



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:21 AM UTC

PDB ID : 8XHU / pdb_00008xhu
Title : Crystal structure of Helicobacter pylori IspDF
Authors : Chen, X.; Wu, D.
Deposited on : 2023-12-18
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

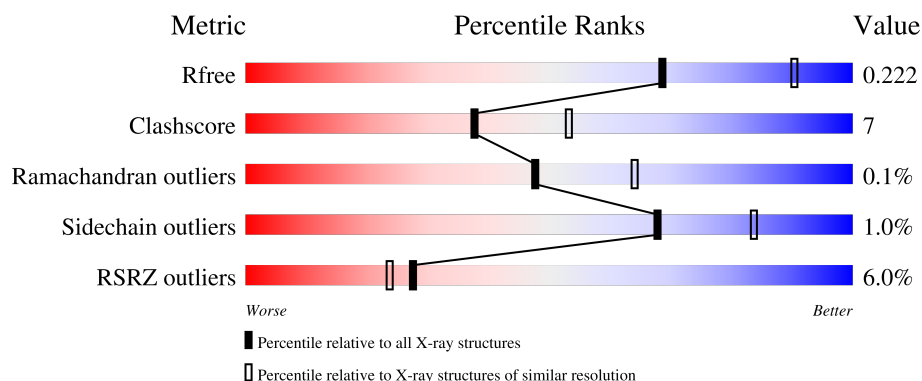
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	381	
1	B	381	
1	C	381	

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
3	EDO	A	505	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8836 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

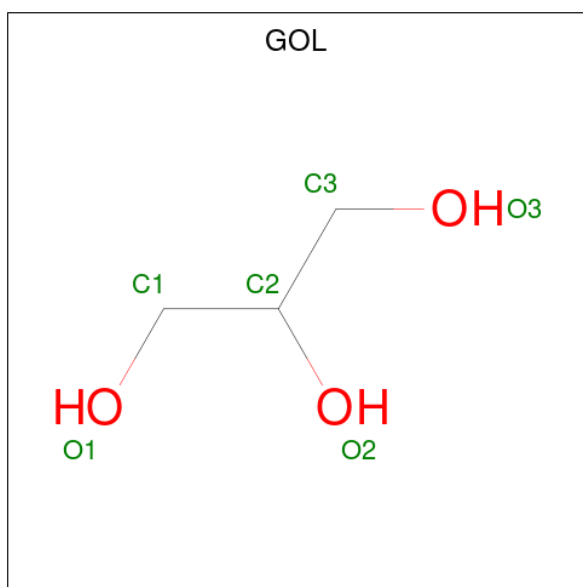
- Molecule 1 is a protein called Bifunctional enzyme IspD/IspF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2796	1808	460	519	9			
1	B	351	Total	C	N	O	S	0	0	0
			2774	1794	455	516	9			
1	C	353	Total	C	N	O	S	0	0	0
			2785	1800	458	518	9			

There are 21 discrepancies between the modelled and reference sequences:

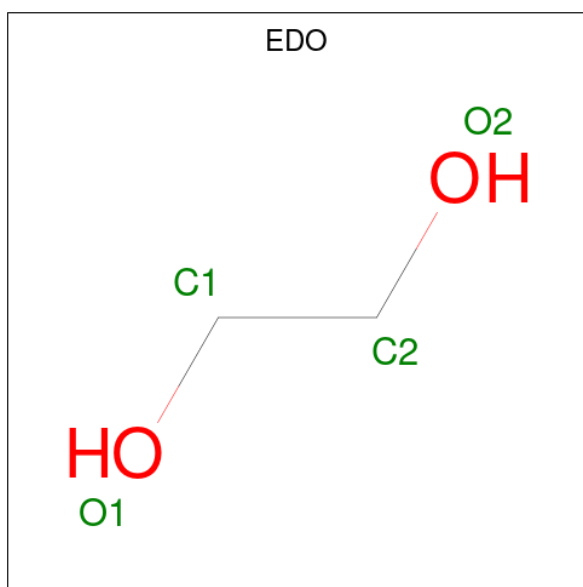
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP O25664
A	27	HIS	-	expression tag	UNP O25664
A	28	HIS	-	expression tag	UNP O25664
A	29	HIS	-	expression tag	UNP O25664
A	30	HIS	-	expression tag	UNP O25664
A	31	HIS	-	expression tag	UNP O25664
A	32	HIS	-	expression tag	UNP O25664
B	26	MET	-	initiating methionine	UNP O25664
B	27	HIS	-	expression tag	UNP O25664
B	28	HIS	-	expression tag	UNP O25664
B	29	HIS	-	expression tag	UNP O25664
B	30	HIS	-	expression tag	UNP O25664
B	31	HIS	-	expression tag	UNP O25664
B	32	HIS	-	expression tag	UNP O25664
C	26	MET	-	initiating methionine	UNP O25664
C	27	HIS	-	expression tag	UNP O25664
C	28	HIS	-	expression tag	UNP O25664
C	29	HIS	-	expression tag	UNP O25664
C	30	HIS	-	expression tag	UNP O25664
C	31	HIS	-	expression tag	UNP O25664
C	32	HIS	-	expression tag	UNP O25664

