64
1:C:395:LEU:HG	1:C:395:LEU:O	1.97	0.64
1:F:202:ASP:O	1:F:206:VAL:HG23	1.97	0.64
1:B:323:LEU:CD2	1:B:359:TYR:HB2	2.27	0.64
1:B:198:LEU:CD2	1:B:202:ASP:HB3	2.27	0.63
1:A:221:LYS:HG3	1:A:266:HIS:HB2	1.81	0.63
1:C:419:GLU:HG2	6:C:802:HOH:O	1.98	0.63
1:E:440:ARG:HD2	1:F:302:SER:CB	2.28	0.63
1:B:323:LEU:HD21	1:B:359:TYR:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:ASN:HA	1:F:167:VAL:CG1	2.26	0.63
1:D:142:VAL:HG12	1:D:162:MET:HB3	1.80	0.63
1:E:297:LEU:O	1:E:400:MET:HE1	1.99	0.63
1:F:134:ASN:ND2	1:F:141:PRO:HD2	2.13	0.63
1:F:302:SER:OG	1:F:378:PHE:HB2	1.99	0.63
1:A:391:SER:O	6:A:807:HOH:O	2.15	0.63
1:C:142:VAL:HG23	1:C:165:PHE:O	1.99	0.63
1:C:391:SER:OG	6:C:805:HOH:O	2.16	0.63
1:F:88:VAL:HG22	1:F:308:VAL:CG1	2.29	0.63
1:F:318:ALA:HB2	1:F:357:LEU:HD21	1.81	0.63
1:B:419:GLU:HB3	1:B:420:ASN:OD1	1.99	0.63
1:D:152:GLN:HG2	1:D:180:ASP:OD1	1.99	0.62
1:C:99:ILE:HG22	1:C:101:ILE:HD11	1.82	0.62
1:D:395:LEU:O	1:D:395:LEU:HG	1.99	0.62
1:A:529:ILE:CG2	1:A:560:LEU:HD12	2.27	0.62
1:B:198:LEU:HD22	1:B:202:ASP:HB3	1.81	0.61
1:C:236:ARG:HD2	1:C:283:LYS:HG2	1.81	0.61
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.81	0.61
1:D:573:HIS:NE2	6:D:810:HOH:O	2.31	0.61
1:C:317:LEU:CD1	1:C:321:LEU:HD22	2.29	0.61
1:F:298:ILE:HA	1:F:400:MET:HE3	1.82	0.61
1:C:498:SER:O	1:C:523:PRO:HG2	1.99	0.61
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.32	0.60
1:D:230:VAL:HG12	1:D:234:LEU:HD23	1.83	0.60
1:A:88:VAL:HG22	1:A:308:VAL:CG1	2.31	0.60
1:B:367:LYS:CG	1:B:369:ILE:HD11	2.31	0.60
1:C:232:LYS:HE3	1:C:276:THR:O	2.00	0.60
1:D:144:ILE:CD1	1:D:157:LEU:HB3	2.31	0.60
1:D:378:PHE:CD2	1:D:433:MET:HE1	2.35	0.60
1:F:597:THR:O	1:F:600:VAL:HG22	2.01	0.60
1:A:144:ILE:CG1	1:A:157:LEU:HD22	2.30	0.60
1:E:529:ILE:HG23	1:E:560:LEU:HG	1.84	0.60
1:F:318:ALA:HB2	1:F:357:LEU:HD23	1.84	0.60
1:A:286:VAL:HG11	1:A:416:LEU:HD21	1.83	0.60
1:B:330:VAL:O	1:B:334:GLU:HG3	2.01	0.60
1:C:100:PRO:C	1:C:101:ILE:HD13	2.22	0.60
1:F:236:ARG:O	1:F:240:GLU:HG3	2.01	0.60
1:B:369:ILE:HD12	1:B:480:TYR:HB2	1.84	0.60
1:F:121:CYS:HA	1:F:270:TYR:CE2	2.37	0.60
1:F:174:HIS:HB3	1:F:213:MET:CE	2.31	0.59
1:B:463:ARG:NE	2:B:701:CO3:O3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ASP:HB3	1:E:153:VAL:HG22	1.83	0.59
1:F:203:MET:CE	1:F:238:PHE:HD1	2.15	0.59
5:E:704:SO4:O2	1:F:436:LYS:HG2	2.02	0.59
1:F:386:LYS:HB3	1:F:391:SER:HB3	1.84	0.59
1:D:222:LEU:HD23	1:D:223:THR:N	2.18	0.59
1:A:207:VAL:HG11	1:A:241:THR:HG22	1.85	0.59
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.85	0.59
1:B:337:LYS:O	1:B:448:SER:HA	2.03	0.59
1:C:99:ILE:HG22	1:C:101:ILE:CD1	2.32	0.59
1:F:172:SER:HB2	1:F:189:TYR:O	2.02	0.59
1:F:203:MET:HB3	1:F:237:PHE:HE2	1.67	0.59
1:E:278:LYS:O	1:E:281:VAL:HG12	2.03	0.58
1:E:302:SER:OG	1:E:377:THR:O	2.19	0.58
1:C:130:PHE:CD1	1:C:225:VAL:HB	2.39	0.58
1:A:102:GLU:HG2	1:A:105:THR:HG22	1.86	0.58
1:B:368:LYS:C	1:B:369:ILE:HD13	2.22	0.58
1:C:271:ILE:HD13	1:C:277:TYR:CD1	2.38	0.58
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.86	0.58
1:F:203:MET:HE2	1:F:238:PHE:HD1	1.69	0.58
1:F:198:LEU:HD22	1:F:202:ASP:CB	2.32	0.58
1:E:272:ASN:O	1:E:273:ASN:HB2	2.03	0.58
1:E:302:SER:OG	1:E:378:PHE:HB2	2.04	0.58
1:A:297:LEU:O	1:A:400:MET:HE1	2.04	0.57
1:F:534:ARG:HD2	1:F:534:ARG:O	2.04	0.57
1:B:488:THR:HG21	1:B:555:SER:HA	1.86	0.57
1:D:440:ARG:HD3	1:D:443:ASP:CG	2.25	0.57
1:C:463:ARG:HG3	1:C:561:PHE:CE2	2.39	0.57
1:D:480:TYR:HD1	1:D:509:LEU:HD22	1.69	0.57
1:F:219:LEU:HD22	1:F:219:LEU:H	1.69	0.57
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.86	0.57
1:B:349:MET:HE3	1:B:350:TYR:CZ	2.40	0.57
1:F:121:CYS:HA	1:F:270:TYR:HE2	1.68	0.57
1:D:287:TYR:CE1	1:D:597:THR:HG21	2.40	0.57
1:A:376:ILE:HB	1:A:399:ASP:HB3	1.86	0.57
1:A:534:ARG:HD2	1:A:534:ARG:O	2.04	0.57
1:E:168:LYS:O	1:E:171:THR:HG22	2.04	0.57
1:E:226:PHE:CB	1:E:271:ILE:HG13	2.34	0.57
1:F:324:GLU:CB	1:F:358:THR:HG23	2.34	0.57
1:E:222:LEU:HD22	1:E:267:LEU:HD13	1.87	0.57
1:A:418:PRO:HG3	1:A:601:LEU:CD2	2.31	0.56
1:A:502:VAL:HG12	1:A:526:TRP:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ILE:O	1:A:514:LEU:HG	2.05	0.56
1:C:321:LEU:HD21	1:C:411:TYR:HA	1.86	0.56
1:E:323:LEU:HD22	1:E:359:TYR:HB2	1.87	0.56
1:F:228:ILE:HD12	1:F:230:VAL:HG13	1.86	0.56
1:B:522:GLU:OE1	6:B:802:HOH:O	2.17	0.56
1:C:216:ASP:HB2	1:E:173:LYS:NZ	2.19	0.56
1:A:203:MET:HA	1:A:203:MET:CE	2.36	0.56
1:B:117:ILE:HG22	1:B:272:ASN:HA	1.87	0.56
1:B:368:LYS:HE2	1:B:477:GLY:O	2.05	0.56
1:D:352:ASN:H	4:D:701:MPD:C5	2.19	0.56
1:E:374:LYS:HE3	1:E:376:ILE:HG13	1.88	0.56
1:F:460:ALA:HB1	1:F:463:ARG:CD	2.35	0.56
1:C:595:LEU:HD23	1:C:595:LEU:C	2.26	0.56
1:F:247:MET:HE3	1:F:247:MET:HA	1.86	0.56
1:B:581:TRP:CZ3	1:B:588:PRO:HG3	2.40	0.56
1:C:137:LYS:H	1:C:137:LYS:HD2	1.70	0.56
1:C:316:GLU:O	1:C:320:LYS:HG3	2.06	0.56
1:A:253:LYS:O	1:A:257:LYS:NZ	2.39	0.55
1:B:266:HIS:NE2	6:B:805:HOH:O	2.22	0.55
1:A:372:VAL:O	1:A:483:ASP:HA	2.05	0.55
1:B:406:VAL:HG12	1:B:425:PHE:HB3	1.89	0.55
1:D:359:TYR:OH	1:D:418:PRO:O	2.20	0.55
1:F:150:ASP:HA	1:F:180:ASP:OD2	2.07	0.55
1:F:356:HIS:CD2	1:F:356:HIS:O	2.59	0.55
1:C:117:ILE:HD11	1:C:146:SER:OG	2.06	0.55
1:D:494:SER:OG	6:D:805:HOH:O	2.18	0.55
1:C:100:PRO:O	1:C:101:ILE:HD13	2.05	0.55
1:C:326:LYS:O	1:C:327:ILE:HD13	2.06	0.55
1:E:449:ASN:HD21	1:E:451:LYS:HD2	1.72	0.55
1:F:338:MET:CE	1:F:468:ASP:HB3	2.36	0.55
1:E:287:TYR:CD2	1:E:594:ARG:HG2	2.42	0.55
1:A:302:SER:OG	1:A:378:PHE:HB2	2.07	0.55
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.88	0.55
1:E:513:ILE:HD13	1:E:574:ILE:HD11	1.89	0.55
1:F:481:ILE:O	1:F:571:TRP:HA	2.07	0.55
1:A:330:VAL:O	1:A:334:GLU:HG3	2.07	0.55
1:C:138:GLU:O	1:C:139:ASN:HB2	2.06	0.55
1:D:444:ILE:HD12	1:E:301:PRO:CG	2.37	0.54
1:F:579:VAL:O	1:F:589:LYS:HD3	2.06	0.54
1:B:321:LEU:HB2	1:B:323:LEU:HD12	1.90	0.54
1:C:512:LYS:NZ	1:C:603:ASP:OD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:ARG:HD2	1:D:534:ARG:O	2.07	0.54
1:A:139:ASN:O	1:A:166:ASN:HB2	2.07	0.54
1:E:330:VAL:O	1:E:334:GLU:HG3	2.08	0.54
1:E:491:MET:HA	6:E:803:HOH:O	2.08	0.54
1:F:142:VAL:HG12	1:F:165:PHE:O	2.08	0.54
1:A:481:ILE:O	1:A:571:TRP:HA	2.08	0.54
1:B:176:TYR:CD1	1:F:177:MET:HE3	2.43	0.54
1:D:440:ARG:N	1:D:440:ARG:HD2	2.22	0.53
1:D:337:LYS:O	1:D:448:SER:HA	2.07	0.53
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.89	0.53
1:F:413:VAL:HG22	1:F:600:VAL:HG21	1.89	0.53
1:D:444:ILE:HD12	1:E:301:PRO:HG2	1.90	0.53
1:B:528:PRO:HG2	1:B:530:ILE:HD11	1.91	0.53
1:C:98:SER:HA	6:C:812:HOH:O	2.08	0.53
1:F:372:VAL:O	1:F:483:ASP:HA	2.08	0.53
1:B:176:TYR:CE1	1:F:156:PHE:HB2	2.44	0.53
1:D:530:ILE:HD12	1:D:556:ILE:HD13	1.91	0.53
1:F:218:LYS:C	1:F:219:LEU:HD13	2.30	0.53
1:A:306:ASN:HB2	1:A:307:PRO:HD2	1.91	0.53
1:F:323:LEU:CD1	1:F:359:TYR:HB2	2.39	0.53
1:B:448:SER:OG	1:B:471:VAL:HG11	2.09	0.53
1:D:378:PHE:HD2	1:D:433:MET:CE	2.22	0.53
1:F:365:VAL:HA	6:F:813:HOH:O	2.09	0.52
1:B:133:ASN:CA	1:B:167:VAL:HG11	2.23	0.52
1:B:540:LYS:O	1:B:540:LYS:HG3	2.08	0.52
1:B:192:CYS:SG	1:B:228:ILE:HD13	2.49	0.52
1:D:287:TYR:HE1	1:D:597:THR:HG21	1.74	0.52
1:D:378:PHE:HD2	1:D:433:MET:HE1	1.74	0.52
1:D:298:ILE:HG21	1:D:588:PRO:HB3	1.92	0.52
1:F:355:ILE:CG2	1:F:357:LEU:HD12	2.40	0.52
1:F:356:HIS:O	1:F:357:LEU:C	2.47	0.52
1:F:536:THR:HG21	1:F:551:VAL:CG2	2.40	0.52
1:C:534:ARG:NH1	1:C:538:ASN:OD1	2.43	0.52
1:E:463:ARG:HG3	1:E:561:PHE:CE2	2.45	0.52
1:F:463:ARG:CD	2:F:701:CO3:O3	2.48	0.52
1:B:365:VAL:HG13	1:B:365:VAL:O	2.09	0.52
1:C:368:LYS:C	1:C:478:VAL:HG22	2.31	0.52
1:D:249:ASP:OD2	1:D:251:ARG:NH2	2.34	0.52
1:F:287:TYR:O	1:F:291:THR:HG23	2.10	0.52
1:A:534:ARG:HA	1:A:560:LEU:HD23	1.92	0.52
1:D:275:ASP:HA	1:D:278:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:541:TYR:OH	1:F:588:PRO:HD3	2.10	0.52
1:F:367:LYS:HA	1:F:479:ASP:OD2	2.10	0.51
1:A:303:ASN:HB3	1:C:440:ARG:HH21	1.74	0.51
1:B:176:TYR:HD1	1:F:177:MET:HE3	1.75	0.51
1:B:306:ASN:HB2	1:B:307:PRO:CD	2.40	0.51
1:D:454:GLU:OE2	6:D:806:HOH:O	2.18	0.51
1:D:254:SER:OG	1:D:255:THR:N	2.42	0.51
1:A:150:ASP:OD1	1:A:153:VAL:HG23	2.11	0.51
1:C:379:ASP:O	1:C:396:MET:HG3	2.10	0.51
1:E:131:LEU:O	1:E:228:ILE:HG23	2.11	0.51
1:E:414:GLY:O	1:E:417:LYS:HG3	2.11	0.51
1:D:235:PHE:CE1	1:D:269:VAL:HG11	2.45	0.51
1:D:351:PRO:HA	4:D:701:MPD:H52	1.92	0.51
1:B:172:SER:HA	1:B:189:TYR:O	2.11	0.51
1:D:148:VAL:HG21	1:D:153:VAL:HG12	1.93	0.51
1:E:156:PHE:CD2	1:E:157:LEU:HD23	2.46	0.51
1:E:578:GLY:N	6:E:809:HOH:O	2.30	0.51
1:B:444:ILE:HD12	1:C:301:PRO:HG3	1.93	0.51
1:B:372:VAL:O	1:B:483:ASP:HA	2.11	0.51
1:F:112:VAL:HG23	1:F:267:LEU:O	2.10	0.51
1:F:121:CYS:O	1:F:149:ASN:HB2	2.11	0.51
1:F:142:VAL:HG13	1:F:162:MET:HB3	1.92	0.51
1:B:503:PHE:O	1:B:573:HIS:N	2.42	0.50
1:E:420:ASN:N	1:E:420:ASN:HD22	2.09	0.50
1:F:369:ILE:O	1:F:423:ILE:HA	2.12	0.50
1:D:278:LYS:N	6:D:807:HOH:O	2.44	0.50
1:E:144:ILE:HG21	1:E:157:LEU:HD13	1.94	0.50
1:E:444:ILE:HG13	1:F:301:PRO:HG3	1.93	0.50
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.92	0.50
1:B:341:TYR:CE1	1:B:428:ALA:HB1	2.46	0.50
1:F:356:HIS:O	1:F:356:HIS:HD2	1.94	0.50
1:A:106:PRO:HD2	1:A:247:MET:SD	2.52	0.50
1:A:174:HIS:HB3	1:D:175:PHE:CD1	2.47	0.50
1:B:278:LYS:O	1:B:281:VAL:HG23	2.11	0.50
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.92	0.50
1:B:374:LYS:HE3	1:B:462:GLY:HA3	1.94	0.50
1:D:306:ASN:OD1	1:D:306:ASN:N	2.44	0.50
1:E:134:ASN:HB2	1:E:167:VAL:HG11	1.93	0.50
1:B:120:GLY:HA2	1:B:147:LYS:O	2.11	0.50
1:C:99:ILE:CG2	1:C:101:ILE:HD11	2.41	0.50
1:C:100:PRO:O	1:C:251:ARG:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:LEU:HD22	1:F:219:LEU:N	2.27	0.50
1:F:374:LYS:HB2	1:F:485:ALA:CB	2.42	0.50
1:A:123:VAL:HG12	1:A:123:VAL:O	2.12	0.50
1:C:207:VAL:HG11	1:C:241:THR:HG22	1.93	0.50
1:B:431:GLU:OE1	6:B:803:HOH:O	2.20	0.49
1:C:539:SER:HB2	1:C:545:ASN:ND2	2.26	0.49
1:E:449:ASN:ND2	1:E:451:LYS:HD2	2.26	0.49
1:E:517:SER:OG	1:E:522:GLU:O	2.19	0.49
1:A:306:ASN:HB2	1:A:307:PRO:CD	2.42	0.49
1:A:532:GLU:OE1	1:F:498:SER:OG	2.30	0.49
1:E:343:SER:HA	1:E:346:LYS:HG3	1.94	0.49
1:B:445:ILE:CD1	1:B:453:ILE:HB	2.42	0.49
1:C:546:GLN:HG2	1:C:547:ILE:HG23	1.93	0.49
1:D:99:ILE:O	1:D:101:ILE:HG12	2.12	0.49
1:E:157:LEU:HD21	1:E:187:VAL:HG11	1.94	0.49
1:E:306:ASN:HB2	1:E:307:PRO:HD2	1.94	0.49
1:A:127:LEU:CD2	1:A:129:ILE:HD11	2.40	0.49
1:B:442:GLY:O	1:C:301:PRO:HB3	2.12	0.49
1:D:236:ARG:NE	1:D:240:GLU:OE2	2.42	0.49
1:F:374:LYS:HE3	1:F:462:GLY:HA3	1.94	0.49
1:D:222:LEU:HD22	1:D:224:VAL:HG23	1.94	0.49
1:C:122:ASN:O	6:C:803:HOH:O	2.19	0.49
1:E:200:GLU:OE1	1:E:204:LYS:NZ	2.43	0.49
1:F:86:SER:N	6:F:809:HOH:O	2.44	0.49
1:B:487:LEU:HB3	1:B:488:THR:HG23	1.95	0.49
1:D:127:LEU:HD12	1:D:186:ALA:HB3	1.95	0.49
1:D:302:SER:HB3	1:F:440:ARG:HE	1.78	0.49
1:E:441:PRO:HD2	1:F:378:PHE:CZ	2.47	0.49
1:F:133:ASN:CA	1:F:167:VAL:HG11	2.31	0.49
1:F:286:VAL:HG21	1:F:416:LEU:HD21	1.95	0.49
1:A:106:PRO:HD2	1:A:247:MET:CE	2.43	0.49
1:B:444:ILE:HB	1:C:301:PRO:HG2	1.95	0.49
1:C:134:ASN:ND2	1:C:141:PRO:HD2	2.28	0.49
1:D:334:GLU:HB3	1:E:93:SER:OG	2.13	0.49
1:A:286:VAL:HG11	1:A:416:LEU:HD22	1.95	0.48
1:B:144:ILE:HD12	1:B:162:MET:HG3	1.94	0.48
1:E:167:VAL:O	1:E:167:VAL:CG2	2.60	0.48
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.94	0.48
1:E:141:PRO:HA	1:E:165:PHE:O	2.14	0.48
1:F:536:THR:HG21	1:F:551:VAL:HG23	1.93	0.48
1:C:255:THR:O	1:C:255:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:ILE:HG12	1:C:576:ILE:HD13	1.94	0.48
1:C:494:SER:CB	1:D:494:SER:HB3	2.44	0.48
1:F:328:LEU:HD12	1:F:328:LEU:N	2.29	0.48
1:B:502:VAL:HG13	1:B:526:TRP:HA	1.96	0.48
1:C:317:LEU:HD11	1:C:321:LEU:CD2	2.42	0.48
1:D:172:SER:O	1:D:173:LYS:HG2	2.13	0.48
1:D:509:LEU:HD12	1:D:509:LEU:O	2.13	0.48
1:E:286:VAL:HG11	1:E:416:LEU:HD21	1.93	0.48
1:F:552:LYS:NZ	6:F:802:HOH:O	2.17	0.48
1:D:330:VAL:HG22	4:D:701:MPD:H53	1.95	0.48
1:E:166:ASN:ND2	1:E:168:LYS:HE2	2.28	0.48
1:F:386:LYS:HE3	1:F:396:MET:SD	2.54	0.48
1:C:130:PHE:CE1	1:C:225:VAL:HG11	2.49	0.48
1:E:292:TYR:O	1:E:296:GLN:HG3	2.13	0.48
1:E:332:GLU:O	1:E:336:LEU:HD22	2.14	0.48
1:C:453:ILE:HG12	1:C:544:ILE:HD11	1.96	0.48
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.96	0.48
1:E:190:VAL:CG1	1:E:206:VAL:HG13	2.41	0.48
1:F:338:MET:HE2	1:F:468:ASP:HB3	1.94	0.48
1:A:128:THR:O	1:A:187:VAL:HA	2.13	0.48
1:C:106:PRO:HG2	1:C:263:TYR:CE2	2.49	0.48
1:C:460:ALA:CA	2:C:702:CO3:O2	2.61	0.48
1:D:330:VAL:O	1:D:334:GLU:HG3	2.13	0.48
1:D:236:ARG:HG2	1:D:240:GLU:OE2	2.14	0.48
1:B:364:ASP:O	1:B:420:ASN:HA	2.14	0.47
1:E:156:PHE:HD2	1:E:157:LEU:HD23	1.79	0.47
1:F:237:PHE:CZ	1:F:241:THR:HG21	2.49	0.47
1:C:130:PHE:HE1	1:C:225:VAL:HG11	1.79	0.47
1:D:88:VAL:CG1	1:D:306:ASN:HD21	2.27	0.47
1:D:306:ASN:HB2	1:D:307:PRO:CD	2.44	0.47
1:D:529:ILE:HG23	1:D:560:LEU:HG	1.95	0.47
1:E:318:ALA:O	1:E:322:ASN:N	2.47	0.47
1:F:483:ASP:C	1:F:483:ASP:OD1	2.53	0.47
1:E:147:LYS:HA	6:E:813:HOH:O	2.13	0.47
1:F:343:SER:O	1:F:346:LYS:HG3	2.15	0.47
1:A:328:LEU:HD22	1:A:332:GLU:OE1	2.14	0.47
1:B:142:VAL:HG13	1:B:165:PHE:O	2.14	0.47
1:B:152:GLN:HG2	1:B:178:PHE:O	2.14	0.47
1:B:217:ASN:ND2	1:F:165:PHE:HE1	2.13	0.47
1:B:247:MET:HG3	1:B:292:TYR:CE1	2.50	0.47
1:C:409:CYS:O	1:C:413:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ARG:HG3	1:C:561:PHE:CD2	2.49	0.47
1:D:235:PHE:CE2	1:D:239:LEU:HD11	2.50	0.47
1:E:198:LEU:CD1	1:E:228:ILE:HD12	2.44	0.47
1:E:539:SER:HB3	1:E:542:ALA:O	2.15	0.47
1:F:590:GLY:N	6:F:808:HOH:O	2.46	0.47
1:D:207:VAL:HG11	1:D:241:THR:HG22	1.97	0.47
1:D:431:GLU:CG	1:D:433:MET:HE3	2.45	0.47
1:E:134:ASN:CB	1:E:167:VAL:HG11	2.45	0.47
1:E:372:VAL:O	1:E:483:ASP:HA	2.14	0.47
1:E:539:SER:HA	1:E:545:ASN:OD1	2.15	0.47
1:F:235:PHE:CE1	1:F:269:VAL:HG11	2.50	0.47
1:A:540:LYS:O	1:A:540:LYS:HG3	2.13	0.47
1:B:339:GLY:HA3	1:B:446:THR:O	2.15	0.47
1:D:150:ASP:HB3	1:D:153:VAL:HB	1.96	0.47
1:C:107:ILE:HG12	1:C:247:MET:HG2	1.97	0.47
1:C:235:PHE:O	1:C:238:PHE:HB3	2.15	0.47
1:F:306:ASN:HB2	1:F:307:PRO:HD2	1.96	0.47
1:A:174:HIS:HB3	1:D:175:PHE:CE1	2.50	0.46
1:B:528:PRO:HG3	1:E:525:TRP:CE3	2.51	0.46
1:A:366:LYS:CD	1:A:420:ASN:HB3	2.46	0.46
1:B:251:ARG:HD3	1:B:296:GLN:OE1	2.15	0.46
1:B:481:ILE:O	1:B:571:TRP:HA	2.15	0.46
1:C:107:ILE:CG1	1:C:247:MET:HG2	2.45	0.46
1:E:174:HIS:CE1	1:E:213:MET:HG2	2.49	0.46
1:F:460:ALA:HB1	1:F:463:ARG:HD3	1.97	0.46
1:A:208:LEU:HD12	1:A:208:LEU:O	2.15	0.46
1:C:150:ASP:OD2	1:C:179:ASN:HB2	2.14	0.46
1:C:524:VAL:HG21	1:C:595:LEU:HD11	1.95	0.46
1:E:222:LEU:C	1:E:222:LEU:HD23	2.36	0.46
1:E:530:ILE:HD12	1:E:556:ILE:HD13	1.97	0.46
1:B:90:GLN:HB3	1:B:95:ASP:HB2	1.98	0.46
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.97	0.46
1:F:375:GLY:O	1:F:429:VAL:HA	2.16	0.46
1:C:271:ILE:HD13	1:C:277:TYR:CE1	2.51	0.46
1:C:306:ASN:HB2	1:C:307:PRO:CD	2.46	0.46
1:F:174:HIS:ND1	1:F:174:HIS:O	2.49	0.46
1:B:135:PRO:HA	1:B:194:SER:O	2.16	0.46
1:B:144:ILE:CD1	1:B:162:MET:HG3	2.44	0.46
1:C:113:GLN:OE1	1:C:113:GLN:HA	2.15	0.46
1:E:225:VAL:HG22	1:E:270:TYR:HB2	1.97	0.46
1:A:203:MET:HA	1:A:203:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:ILE:HG22	1:D:591:PHE:CE1	2.51	0.46
1:B:204:LYS:HG3	1:B:208:LEU:CD2	2.46	0.46
1:C:222:LEU:HD12	1:C:223:THR:H	1.81	0.46
1:D:90:GLN:HB3	1:D:95:ASP:HB2	1.97	0.46
1:D:372:VAL:O	1:D:483:ASP:HA	2.16	0.46
1:F:203:MET:HE1	1:F:238:PHE:CD1	2.51	0.46
1:F:410:ALA:HA	1:F:425:PHE:CE2	2.51	0.46
1:F:491:MET:HE3	1:F:555:SER:HB3	1.98	0.46
1:C:107:ILE:HG21	1:C:243:PHE:HB3	1.97	0.46
1:D:306:ASN:HB2	1:D:307:PRO:HD2	1.97	0.46
1:D:380:SER:O	1:D:386:LYS:HG3	2.16	0.46
1:E:364:ASP:O	1:E:420:ASN:HA	2.15	0.46
1:C:321:LEU:HD12	1:C:321:LEU:HA	1.77	0.45
1:D:256:ASP:HB3	1:D:257:LYS:H	1.50	0.45
1:E:481:ILE:O	1:E:571:TRP:HA	2.16	0.45
1:E:536:THR:OG1	1:E:548:SER:OG	2.28	0.45
1:B:375:GLY:O	1:B:429:VAL:HA	2.16	0.45
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.97	0.45
1:E:106:PRO:HD2	1:E:247:MET:SD	2.56	0.45
1:B:460:ALA:HB1	2:B:701:CO3:O3	2.16	0.45
1:C:187:VAL:HG12	1:C:188:GLY:N	2.31	0.45
1:D:107:ILE:HG21	1:D:288:TYR:CE2	2.52	0.45
1:D:517:SER:OG	1:D:524:VAL:HG23	2.16	0.45
1:F:203:MET:CE	1:F:238:PHE:CD1	2.98	0.45
1:F:221:LYS:HA	1:F:266:HIS:O	2.16	0.45
1:F:534:ARG:HA	1:F:560:LEU:HD13	1.98	0.45
1:B:352:ASN:O	1:B:353:LYS:HD2	2.16	0.45
1:C:481:ILE:O	1:C:571:TRP:HA	2.16	0.45
1:E:140:GLY:O	1:E:167:VAL:HG12	2.17	0.45
1:F:219:LEU:HD13	1:F:219:LEU:N	2.31	0.45
1:F:484:ILE:HG23	1:F:484:ILE:O	2.16	0.45
1:E:192:CYS:SG	1:E:228:ILE:HD13	2.57	0.45
1:F:410:ALA:HB2	1:F:425:PHE:CD2	2.51	0.45
1:A:291:THR:HG22	1:A:593:VAL:HB	1.98	0.45
1:B:225:VAL:HG13	1:B:270:TYR:HB2	1.98	0.45
1:D:316:GLU:O	1:D:320:LYS:HG3	2.17	0.45
1:D:419:GLU:O	1:D:421:VAL:HG13	2.17	0.45
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.99	0.45
1:B:198:LEU:HD22	1:B:202:ASP:CB	2.47	0.45
1:B:133:ASN:HB2	1:B:193:GLY:O	2.17	0.45
1:D:301:PRO:HA	1:D:397:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLU:HG3	6:E:808:HOH:O	2.17	0.45
1:F:306:ASN:HB2	1:F:307:PRO:CD	2.47	0.45
1:F:487:LEU:HD11	2:F:701:CO3:O3	2.17	0.45
1:F:591:PHE:N	6:F:808:HOH:O	2.41	0.45
1:A:298:ILE:HA	1:A:400:MET:HE3	1.99	0.45
1:A:587:LYS:HB2	1:A:588:PRO:HD2	1.98	0.45
1:B:167:VAL:HG13	1:B:191:GLY:HA2	1.99	0.45
1:B:466:LEU:O	1:B:470:LEU:HG	2.16	0.45
1:E:99:ILE:HG22	1:E:101:ILE:CD1	2.47	0.45
1:B:571:TRP:CZ2	1:B:573:HIS:HB2	2.52	0.44