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



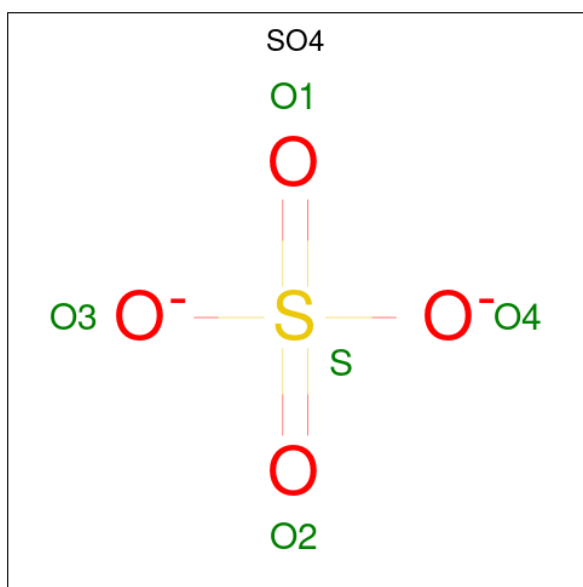
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	165	Total	O	0	0
			165	165		
7	B	100	Total	O	0	0
			100	100		

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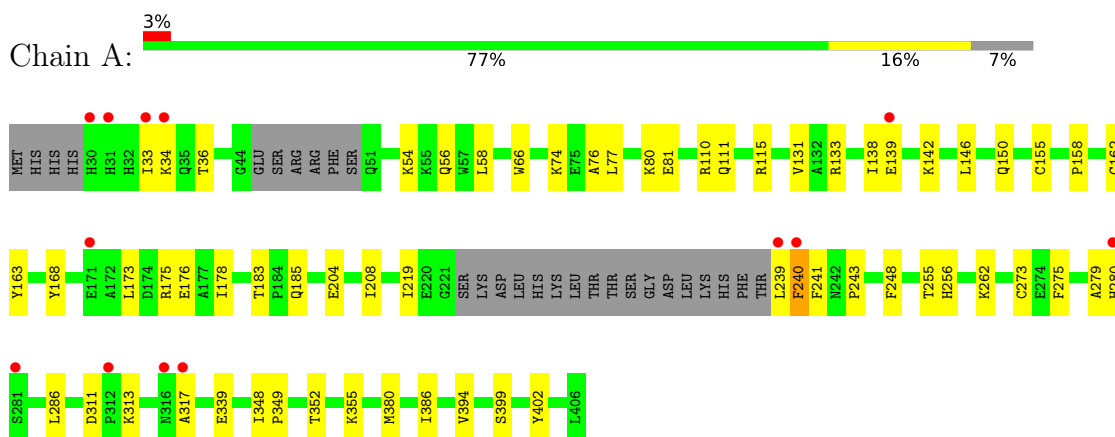
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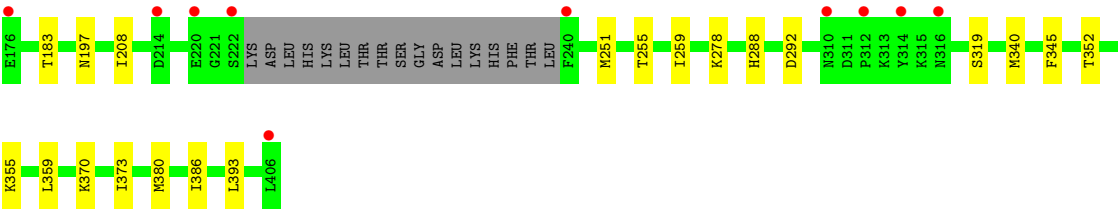
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	133	Total 133	O 133	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Bifunctional enzyme IspD/IspF





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.27Å 145.27Å 138.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.90 – 2.40 35.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (35.90-2.40) 97.5 (35.90-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.198 , 0.223 0.202 , 0.222	Depositor DCC
R_{free} test set	3146 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8836	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, CL, SO4, EDO

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	0.42	1/2854 (0.0%)	0.50	2/3853 (0.1%)
1	B	0.30	0/2831	0.51	3/3822 (0.1%)
1	C	0.25	0/2843	0.47	1/3838 (0.0%)
All	All	0.33	1/8528 (0.0%)	0.49	6/11513 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	ASP	C-O	-5.81	1.19	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	GLU	N-CA-C	6.19	118.94	107.99
1	B	59	ARG	N-CA-C	6.01	118.70	108.90
1	A	280	HIS	N-CA-C	-5.57	105.13	111.14
1	A	139	GLU	CB-CA-C	-5.40	102.40	110.88
1	B	198	GLN	N-CA-C	5.21	119.33	112.92
1	B	32	HIS	N-CA-C	-5.12	105.88	111.82

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	2796	0	2834	49	0
1	B	2774	0	2813	47	0
1	C	2785	0	2820	26	0
2	A	18	0	24	0	0
2	B	6	0	8	1	0
2	C	18	0	24	2	0
3	A	16	0	24	6	0
3	B	8	0	12	1	0
3	C	8	0	12	0	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	C	1	0	0	0	0
7	A	165	0	0	5	0
7	B	100	0	0	1	0
7	C	133	0	0	2	0
All	All	8836	0	8571	119	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 7.

All (119) 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:107:GLY:HA3	1:B:112:GLU:HG2	1.32	1.08
1:B:280:HIS:CE1	1:B:315:LYS:HB2	2.04	0.93
1:B:127:LEU:HD11	1:B:184:PRO:HB2	1.66	0.77
1:B:107:GLY:HA3	1:B:112:GLU:CG	2.15	0.75
1:A:163:TYR:H	3:A:505:EDO:H21	1.51	0.74
1:B:59:ARG:HG2	1:B:63:THR:C	2.12	0.73
1:C:88:GLU:OE1	1:C:105:LYS:HD3	1.89	0.72
1:B:59:ARG:HG2	1:B:64:PRO:N	2.05	0.71
1:A:339:GLU:HB3	1:A:399:SER:HB2	1.73	0.70
1:A:115:ARG:HH11	1:A:115:ARG:HB3	1.57	0.70
1:B:339:GLU:HB3	1:B:399:SER:HB2	1.74	0.68
1:A:162:CYS:HA	3:A:505:EDO:H22	1.78	0.65
1:B:153:HIS:CD2	1:B:215:ARG:HA	2.31	0.65
1:C:72:SER:HB3	1:C:135:LEU:HD23	1.79	0.65
1:A:34:LYS:O	1:A:80:LYS:HB2	1.97	0.64
1:A:163:TYR:H	3:A:505:EDO:C2	2.10	0.64
1:B:280:HIS:HE1	1:B:315:LYS:HB2	1.59	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:H	1:B:112:GLU:CD	2.07	0.62
1:B:144:LEU:HD23	1:B:219:ILE:HD11	1.81	0.62
1:A:115:ARG:HB3	1:A:115:ARG:NH1	2.15	0.62
1:A:175:ARG:HA	1:A:178:ILE:HD12	1.83	0.61
1:B:32:HIS:CD2	1:B:125:TYR:HE2	2.20	0.59
1:C:345:PHE:HD2	1:C:380:MET:HE3	1.68	0.59
1:B:133:ARG:HD2	1:B:183:THR:OG1	2.04	0.57
1:B:110:ARG:NH1	1:B:204:GLU:OE2	2.30	0.57
1:B:153:HIS:HD2	1:B:215:ARG:HA	1.69	0.57
1:A:33:ILE:HD13	1:A:77:LEU:HD13	1.87	0.56
1:B:154:TYR:CD2	1:B:215:ARG:HG3	2.40	0.56
1:C:380:MET:HG3	1:C:386:ILE:HB	1.87	0.56
1:A:111:GLN:O	1:A:115:ARG:HG3	2.05	0.56
1:C:116:ASN:HA	1:C:119:LYS:HD2	1.87	0.55
1:B:255:THR:HB	1:B:393:LEU:HD12	1.87	0.55
1:B:351:ILE:H	2:B:501:GOL:H31	1.72	0.55
1:C:155:CYS:HB2	1:C:208:ILE:HD12	1.89	0.55
1:C:340:MET:HE3	1:C:373:ILE:HG23	1.88	0.55
1:C:359:LEU:HG	1:C:370:LYS:HG2	1.89	0.55
1:A:76:ALA:HA	1:A:138:ILE:HD11	1.89	0.54
1:B:59:ARG:HG2	1:B:64:PRO:CA	2.38	0.54
1:B:153:HIS:ND1	1:B:217:SER:OG	2.36	0.54
1:A:110:ARG:NH1	1:A:204:GLU:OE2	2.39	0.54
1:A:241:PHE:CE1	1:A:243:PRO:HG3	2.42	0.53
1:A:115:ARG:HH11	1:A:115:ARG:CB	2.21	0.53
1:A:240:PHE:C	1:A:240:PHE:CD2	2.86	0.53
1:B:280:HIS:CE1	1:B:315:LYS:CB	2.87	0.53
1:A:183:THR:HG22	1:A:185:GLN:HG3	1.91	0.52
1:B:286:LEU:HA	1:B:394:VAL:HG11	1.90	0.52
1:C:165:THR:N	7:C:601:HOH:O	2.29	0.52
1:A:248:PHE:CE1	2:C:501:GOL:H31	2.45	0.51
1:A:133:ARG:HD2	1:A:183:THR:OG1	2.09	0.51
1:C:352:THR:HA	1:C:355:LYS:HD2	1.93	0.50
1:A:380:MET:HG3	1:A:386:ILE:HB	1.93	0.50
1:C:255:THR:HB	1:C:393:LEU:HD12	1.93	0.49
1:A:74:LYS:NZ	7:A:606:HOH:O	2.34	0.49
1:B:80:LYS:HD2	1:B:123:SER:HB3	1.95	0.49
1:B:154:TYR:HB2	1:B:215:ARG:HB3	1.95	0.49
1:B:59:ARG:CG	1:B:64:PRO:HA	2.42	0.48
1:B:183:THR:HG22	1:B:185:GLN:HG3	1.94	0.48
1:B:53:ILE:HG12	1:B:334:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASN:HB3	1:C:140:ALA:HB3	1.95	0.48
1:A:158:PRO:HA	1:A:219:ILE:O	2.14	0.48
1:A:352:THR:HA	1:A:355:LYS:HD2	1.94	0.48
1:A:163:TYR:CD2	3:A:505:EDO:H21	2.49	0.48