1:C:368:LYS:HG2	1:C:422:GLU:HB3	1.98	0.44
1:D:397:LYS:NZ	6:F:804:HOH:O	2.49	0.44
1:E:169:LEU:HD13	1:E:169:LEU:C	2.38	0.44
1:F:395:LEU:HG	1:F:395:LEU:O	2.17	0.44
1:A:222:LEU:O	1:A:267:LEU:HA	2.16	0.44
1:E:127:LEU:HD11	1:E:129:ILE:HD11	1.99	0.44
1:E:222:LEU:HD21	1:E:224:VAL:CG2	2.42	0.44
1:F:156:PHE:CB	1:F:177:MET:HE1	2.47	0.44
1:B:365:VAL:O	1:B:365:VAL:CG1	2.65	0.44
1:B:491:MET:HA	1:B:494:SER:OG	2.18	0.44
1:D:374:LYS:NZ	1:D:399:ASP:OD1	2.47	0.44
1:F:236:ARG:HD2	1:F:283:LYS:HD3	1.99	0.44
1:A:222:LEU:O	1:A:267:LEU:HD12	2.16	0.44
1:A:341:TYR:CE1	1:A:428:ALA:HB1	2.51	0.44
1:B:544:ILE:CD1	1:B:564:GLU:HG3	2.48	0.44
1:E:365:VAL:HG21	1:E:422:GLU:HB2	1.99	0.44
1:A:117:ILE:HD11	1:A:146:SER:CB	2.48	0.44
1:A:123:VAL:HG21	1:A:153:VAL:HG11	2.00	0.44
1:B:174:HIS:HB2	1:F:174:HIS:O	2.17	0.44
1:B:423:ILE:HD11	1:B:600:VAL:HG13	1.99	0.44
1:C:342:LEU:HD23	1:C:352:ASN:HD22	1.82	0.44
1:E:395:LEU:O	1:E:395:LEU:HG	2.17	0.44
1:A:375:GLY:O	1:A:429:VAL:HA	2.18	0.44
1:C:510:ILE:HD13	1:C:526:TRP:NE1	2.33	0.44
1:F:503:PHE:CE2	1:F:527:LEU:HB2	2.52	0.44
1:C:216:ASP:HB2	1:E:173:LYS:HZ2	1.83	0.44
1:C:236:ARG:NE	1:C:240:GLU:OE2	2.32	0.44
1:D:127:LEU:HD12	1:D:186:ALA:CB	2.48	0.44
1:D:321:LEU:CD1	1:D:411:TYR:HA	2.47	0.44
1:D:352:ASN:H	4:D:701:MPD:H51	1.83	0.44
1:D:463:ARG:HE	1:D:463:ARG:HB3	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:SER:OG	1:F:445:ILE:HG21	2.18	0.44
1:A:298:ILE:HA	1:A:400:MET:CE	2.48	0.44
1:B:380:SER:O	1:B:385:LEU:HD12	2.17	0.44
1:E:306:ASN:HB2	1:E:307:PRO:CD	2.47	0.44
1:B:236:ARG:NE	1:B:240:GLU:OE2	2.48	0.44
1:B:440:ARG:NH2	6:B:808:HOH:O	2.51	0.44
1:C:292:TYR:O	1:C:296:GLN:HG3	2.18	0.44
1:A:195:VAL:CG2	1:A:198:LEU:HD23	2.48	0.43
1:B:463:ARG:NH2	1:B:558:ALA:HB2	2.33	0.43
1:C:302:SER:OG	1:C:378:PHE:HB2	2.18	0.43
1:D:275:ASP:HA	1:D:278:LYS:HZ2	1.82	0.43
1:E:342:LEU:HA	1:E:352:ASN:ND2	2.33	0.43
1:A:499:TYR:CD1	1:A:523:PRO:HB2	2.53	0.43
1:C:216:ASP:O	1:E:173:LYS:NZ	2.51	0.43
1:E:386:LYS:HE3	1:E:396:MET:SD	2.58	0.43
1:F:340:ALA:HB1	1:F:464:LEU:HB3	2.00	0.43
1:A:332:GLU:OE1	6:A:810:HOH:O	2.21	0.43
1:A:337:LYS:O	1:A:448:SER:HA	2.19	0.43
1:D:99:ILE:HD11	1:D:305:CYS:HA	2.00	0.43
1:C:579:VAL:O	1:C:589:LYS:HE3	2.18	0.43
1:F:167:VAL:O	1:F:167:VAL:CG1	2.65	0.43
1:F:327:ILE:HD13	1:F:355:ILE:HA	2.00	0.43
1:B:117:ILE:O	1:B:119:GLY:N	2.50	0.43
1:C:372:VAL:O	1:C:483:ASP:HA	2.19	0.43
1:E:416:LEU:HD13	1:E:416:LEU:HA	1.88	0.43
1:B:346:LYS:HB3	1:B:437:ASN:O	2.18	0.43
1:B:349:MET:CE	1:B:350:TYR:CZ	3.01	0.43
1:C:530:ILE:HB	1:C:533:TYR:CE2	2.53	0.43
1:D:379:ASP:O	1:D:396:MET:HG3	2.19	0.43
1:D:461:GLU:O	1:D:465:THR:HG23	2.18	0.43
1:E:124:GLU:O	1:E:125:GLU:HB3	2.19	0.43
1:E:467:ALA:O	1:E:471:VAL:HG23	2.19	0.43
1:F:355:ILE:HG22	1:F:357:LEU:HD12	2.00	0.43
1:A:495:LEU:HD11	1:A:527:LEU:CD2	2.32	0.43
1:B:374:LYS:HE2	1:B:376:ILE:HG13	2.01	0.43
1:D:503:PHE:CE2	1:D:527:LEU:HB2	2.53	0.43
1:F:463:ARG:HG2	1:F:463:ARG:HH11	1.84	0.43
1:A:165:PHE:HB3	1:A:189:TYR:OH	2.18	0.43
1:B:568:ASN:O	1:B:568:ASN:ND2	2.48	0.43
1:D:131:LEU:HD22	1:D:206:VAL:HG11	2.00	0.43
1:D:302:SER:CB	1:F:440:ARG:HE	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLU:HG2	1:E:296:GLN:OE1	2.19	0.43
1:E:365:VAL:HG13	1:E:365:VAL:O	2.17	0.43
1:F:108:HIS:CD2	6:F:801:HOH:O	2.72	0.43
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.01	0.43
1:B:129:ILE:HG13	1:B:213:MET:CE	2.49	0.43
1:B:225:VAL:HG13	1:B:270:TYR:CB	2.49	0.43
1:B:302:SER:OG	1:B:378:PHE:HB2	2.19	0.43
1:C:210:LEU:HA	1:C:213:MET:HE2	2.00	0.43
1:D:144:ILE:HD11	1:D:157:LEU:HB3	2.00	0.43
1:B:230:VAL:O	1:B:230:VAL:HG13	2.18	0.43
1:D:251:ARG:NH2	1:D:296:GLN:HA	2.34	0.43
1:D:431:GLU:HG2	1:D:433:MET:HE3	2.01	0.43
1:E:242:LEU:O	1:E:246:TYR:HB2	2.19	0.43
1:C:552:LYS:O	1:C:554:SER:N	2.52	0.42
1:F:142:VAL:HG11	1:F:165:PHE:HB2	2.01	0.42
1:B:171:THR:O	1:B:190:VAL:HA	2.19	0.42
1:B:174:HIS:HE1	1:B:213:MET:HG2	1.74	0.42
1:C:339:GLY:O	1:C:343:SER:OG	2.29	0.42
1:D:597:THR:HG22	1:D:601:LEU:HD22	2.01	0.42
1:E:136:GLY:O	1:E:138:GLU:N	2.53	0.42
1:B:217:ASN:HD22	1:F:173:LYS:NZ	2.17	0.42
1:E:509:LEU:HD12	1:E:509:LEU:O	2.19	0.42
1:A:123:VAL:HG12	1:A:185:VAL:HG11	2.00	0.42
1:B:99:ILE:HD12	1:B:305:CYS:HA	2.01	0.42
1:A:103:TYR:OH	6:A:809:HOH:O	2.21	0.42
1:A:368:LYS:HB2	1:A:478:VAL:HA	2.01	0.42
1:B:423:ILE:HD11	1:B:600:VAL:CG1	2.49	0.42
1:B:582:ASN:HB3	1:B:587:LYS:O	2.19	0.42
1:C:360:LYS:HE2	1:C:365:VAL:HG21	2.01	0.42
1:D:375:GLY:O	1:D:429:VAL:HA	2.18	0.42
1:A:103:TYR:CE2	1:A:320:LYS:HE3	2.55	0.42
1:A:524:VAL:HG21	1:A:595:LEU:HD21	2.01	0.42
1:D:230:VAL:HG12	1:D:234:LEU:CD2	2.48	0.42
1:E:153:VAL:HA	1:E:177:MET:CE	2.49	0.42
1:E:160:GLU:H	1:E:160:GLU:CD	2.22	0.42
1:E:200:GLU:O	1:E:204:LYS:HG3	2.19	0.42
1:F:340:ALA:HA	1:F:445:ILE:HD12	2.02	0.42
1:A:207:VAL:O	1:A:211:VAL:HG23	2.20	0.42
1:C:222:LEU:HD12	1:C:223:THR:N	2.34	0.42
1:D:303:ASN:CA	1:F:440:ARG:HH21	2.33	0.42
1:E:140:GLY:O	1:E:166:ASN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:HD12	1:A:288:TYR:OH	2.20	0.42
1:B:117:ILE:HD12	1:B:225:VAL:CG1	2.50	0.42
1:D:440:ARG:HD3	1:D:443:ASP:OD2	2.20	0.42
1:B:142:VAL:CG2	1:B:162:MET:HB3	2.50	0.42
1:B:440:ARG:HD2	1:C:302:SER:HB2	2.01	0.42
1:C:215:HIS:O	1:E:173:LYS:NZ	2.53	0.42
1:A:368:LYS:O	1:A:478:VAL:HB	2.20	0.41
1:A:497:THR:O	1:A:589:LYS:NZ	2.53	0.41
1:C:99:ILE:HD11	1:C:305:CYS:HA	2.02	0.41
1:C:486:THR:HG22	1:C:576:ILE:HG13	2.02	0.41
1:B:297:LEU:O	6:B:804:HOH:O	2.22	0.41
1:C:466:LEU:O	1:C:470:LEU:HG	2.19	0.41
1:E:148:VAL:N	6:E:813:HOH:O	2.41	0.41
1:E:226:PHE:CD1	1:E:271:ILE:HD12	2.56	0.41
1:E:376:ILE:HD11	1:E:465:THR:HG21	2.02	0.41
1:E:379:ASP:HB3	1:E:396:MET:HG3	2.02	0.41
1:F:323:LEU:HD12	1:F:358:THR:O	2.19	0.41
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.94	0.41
1:A:502:VAL:HB	1:A:524:VAL:CG1	2.51	0.41
1:B:235:PHE:O	1:B:238:PHE:HB3	2.21	0.41
1:A:230:VAL:O	1:A:277:TYR:OH	2.27	0.41
1:E:127:LEU:HB2	1:E:219:LEU:HD22	2.02	0.41
1:B:178:PHE:HA	1:B:183:ASN:O	2.20	0.41
1:B:431:GLU:O	6:B:807:HOH:O	2.22	0.41
1:B:445:ILE:HD11	1:B:453:ILE:HB	2.03	0.41
1:C:144:ILE:N	1:C:144:ILE:HD13	2.35	0.41
1:C:174:HIS:HB3	1:E:175:PHE:CD2	2.55	0.41
1:D:526:TRP:NE1	6:D:803:HOH:O	2.15	0.41
4:D:701:MPD:H52	4:D:701:MPD:HM1	2.03	0.41
1:E:320:LYS:NZ	6:E:817:HOH:O	2.48	0.41
1:F:287:TYR:HB3	1:F:594:ARG:HD3	2.02	0.41
1:A:440:ARG:HH11	1:B:433:MET:HE2	1.85	0.41
1:A:587:LYS:HB2	1:A:588:PRO:CD	2.51	0.41
1:B:177:MET:HE1	1:B:187:VAL:HG21	2.03	0.41
1:B:250:GLU:OE2	6:B:806:HOH:O	2.22	0.41
1:B:528:PRO:HB3	1:E:525:TRP:CH2	2.55	0.41
1:C:247:MET:HG3	1:C:288:TYR:OH	2.20	0.41
1:E:249:ASP:OD2	1:E:251:ARG:NH1	2.49	0.41
1:E:440:ARG:HG2	1:E:443:ASP:OD1	2.21	0.41
1:E:461:GLU:O	1:E:465:THR:HG23	2.21	0.41
1:F:112:VAL:HG23	1:F:267:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:VAL:CA	6:F:813:HOH:O	2.69	0.41
1:B:117:ILE:HG22	1:B:272:ASN:CA	2.49	0.41
1:B:369:ILE:HD13	1:B:369:ILE:N	2.34	0.41
1:D:306:ASN:OD1	1:D:309:SER:OG	2.31	0.41
1:D:487:LEU:HD23	1:D:573:HIS:CE1	2.55	0.41
1:F:142:VAL:CG1	1:F:165:PHE:HB2	2.51	0.41
1:A:192:CYS:HB3	1:A:198:LEU:HD11	2.03	0.40
1:B:237:PHE:HB2	1:B:521:ASN:HD22	1.86	0.40
1:B:484:ILE:HG23	1:B:484:ILE:O	2.21	0.40
1:C:174:HIS:NE2	1:C:213:MET:HG2	2.36	0.40
1:C:177:MET:HE2	1:C:187:VAL:CG2	2.51	0.40
1:C:250:GLU:HG2	1:C:253:LYS:HG3	2.03	0.40
1:C:322:ASN:OD1	6:C:807:HOH:O	2.22	0.40
1:C:565:PHE:O	6:C:808:HOH:O	2.22	0.40
1:E:153:VAL:HA	1:E:177:MET:HE3	2.04	0.40
1:A:493:TYR:N	1:A:493:TYR:CD2	2.88	0.40
1:C:317:LEU:HD12	1:C:321:LEU:HD22	2.03	0.40
1:D:423:ILE:HD13	1:D:600:VAL:HG21	2.03	0.40
1:D:436:LYS:HE3	6:E:815:HOH:O	2.22	0.40
1:E:210:LEU:HD12	1:E:210:LEU:HA	1.86	0.40
1:F:121:CYS:O	1:F:149:ASN:N	2.50	0.40
1:A:134:ASN:ND2	1:A:141:PRO:HD2	2.37	0.40
1:B:128:THR:HB	1:B:223:THR:HB	2.04	0.40
1:B:341:TYR:CZ	1:B:428:ALA:HB1	2.56	0.40
1:C:115:TYR:HB2	1:C:270:TYR:CE1	2.57	0.40
1:C:216:ASP:HB2	1:E:173:LYS:HZ1	1.83	0.40
1:C:491:MET:HE2	1:C:491:MET:HB3	1.89	0.40
1:D:374:LYS:HE3	1:D:462:GLY:HA3	2.03	0.40
1:F:503:PHE:O	1:F:573:HIS:N	2.50	0.40
1:C:115:TYR:HB2	1:C:270:TYR:CD1	2.56	0.40
1:C:133:ASN:HB3	1:C:228:ILE:HG22	2.03	0.40
1:C:454:GLU:OE2	6:C:806:HOH:O	2.22	0.40
1:D:303:ASN:OD1	1:D:303:ASN:N	2.54	0.40
1:E:99:ILE:CG2	1:E:101:ILE:HD11	2.51	0.40
1:F:239:LEU:HD23	1:F:239:LEU:HA	1.83	0.40
1:A:412:CYS:O	1:A:416:LEU:HD22	2.21	0.40
1:A:506:ASN:OD1	1:A:508:GLU:OE1	2.40	0.40
1:B:130:PHE:CD1	1:B:225:VAL:HB	2.57	0.40
1:C:127:LEU:HD21	1:C:129:ILE:HD11	2.03	0.40
1:F:248:THR:HG23	1:F:263:TYR:OH	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LYS:NZ	1:E:364:ASP:OD2[3_555]	2.07	0.13
1:C:181:ASN:O	1:F:326:LYS:NZ[1_455]	2.18	0.02