1:A:273:CYS:SG	1:A:349:PRO:HG3	2.54	0.47
1:A:110:ARG:HH12	1:A:204:GLU:CD	2.23	0.47
1:A:255:THR:HG21	1:C:380:MET:HA	1.97	0.47
1:A:168:TYR:HB3	1:A:173:LEU:HD21	1.97	0.47
1:B:188:HIS:HB3	1:B:191:ALA:HB3	1.96	0.47
1:B:125:TYR:CZ	1:B:148:LEU:HD21	2.50	0.46
1:A:275:PHE:CZ	1:A:348:ILE:HD12	2.51	0.46
1:A:286:LEU:HA	1:A:394:VAL:HG11	1.98	0.46
1:A:163:TYR:HD2	3:A:505:EDO:H21	1.80	0.45
1:C:35:GLN:O	1:C:123:SER:HB3	2.17	0.45
1:C:173:LEU:HD23	1:C:173:LEU:HA	1.63	0.45
1:B:154:TYR:HB2	1:B:215:ARG:CB	2.46	0.45
1:C:137:ASN:O	1:C:141:LEU:HG	2.17	0.45
1:A:36:THR:O	1:A:80:LYS:HB3	2.16	0.45
1:C:288:HIS:HE2	1:C:319:SER:HG	1.65	0.44
1:B:406:LEU:HD23	1:B:406:LEU:HA	1.86	0.44
1:A:176:GLU:OE2	7:A:601:HOH:O	2.21	0.44
1:C:259:ILE:HB	1:C:278:LYS:HB2	1.99	0.44
1:A:256:HIS:CE1	1:A:279:ALA:HB2	2.53	0.44
1:A:262:LYS:HE2	7:A:693:HOH:O	2.17	0.44
1:A:58:LEU:O	1:A:240:PHE:HE2	2.00	0.44
1:B:111:GLN:HG3	1:B:196:LEU:HD22	2.00	0.44
1:C:115:ARG:NH2	1:C:197:ASN:OD1	2.51	0.44
1:A:402:TYR:OH	2:C:501:GOL:H2	2.17	0.43
1:B:187:SER:HB2	7:B:618:HOH:O	2.18	0.43
1:B:251:MET:HE3	1:B:251:MET:HB3	1.77	0.43
1:A:163:TYR:N	3:A:505:EDO:H21	2.25	0.43
1:B:59:ARG:CG	1:B:64:PRO:CA	2.97	0.43
1:B:59:ARG:HG3	1:B:64:PRO:HA	2.00	0.43
1:A:317:ALA:CA	7:A:611:HOH:O	2.66	0.43
1:A:317:ALA:HA	7:A:611:HOH:O	2.18	0.43
1:B:355:LYS:O	1:B:359:LEU:HB2	2.18	0.43
1:C:370:LYS:HE2	1:C:370:LYS:HB2	1.80	0.43
1:A:80:LYS:HG3	1:A:81:GLU:HG2	2.00	0.43
1:B:136:ALA:HB1	1:B:141:LEU:HD11	2.01	0.43
1:B:313:LYS:HE2	1:B:313:LYS:HB3	1.75	0.43
1:A:146:LEU:O	1:A:150:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASP:HB3	7:C:601:HOH:O	2.18	0.42
1:A:56:GLN:HB2	1:A:66:TRP:HB3	2.00	0.42
1:A:380:MET:HA	1:B:255:THR:HG21	2.01	0.42
1:A:313:LYS:O	1:A:313:LYS:HG3	2.18	0.42
1:C:33:ILE:HG21	1:C:77:LEU:HB3	2.02	0.42
1:B:251:MET:HE1	1:C:251:MET:HE2	2.01	0.42
1:A:155:CYS:HB2	1:A:208:ILE:HD13	2.02	0.42
1:A:239:LEU:HD12	1:A:240:PHE:H	1.85	0.41
1:B:117:ALA:O	1:B:121:ILE:HG13	2.20	0.41
1:B:151:THR:HB	1:B:153:HIS:ND1	2.35	0.41
1:B:370:LYS:HE2	1:B:370:LYS:HB2	1.79	0.41
1:C:164:ASP:O	1:C:175:ARG:HD2	2.21	0.41
1:C:288:HIS:NE2	1:C:319:SER:OG	2.50	0.41
1:A:138:ILE:HG22	1:A:142:LYS:HE3	2.02	0.41
1:A:240:PHE:O	1:A:240:PHE:CG	2.70	0.41
1:A:33:ILE:HG21	1:A:77:LEU:HB3	2.03	0.40
1:B:62:HIS:HB2	3:B:502:EDO:H11	2.04	0.40
1:B:189:THR:O	1:B:193:GLN:HB2	2.22	0.40
1:B:259:ILE:O	1:B:276:GLY:N	2.50	0.40
1:C:77:LEU:HD12	1:C:79:PHE:CZ	2.57	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	348/381 (91%)	338 (97%)	10 (3%)	0	100	100
1	B	345/381 (91%)	338 (98%)	6 (2%)	1 (0%)	36	50
1	C	347/381 (91%)	339 (98%)	8 (2%)	0	100	100
All	All	1040/1143 (91%)	1015 (98%)	24 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	ASP

5.3.2 Protein sidechains ⓘ

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	303/329 (92%)	300 (99%)	3 (1%)	68	84
1	B	301/329 (92%)	298 (99%)	3 (1%)	68	84
1	C	302/329 (92%)	299 (99%)	3 (1%)	68	84
All	All	906/987 (92%)	897 (99%)	9 (1%)	68	84

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

Mol	Chain	Res	Type
1	A	54	LYS
1	A	131	VAL
1	A	240	PHE
1	B	74	LYS
1	B	220	GLU
1	B	315	LYS
1	C	80	LYS
1	C	183	THR
1	C	292	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	143	ASN
1	A	193	GLN
1	A	242	ASN
1	A	256	HIS
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	331	GLN
1	B	32	HIS
1	B	149	GLN
1	B	280	HIS
1	C	32	HIS
1	C	256	HIS
1	C	364	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z > 2$
3	EDO	A	504	-	3,3,3	0.71	0	2,2,2	0.67	0
2	GOL	C	502	-	5,5,5	0.48	0	5,5,5	0.30	0
3	EDO	B	502	-	3,3,3	0.41	0	2,2,2	0.41	0
3	EDO	A	505	-	3,3,3	0.59	0	2,2,2	0.32	0
3	EDO	A	506	-	3,3,3	0.62	0	2,2,2	0.67	0
2	GOL	C	501	-	5,5,5	0.53	0	5,5,5	0.31	0
3	EDO	B	503	-	3,3,3	0.42	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	504	-	3,3,3	0.44	0	2,2,2	0.54	0
2	GOL	A	502	-	5,5,5	0.53	0	5,5,5	0.34	0
2	GOL	C	503	-	5,5,5	0.54	0	5,5,5	0.35	0
3	EDO	C	505	-	3,3,3	0.41	0	2,2,2	0.48	0
2	GOL	A	503	-	5,5,5	0.53	0	5,5,5	0.39	0
3	EDO	A	507	-	3,3,3	0.63	0	2,2,2	0.89	0
2	GOL	B	501	-	5,5,5	0.53	0	5,5,5	0.32	0
2	GOL	A	501	-	5,5,5	0.56	0	5,5,5	0.34	0
4	SO4	A	508	-	4,4,4	0.26	0	6,6,6	0.09	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
3	EDO	A	504	-	-	1/1/1/1	-
2	GOL	C	502	-	-	3/4/4/4	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
2	GOL	C	501	-	-	2/4/4/4	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
2	GOL	A	502	-	-	4/4/4/4	-
2	GOL	C	503	-	-	0/4/4/4	-
3	EDO	C	505	-	-	1/1/1/1	-
2	GOL	A	503	-	-	0/4/4/4	-
3	EDO	A	507	-	-	0/1/1/1	-
2	GOL	B	501	-	-	3/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	A	502	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	502	GOL	C1-C2-C3-O3
2	C	502	GOL	C1-C2-C3-O3
2	B	501	GOL	O1-C1-C2-C3
2	C	501	GOL	C1-C2-C3-O3
2	C	502	GOL	O1-C1-C2-C3
2	A	501	GOL	O2-C2-C3-O3
2	A	502	GOL	O1-C1-C2-O2
2	B	501	GOL	O1-C1-C2-O2
2	C	502	GOL	O2-C2-C3-O3
3	B	502	EDO	O1-C1-C2-O2
2	A	502	GOL	O2-C2-C3-O3
2	C	501	GOL	O2-C2-C3-O3
3	A	506	EDO	O1-C1-C2-O2
3	C	505	EDO	O1-C1-C2-O2
3	C	504	EDO	O1-C1-C2-O2
2	B	501	GOL	O2-C2-C3-O3
3	A	504	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EDO	1	0
3	A	505	EDO	6	0
2	C	501	GOL	2	0
2	B	501	GOL	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, 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	354/381 (92%)	0.01	13 (3%) 45 41	19, 34, 58, 69	0
1	B	351/381 (92%)	0.48	32 (9%) 15 12	23, 44, 69, 80	0
1	C	353/381 (92%)	0.16	18 (5%) 33 30	19, 38, 60, 79	0
All	All	1058/1143 (92%)	0.22	63 (5%) 27 24	19, 38, 64, 80	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	HIS	4.8
1	C	170	ASN	4.7
1	C	222	SER	4.4
1	A	240	PHE	3.9
1	B	240	PHE	3.9
1	B	31	HIS	3.9
1	A	239	LEU	3.8
1	A	316	ASN	3.7
1	B	35	GLN	3.7
1	C	220	GLU	3.5
1	C	240	PHE	3.5
1	B	212	PHE	3.5
1	A	139	GLU	3.4
1	B	152	SER	3.3
1	C	312	PRO	3.3
1	C	30	HIS	3.2
1	C	171	GLU	3.2
1	A	312	PRO	3.0
1	B	214	ASP	3.0
1	B	198	GLN	3.0
1	B	274	GLU	2.8
1	B	200	ASP	2.7
1	A	281	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	260	LYS	2.7
1	B	44	GLY	2.7
1	C	316	ASN	2.7
1	A	31	HIS	2.6
1	B	154	TYR	2.6
1	A	34	LYS	2.6
1	B	59	ARG	2.5
1	B	273	CYS	2.5
1	B	125	TYR	2.5
1	A	317	ALA	2.4
1	B	201	PHE	2.4
1	B	52	THR	2.3
1	B	216	VAL	2.3
1	A	280	HIS	2.3
1	B	138	ILE	2.3
1	A	171	GLU	2.3
1	C	139	GLU	2.3
1	B	149	GLN	2.3
1	C	214	ASP	2.2
1	C	310	ASN	2.2
1	B	217	SER	2.2
1	B	122	ASP	2.2
1	A	33	ILE	2.2
1	B	208	ILE	2.2
1	C	176	GLU	2.2
1	B	275	PHE	2.2
1	C	52	THR	2.2
1	B	148	LEU	2.2
1	B	211	ALA	2.1
1	C	406	LEU	2.1
1	B	112	GLU	2.1
1	B	151	THR	2.1
1	C	142	LYS	2.1
1	B	150	GLN	2.1
1	C	122	ASP	2.1
1	C	314	TYR	2.1
1	B	163	TYR	2.0
1	B	261	ASP	2.0
1	A	30	HIS	2.0
1	B	315	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