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	517/527 (98%)	494 (96%)	23 (4%)	0	100	100
1	B	516/527 (98%)	484 (94%)	29 (6%)	3 (1%)	25	31
1	C	516/527 (98%)	498 (96%)	17 (3%)	1 (0%)	47	58
1	D	513/527 (97%)	492 (96%)	21 (4%)	0	100	100
1	E	507/527 (96%)	486 (96%)	20 (4%)	1 (0%)	47	58
1	F	503/527 (95%)	480 (95%)	21 (4%)	2 (0%)	34	42
All	All	3072/3162 (97%)	2934 (96%)	131 (4%)	7 (0%)	47	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	357	LEU
1	E	137	LYS
1	F	477	GLY
1	B	119	GLY
1	B	553	ALA
1	C	553	ALA
1	B	118	LYS

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	412/454 (91%)	401 (97%)	11 (3%)	44	61
1	B	392/454 (86%)	378 (96%)	14 (4%)	35	49
1	C	411/454 (90%)	388 (94%)	23 (6%)	21	29
1	D	395/454 (87%)	375 (95%)	20 (5%)	24	33
1	E	405/454 (89%)	389 (96%)	16 (4%)	31	44
1	F	369/454 (81%)	353 (96%)	16 (4%)	29	40
All	All	2384/2724 (88%)	2284 (96%)	100 (4%)	30	42

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	113	GLN
1	A	145	SER
1	A	209	SER
1	A	288	TYR
1	A	398	PHE
1	A	399	ASP
1	A	400	MET
1	A	439	TYR
1	A	440	ARG
1	A	474	GLU
1	B	86	SER
1	B	159	ASP
1	B	209	SER
1	B	219	LEU
1	B	254	SER
1	B	288	TYR
1	B	295	SER
1	B	361	SER
1	B	398	PHE
1	B	417	LYS
1	B	439	TYR
1	B	498	SER
1	B	568	ASN
1	B	603	ASP
1	C	86	SER

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Mol	Chain	Res	Type
1	C	102	GLU
1	C	121	CYS
1	C	177	MET
1	C	194	SER
1	C	199	SER
1	C	203	MET
1	C	209	SER
1	C	216	ASP
1	C	220	SER
1	C	251	ARG
1	C	288	TYR
1	C	295	SER
1	C	321	LEU
1	C	398	PHE
1	C	400	MET
1	C	439	TYR
1	C	445	ILE
1	C	461	GLU
1	C	478	VAL
1	C	483	ASP
1	C	534	ARG
1	C	603	ASP
1	D	132	VAL
1	D	154	SER
1	D	216	ASP
1	D	248	THR
1	D	254	SER
1	D	256	ASP
1	D	288	TYR
1	D	337	LYS
1	D	398	PHE
1	D	435	SER
1	D	438	SER
1	D	439	TYR
1	D	440	ARG
1	D	445	ILE
1	D	494	SER
1	D	510	ILE
1	D	513	ILE
1	D	518	LYS
1	D	534	ARG
1	D	573	HIS

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Mol	Chain	Res	Type
1	E	86	SER
1	E	149	ASN
1	E	164	LYS
1	E	219	LEU
1	E	220	SER
1	E	247	MET
1	E	254	SER
1	E	288	TYR
1	E	336	LEU
1	E	396	MET
1	E	400	MET
1	E	439	TYR
1	E	483	ASP
1	E	511	ASN
1	E	538	ASN
1	E	587	LYS
1	F	145	SER
1	F	156	PHE
1	F	172	SER
1	F	174	HIS
1	F	180	ASP
1	F	219	LEU
1	F	248	THR
1	F	253	LYS
1	F	283	LYS
1	F	398	PHE
1	F	400	MET
1	F	401	SER
1	F	429	VAL
1	F	439	TYR
1	F	463	ARG
1	F	483	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	568	ASN
1	B	174	HIS
1	B	217	ASN
1	C	215	HIS
1	E	166	ASN
1	E	420	ASN

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Mol	Chain	Res	Type
1	E	538	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 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	CO3	B	701	-	2,3,3	0.40	0	2,3,3	0.24	0
2	CO3	F	701	1	2,3,3	0.31	0	2,3,3	1.51	0
5	SO4	E	704	-	4,4,4	0.16	0	6,6,6	0.14	0
2	CO3	C	702	-	2,3,3	0.48	0	2,3,3	0.61	0
4	MPD	C	701	-	7,7,7	0.26	0	9,10,10	0.58	0
2	CO3	D	702	1	2,3,3	0.36	0	2,3,3	0.50	0
4	MPD	D	701	-	7,7,7	0.23	0	9,10,10	0.40	0
2	CO3	A	701	-	2,3,3	0.39	0	2,3,3	0.27	0
2	CO3	E	701	-	2,3,3	0.38	0	2,3,3	0.12	0
5	SO4	C	705	-	4,4,4	0.16	0	6,6,6	0.12	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
4	MPD	C	701	-	-	0/5/5/5	-
4	MPD	D	701	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	701	MPD	C2-C3-C4-O4
4	D	701	MPD	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	CO3	2	0
2	F	701	CO3	5	0
5	E	704	SO4	1	0
2	C	702	CO3	2	0
4	D	701	MPD	5	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, 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	519/527 (98%)	0.21	6 (1%) 79 83	41, 52, 74, 92	0
1	B	518/527 (98%)	0.24	19 (3%) 41 48	41, 56, 87, 97	0
1	C	518/527 (98%)	0.20	11 (2%) 63 70	40, 50, 78, 90	0
1	D	517/527 (98%)	0.13	10 (1%) 66 73	41, 53, 76, 89	0
1	E	511/527 (96%)	0.15	9 (1%) 68 74	40, 54, 73, 86	0
1	F	509/527 (96%)	0.27	13 (2%) 56 63	43, 57, 87, 98	0
All	All	3092/3162 (97%)	0.20	68 (2%) 62 69	40, 54, 81, 98	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	140	GLY	4.4
1	F	144	ILE	4.3
1	F	128	THR	4.2
1	C	141	PRO	4.1
1	B	230	VAL	3.9
1	B	226	PHE	3.9
1	F	153	VAL	3.8
1	F	121	CYS	3.6
1	F	175	PHE	3.6
1	D	145	SER	3.5
1	F	177	MET	3.4
1	D	126	GLY	3.4
1	C	142	VAL	3.3
1	C	120	GLY	3.3
1	D	228	ILE	3.3
1	B	603	ASP	3.2
1	B	176	TYR	3.1
1	C	121	CYS	3.1
1	D	195	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	209	SER	3.1
1	D	603	ASP	2.9
1	B	194	SER	2.9
1	A	165	PHE	2.8
1	B	195	VAL	2.8
1	B	142	VAL	2.7
1	B	104	ASN	2.7
1	D	132	VAL	2.7
1	C	270	TYR	2.7
1	B	198	LEU	2.6
1	F	156	PHE	2.6
1	C	271	ILE	2.6
1	A	141	PRO	2.6
1	E	269	VAL	2.6
1	B	162	MET	2.5
1	B	196	ALA	2.5
1	A	603	ASP	2.5
1	C	135	PRO	2.5
1	B	144	ILE	2.5
1	E	161	ASN	2.5
1	E	271	ILE	2.4
1	F	162	MET	2.4
1	E	276	THR	2.4
1	C	145	SER	2.4
1	E	117	ILE	2.4
1	B	165	PHE	2.4
1	F	235	PHE	2.4
1	E	141	PRO	2.3
1	E	270	TYR	2.3
1	A	144	ILE	2.3
1	B	228	ILE	2.3
1	B	177	MET	2.2
1	F	159	ASP	2.2
1	C	148	VAL	2.2
1	F	224	VAL	2.2
1	A	161	ASN	2.2
1	F	323	LEU	2.2
1	A	136	GLY	2.2
1	C	134	ASN	2.1
1	D	85	ALA	2.1
1	B	275	ASP	2.1
1	B	175	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	132	VAL	2.1
1	D	196	ALA	2.1
1	D	222	LEU	2.1
1	B	421	VAL	2.1
1	E	219	LEU	2.1
1	D	229	ASN	2.0
1	C	196	ALA	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(Å ²)	Q<0.9
2	CO3	F	701	4/4	0.61	0.25	49,53,55,62	0
2	CO3	D	702	4/4	0.69	0.19	52,54,62,62	0
3	ZN	B	702	1/1	0.70	0.13	51,51,51,51	0
3	ZN	B	703	1/1	0.73	0.13	52,52,52,52	0
3	ZN	D	704	1/1	0.80	0.12	52,52,52,52	0
2	CO3	C	702	4/4	0.91	0.21	49,50,52,57	0
4	MPD	D	701	8/8	0.91	0.27	51,70,86,90	0
2	CO3	A	701	4/4	0.92	0.19	44,46,48,55	0
3	ZN	F	703	1/1	0.92	0.15	54,54,54,54	0
3	ZN	C	704	1/1	0.92	0.12	50,50,50,50	0
3	ZN	A	702	1/1	0.93	0.13	48,48,48,48	1
3	ZN	E	703	1/1	0.93	0.12	47,47,47,47	0
3	ZN	F	702	1/1	0.93	0.13	55,55,55,55	0
2	CO3	B	701	4/4	0.93	0.15	52,52,53,62	0
3	ZN	D	703	1/1	0.93	0.15	49,49,49,49	0
4	MPD	C	701	8/8	0.94	0.13	51,63,69,69	0

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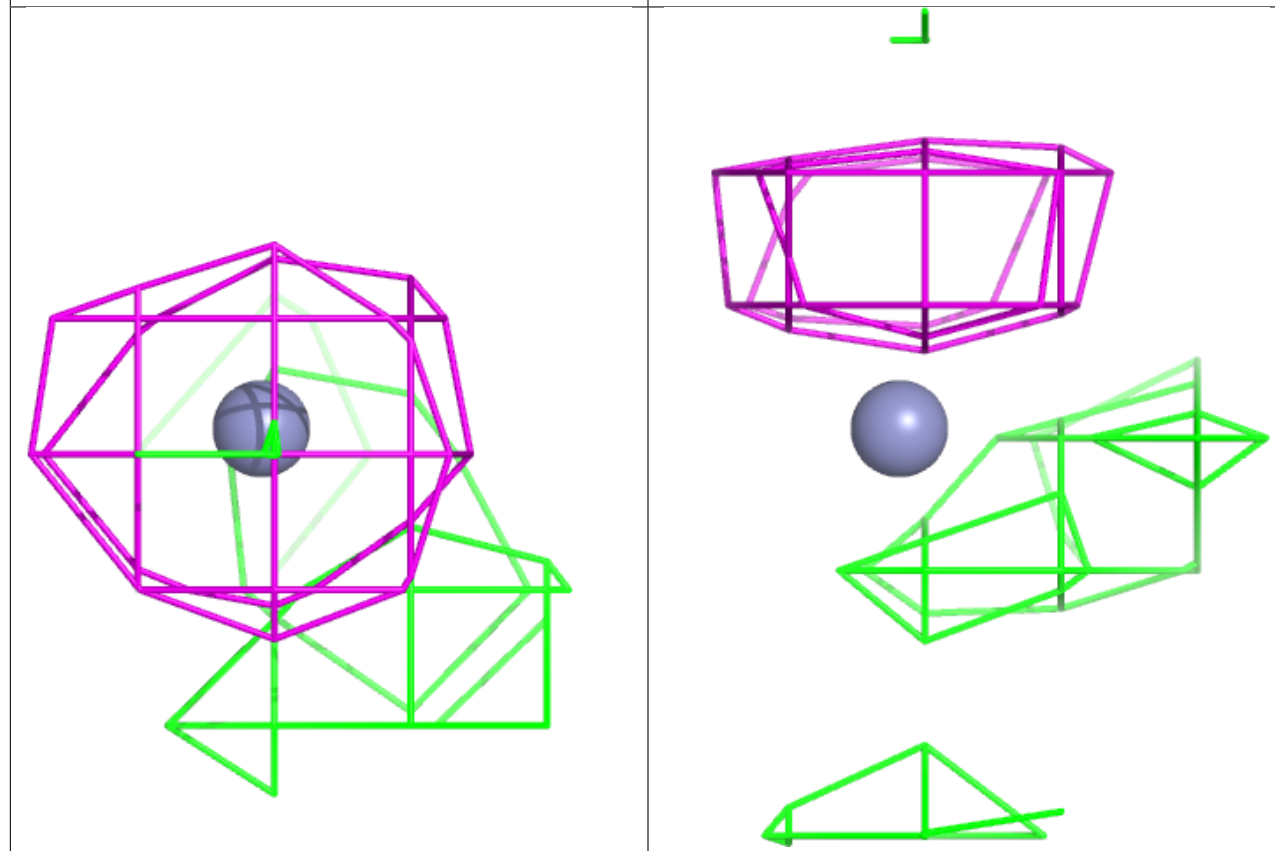
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	C	703	1/1	0.95	0.13	49,49,49,49	0
3	ZN	E	702	1/1	0.96	0.14	50,50,50,50	0
3	ZN	A	703	1/1	0.96	0.12	50,50,50,50	0
2	CO3	E	701	4/4	0.97	0.13	49,52,56,63	0
5	SO4	C	705	5/5	0.97	0.13	42,46,50,57	0
5	SO4	E	704	5/5	0.98	0.12	46,47,51,53	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.