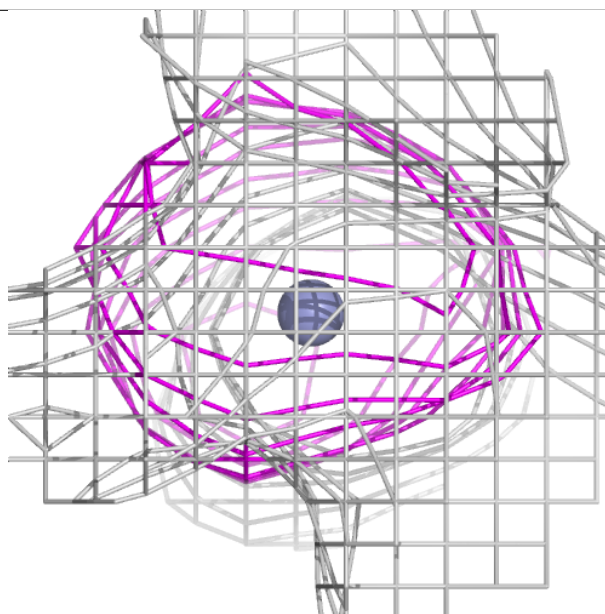
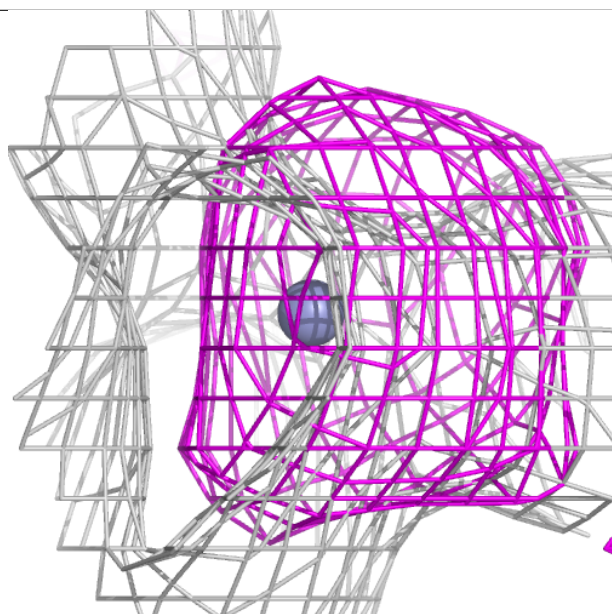
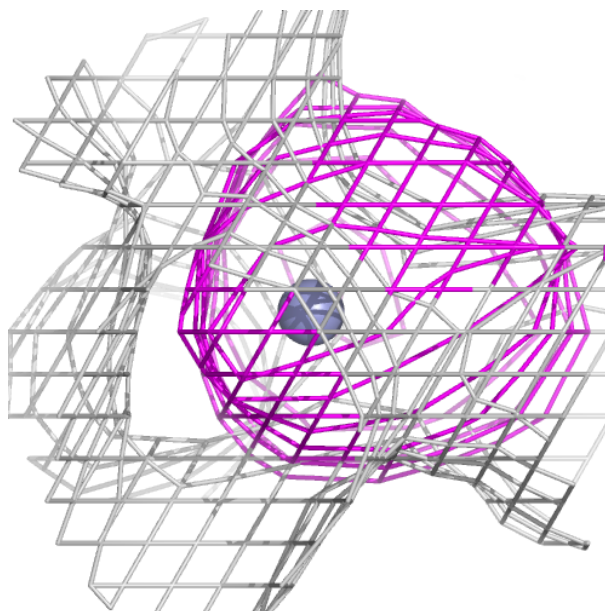
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	502	4/4	0.76	0.18	41,44,51,52	0
3	EDO	B	503	4/4	0.78	0.15	45,49,50,55	0
2	GOL	A	502	6/6	0.80	0.17	43,44,48,48	0
5	ZN	B	504	1/1	0.80	0.29	91,91,91,91	0
3	EDO	A	507	4/4	0.83	0.14	50,51,52,58	0
2	GOL	B	501	6/6	0.84	0.14	47,50,52,53	0
3	EDO	A	506	4/4	0.84	0.15	43,45,45,53	0
6	CL	C	507	1/1	0.84	0.18	71,71,71,71	0
3	EDO	A	505	4/4	0.85	0.18	41,41,48,49	0
3	EDO	C	505	4/4	0.85	0.14	33,35,36,37	0
2	GOL	C	502	6/6	0.86	0.13	32,33,34,36	0
3	EDO	A	504	4/4	0.86	0.13	39,40,41,43	0
2	GOL	C	501	6/6	0.88	0.16	28,28,33,36	0
2	GOL	A	503	6/6	0.88	0.19	31,34,36,37	0
5	ZN	C	506	1/1	0.88	0.24	82,82,82,82	0
3	EDO	C	504	4/4	0.88	0.14	42,42,45,46	0
2	GOL	C	503	6/6	0.92	0.11	30,33,34,39	0
2	GOL	A	501	6/6	0.93	0.09	27,33,34,39	0
5	ZN	A	509	1/1	0.95	0.28	71,71,71,71	0
4	SO4	A	508	5/5	0.97	0.06	28,33,37,38	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.

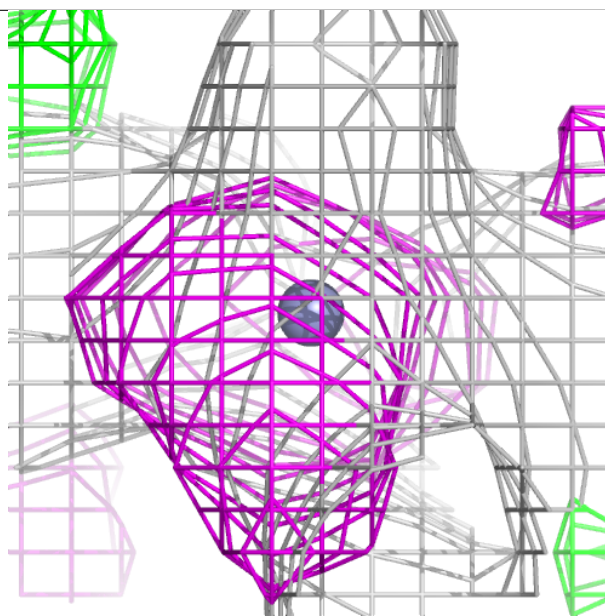
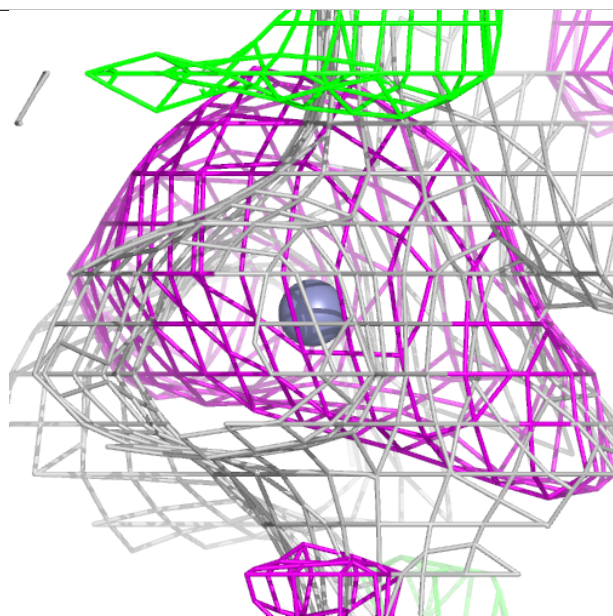
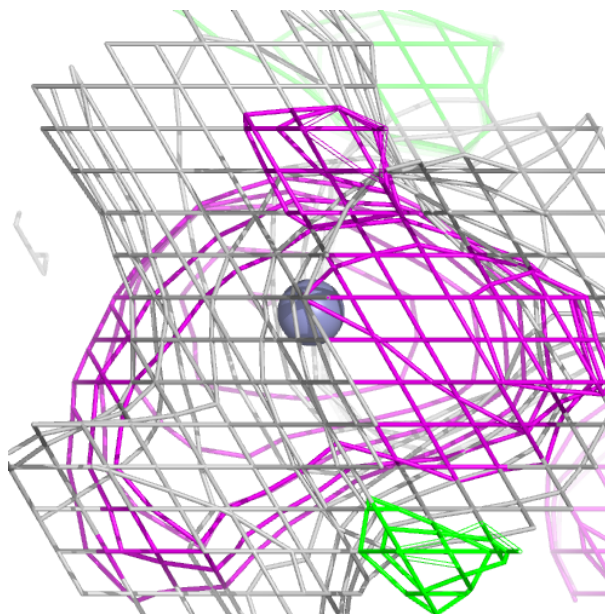
Electron density around ZN B 504:

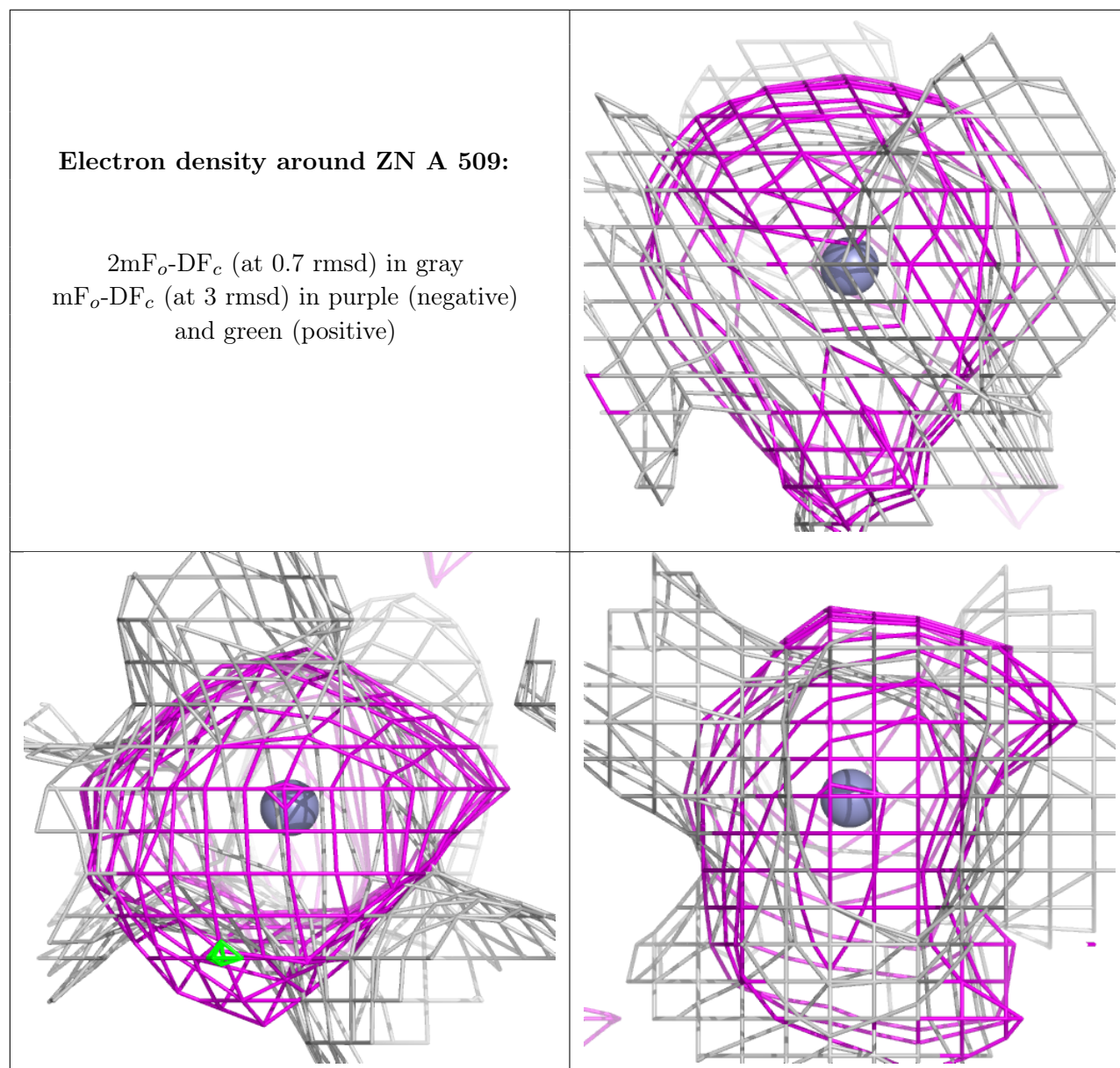
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN C 506:

$2mF_o-DF_c$ (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.