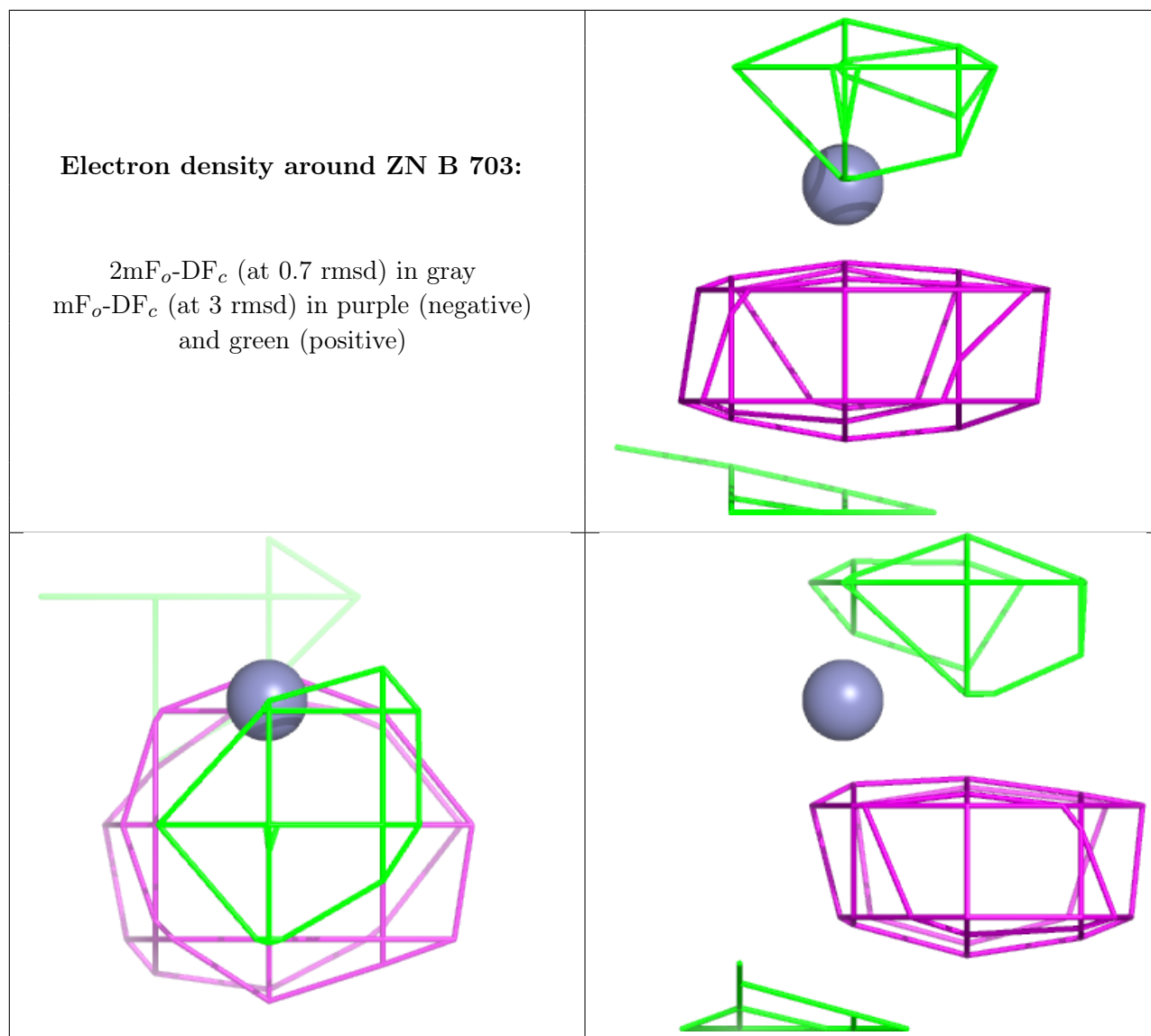
Electron density around ZN B 702:

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



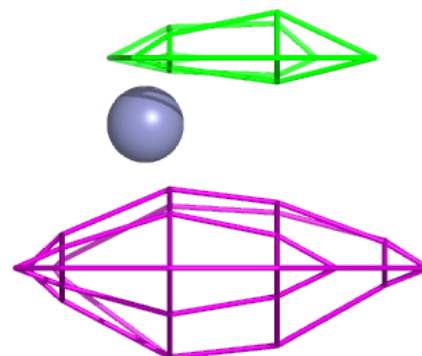
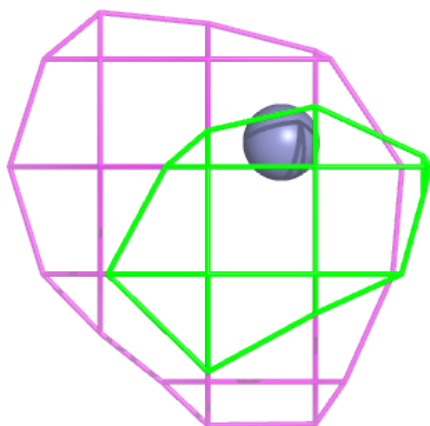
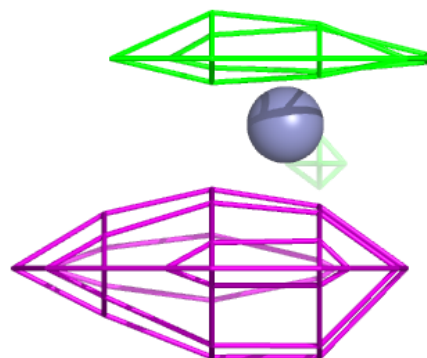
Electron density around ZN B 703:

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



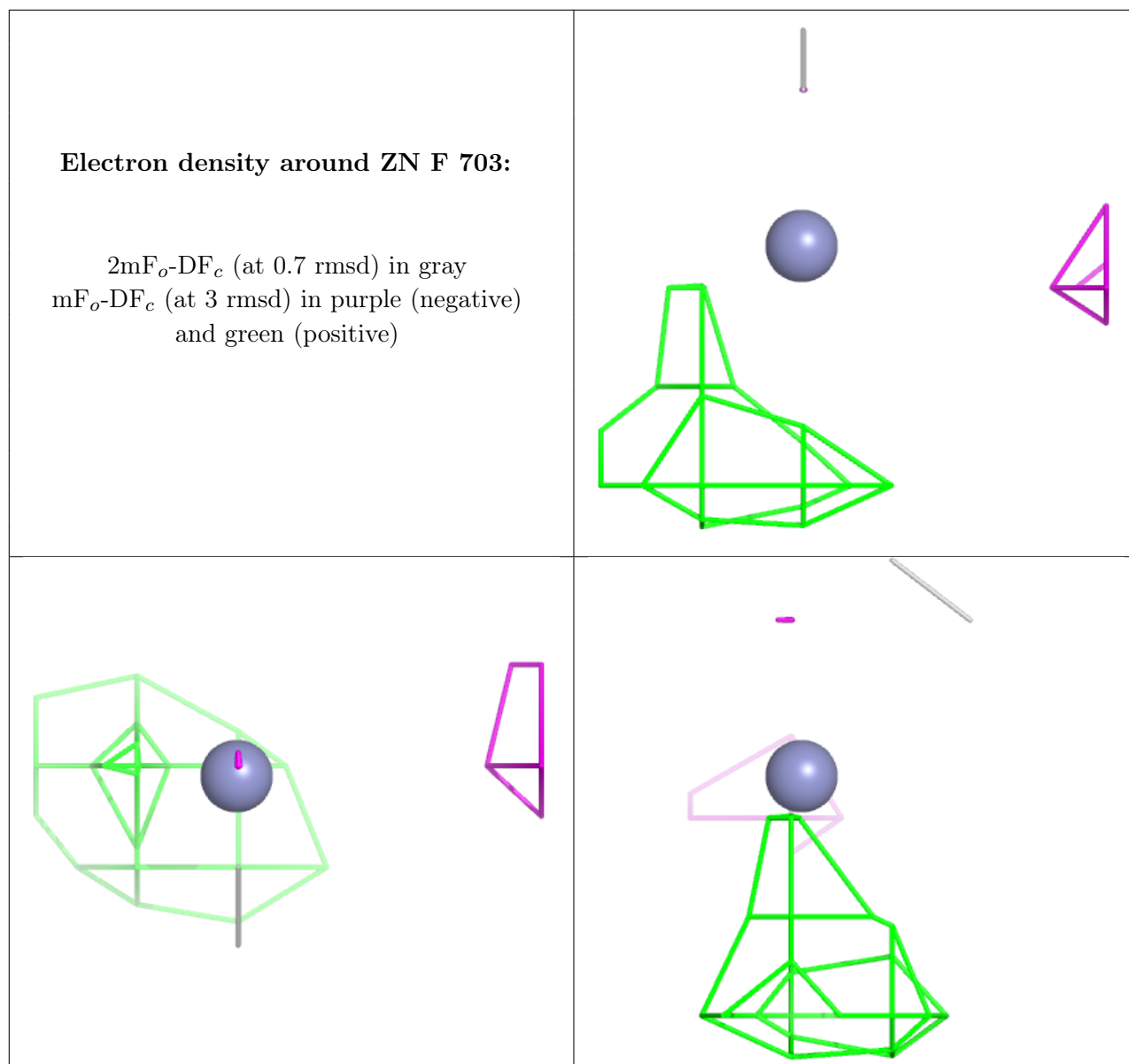
Electron density around ZN D 704:

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



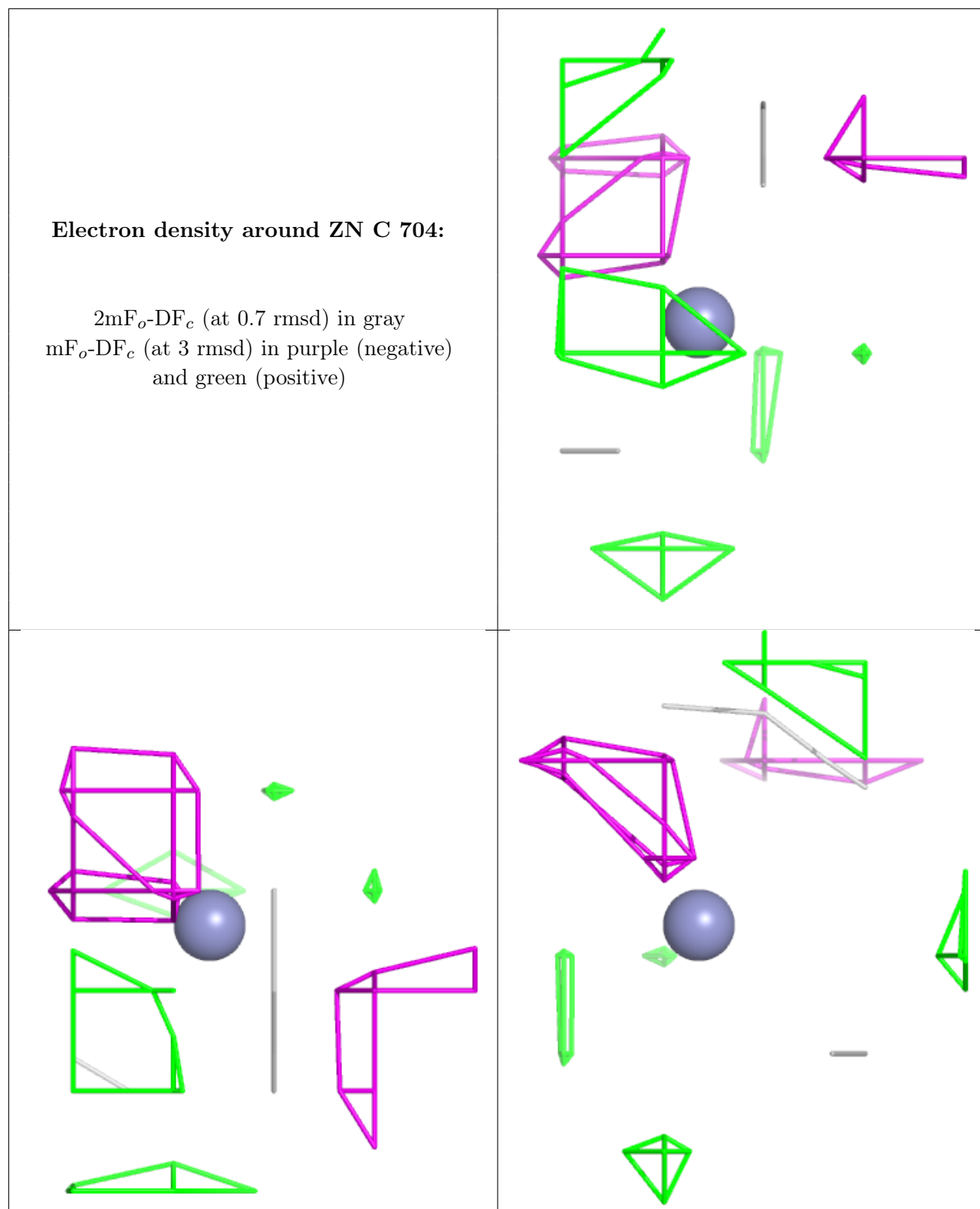
Electron density around ZN F 703:

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



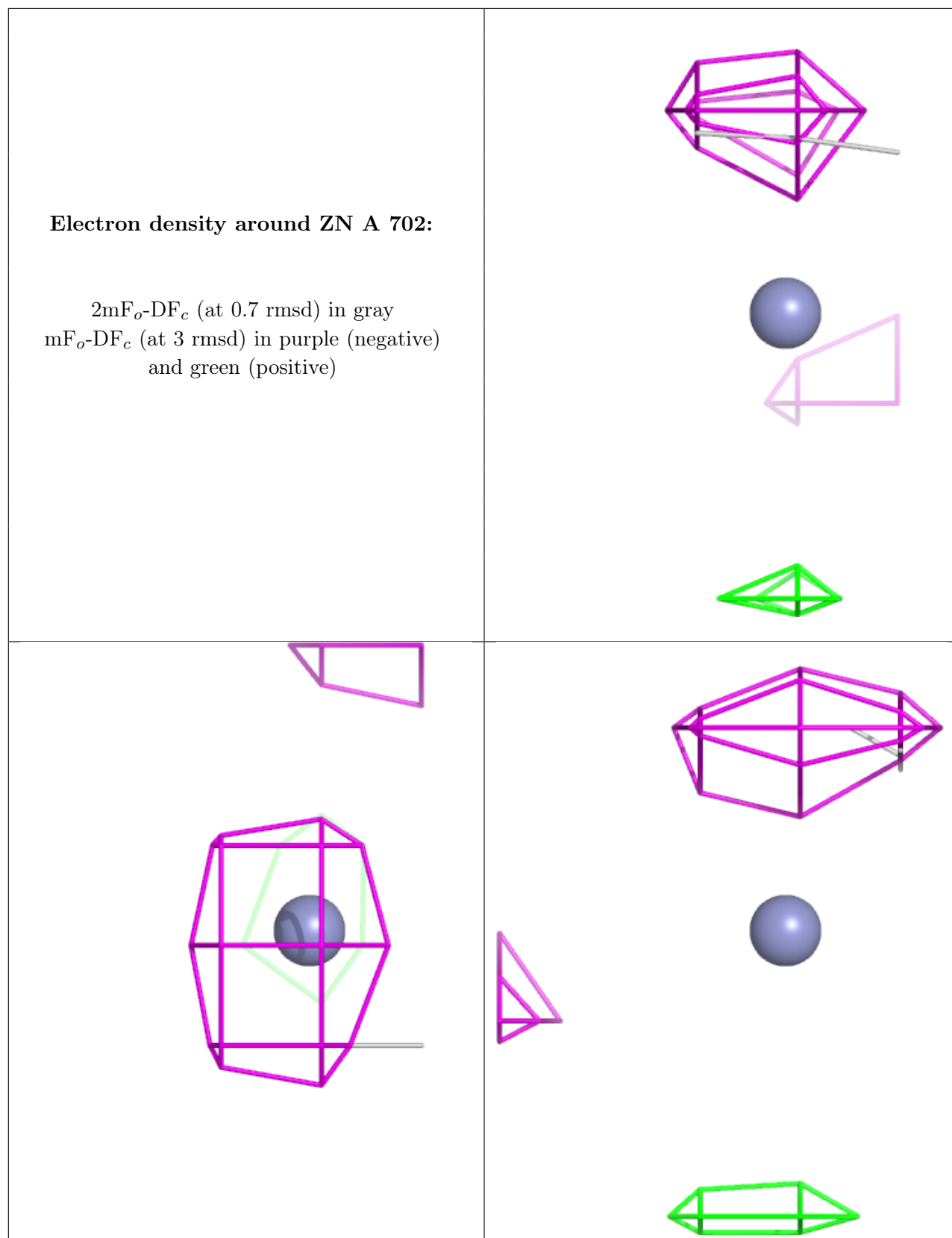
Electron density around ZN C 704:

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and green (positive)



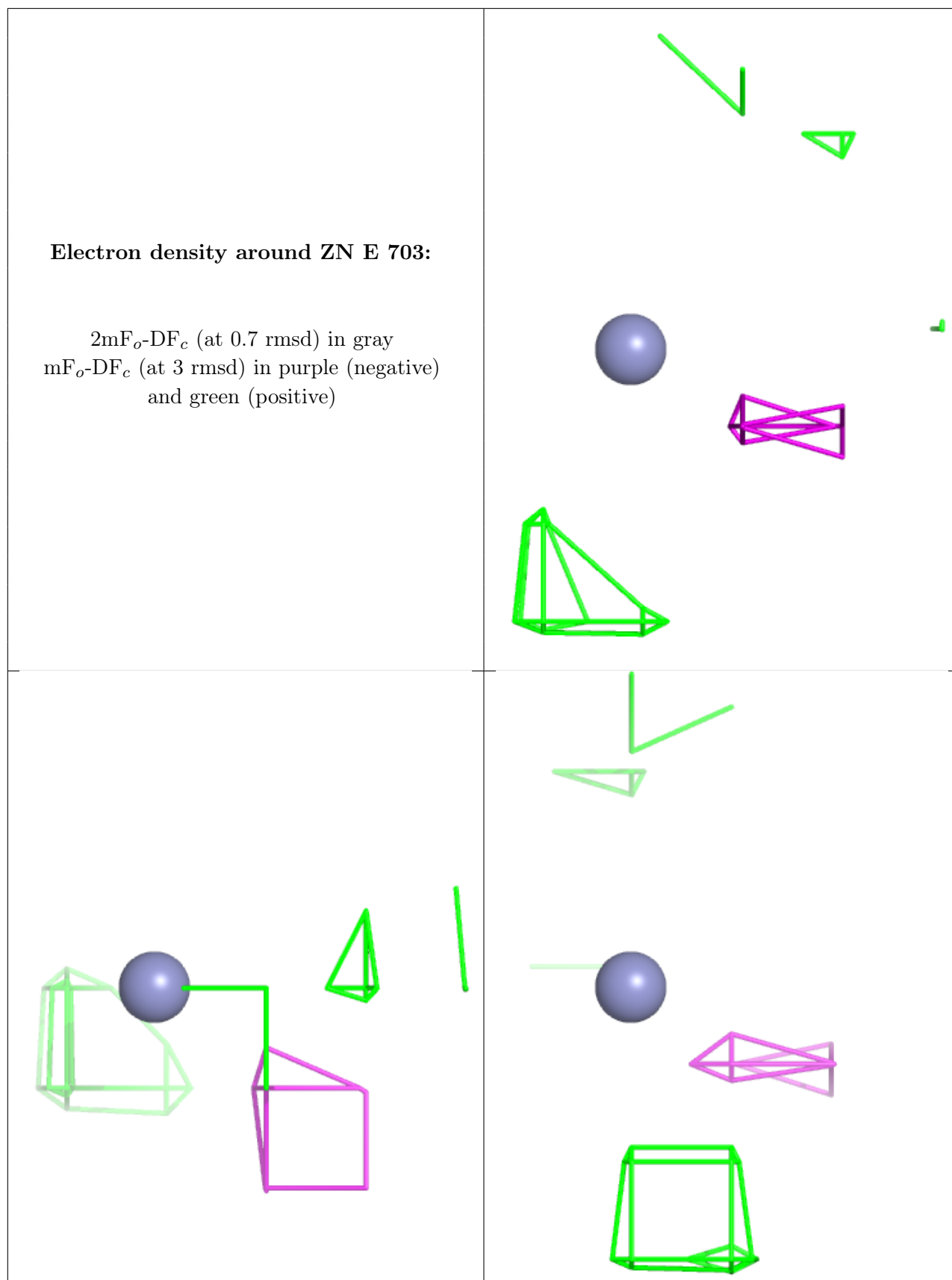
Electron density around ZN A 702:

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and green (positive)



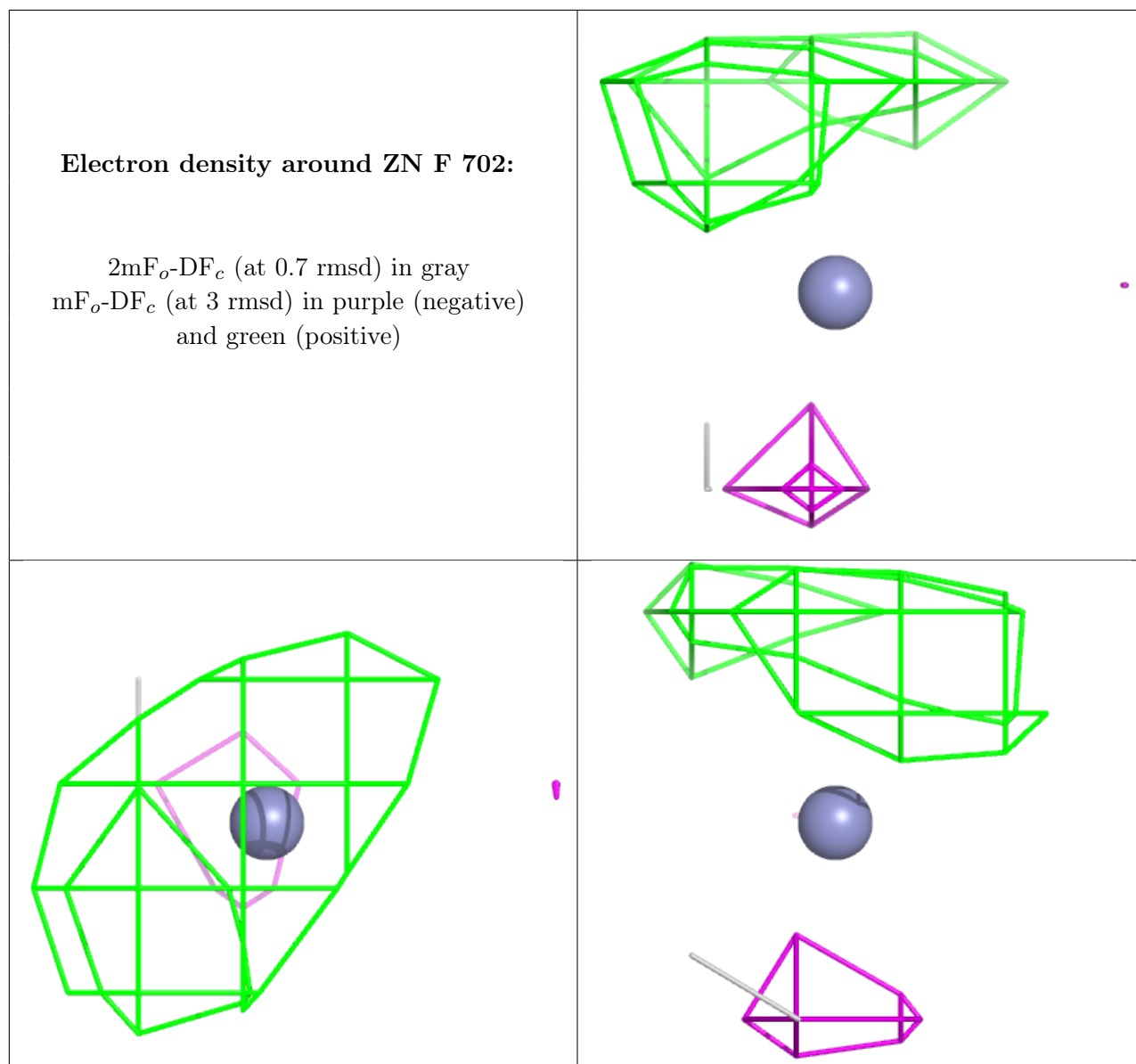
Electron density around ZN E 703:

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and green (positive)



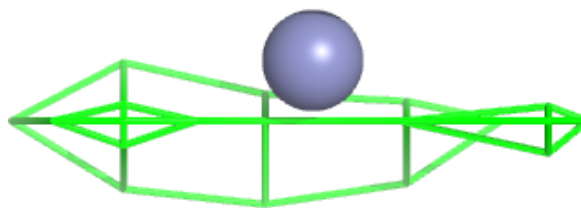
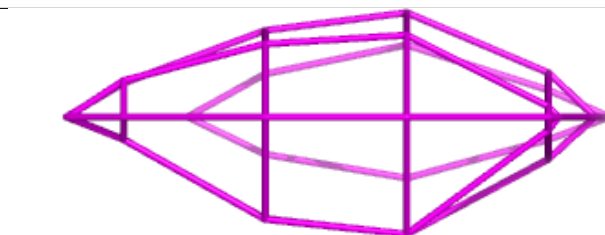
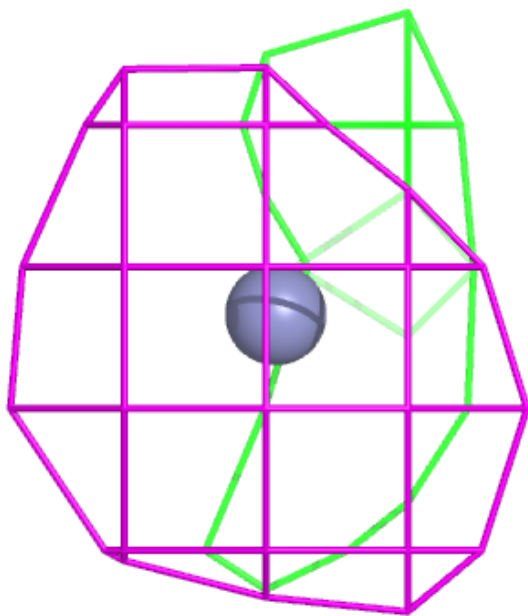
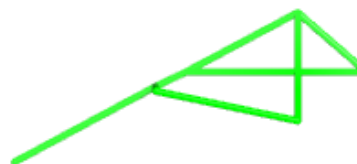
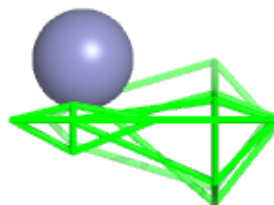
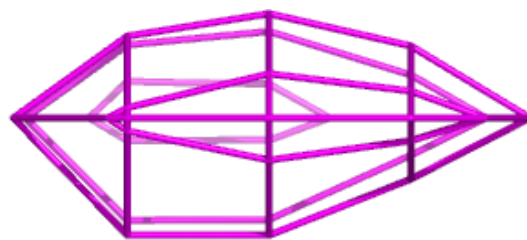
Electron density around ZN F 702:

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



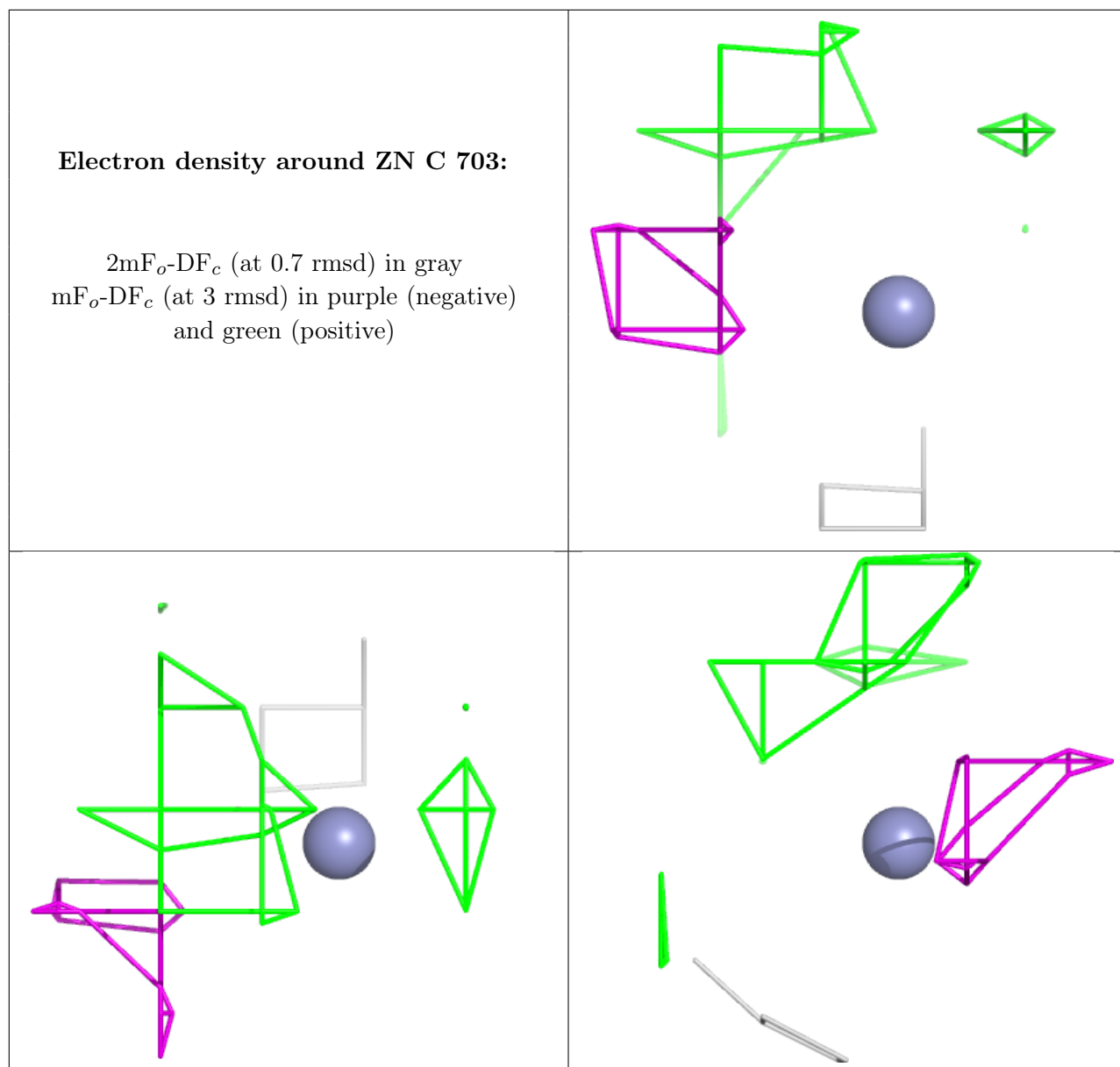
Electron density around ZN D 703:

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



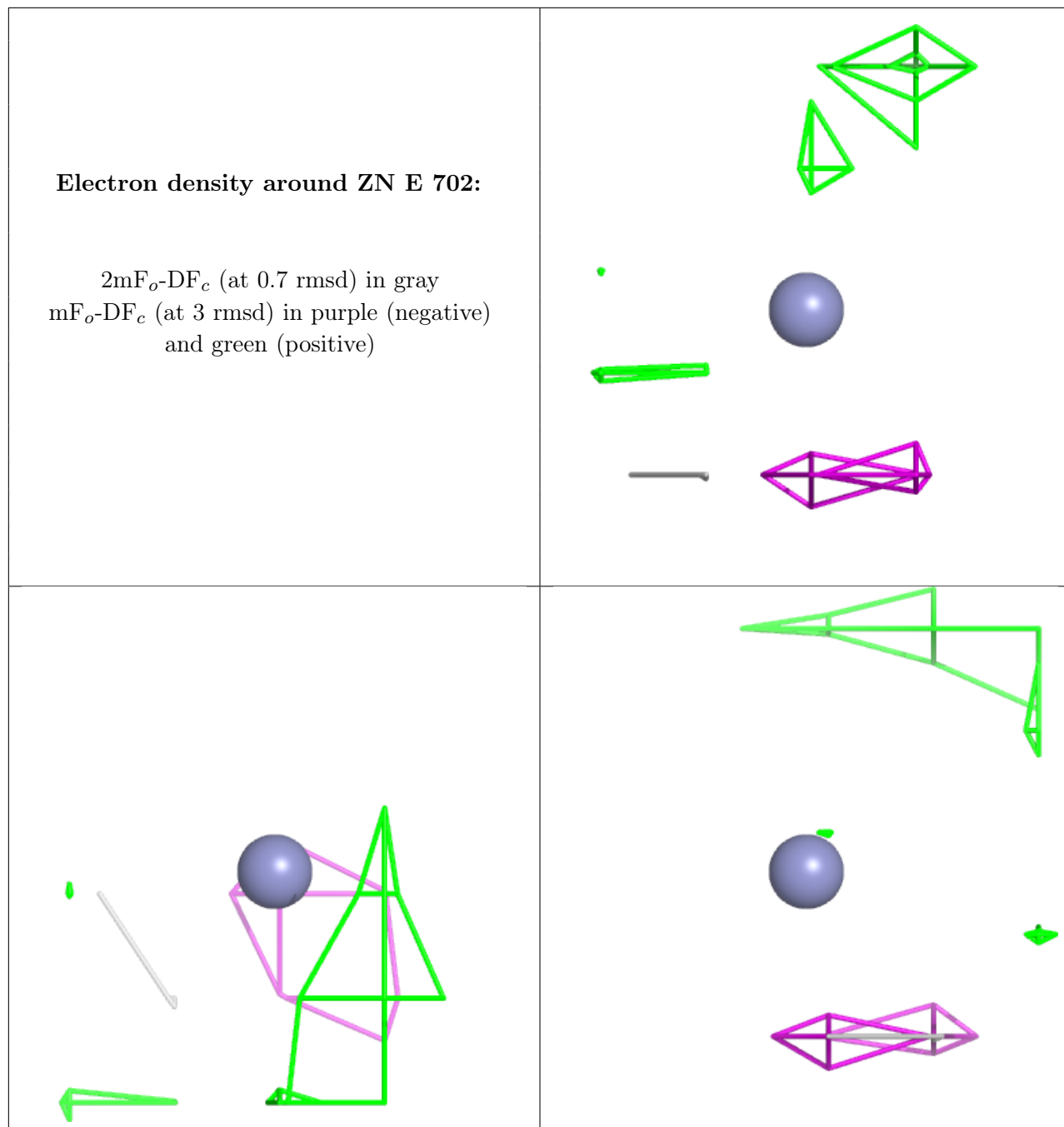
Electron density around ZN C 703:

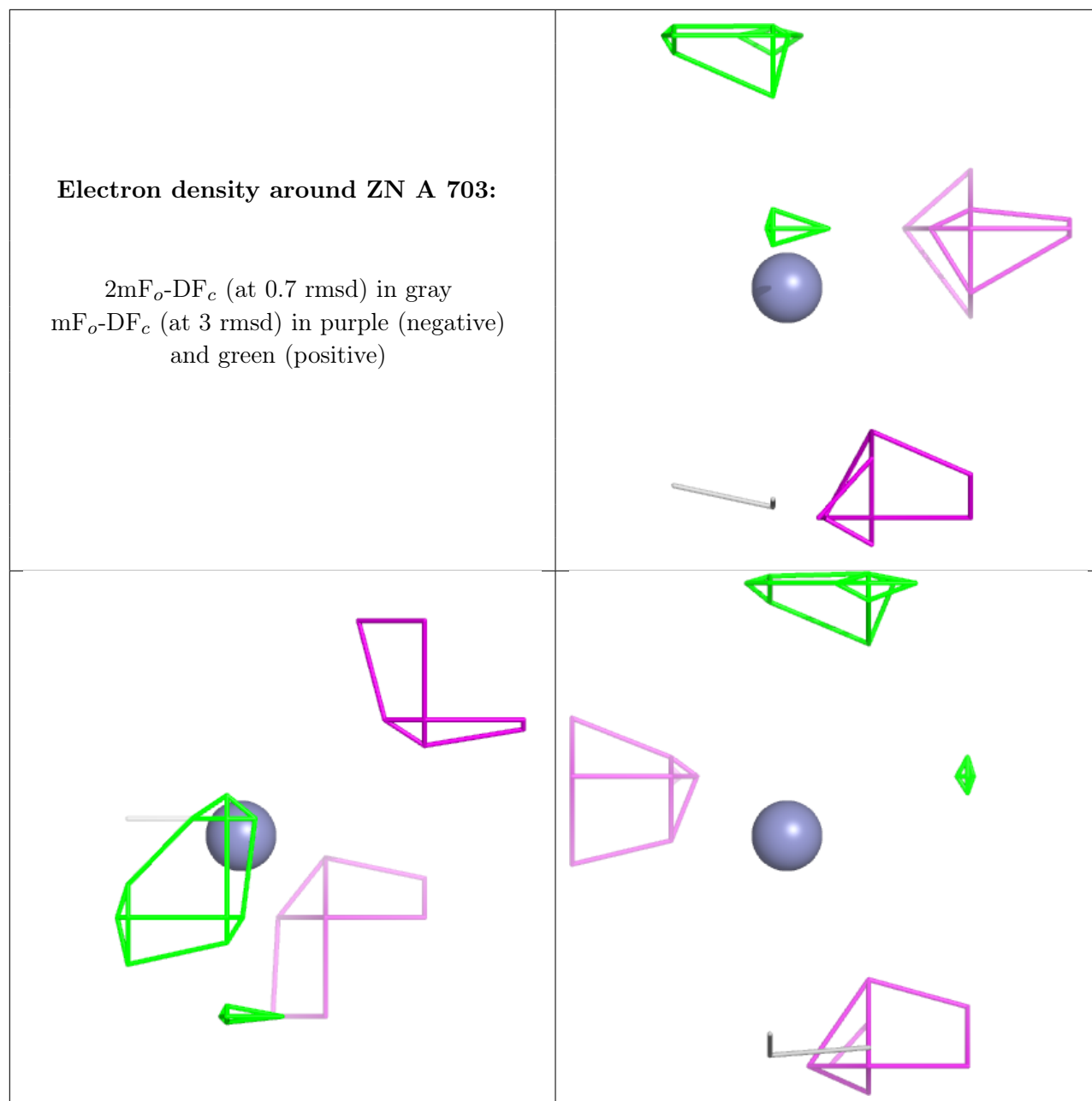
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN E 702:

$2mF_o-DF_c$ (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.