



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 10:05 PM JST

PDB ID : 8ZEV  
Title : Crystal structure of the dehydratase domain of human fatty acid synthase  
Authors : Zhang, L.; Zhang, L.  
Deposited on : 2024-05-07  
Resolution : 1.80 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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

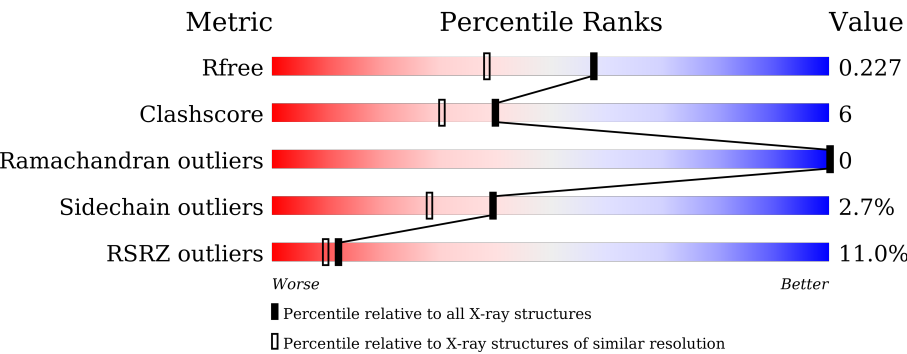
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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  $\geq 3$ , 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	252	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>88%</div><div>12%</div></div>
1	B	252	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>84%</div><div>10%</div><div>• •</div></div>
1	C	252	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>81%</div><div>15%</div><div>• •</div></div>
1	D	252	<div><div>11%</div><div><div></div><div></div><div></div><div></div></div><div>86%</div><div>7%</div><div>• 5%</div></div>

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	IOD	A	2001	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8510 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	3	0
			1995	1278	337	377	3			
1	B	241	Total	C	N	O	S	0	2	0
			1910	1224	325	358	3			
1	C	245	Total	C	N	O	S	0	3	0
			1947	1246	330	368	3			
1	D	240	Total	C	N	O	S	0	1	0
			1904	1219	327	355	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP P49327
A	-6	GLU	-	expression tag	UNP P49327
A	-5	ASN	-	expression tag	UNP P49327
A	-4	LEU	-	expression tag	UNP P49327
A	-3	TYR	-	expression tag	UNP P49327
A	-2	PHE	-	expression tag	UNP P49327
A	-1	GLN	-	expression tag	UNP P49327
B	-7	SER	-	expression tag	UNP P49327
B	-6	GLU	-	expression tag	UNP P49327
B	-5	ASN	-	expression tag	UNP P49327
B	-4	LEU	-	expression tag	UNP P49327
B	-3	TYR	-	expression tag	UNP P49327
B	-2	PHE	-	expression tag	UNP P49327
B	-1	GLN	-	expression tag	UNP P49327
C	-7	SER	-	expression tag	UNP P49327
C	-6	GLU	-	expression tag	UNP P49327
C	-5	ASN	-	expression tag	UNP P49327
C	-4	LEU	-	expression tag	UNP P49327
C	-3	TYR	-	expression tag	UNP P49327
C	-2	PHE	-	expression tag	UNP P49327
C	-1	GLN	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	SER	-	expression tag	UNP P49327
D	-6	GLU	-	expression tag	UNP P49327
D	-5	ASN	-	expression tag	UNP P49327
D	-4	LEU	-	expression tag	UNP P49327
D	-3	TYR	-	expression tag	UNP P49327
D	-2	PHE	-	expression tag	UNP P49327
D	-1	GLN	-	expression tag	UNP P49327

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total I 2 2	0	0
2	B	2	Total I 2 2	0	0
2	C	2	Total I 2 2	0	0
2	D	1	Total I 1 1	0	0

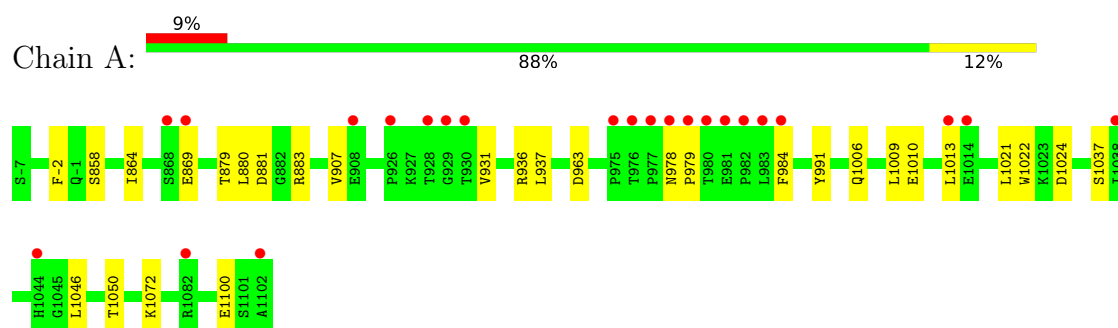
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	196	Total O 196 196	0	0
3	B	206	Total O 206 206	0	0
3	C	169	Total O 169 169	0	0
3	D	176	Total O 176 176	0	0

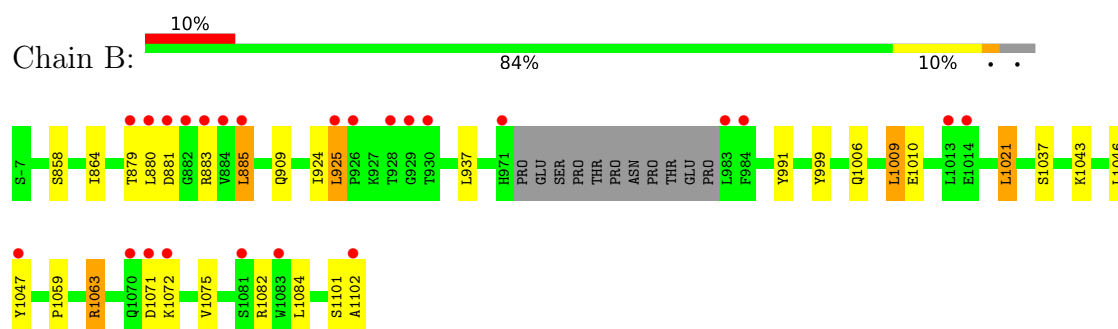
### 3 Residue-property plots

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.

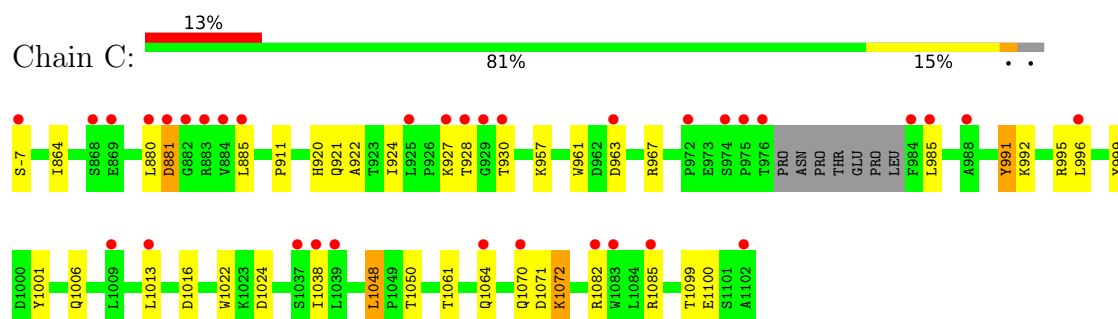
#### • Molecule 1: Fatty acid synthase



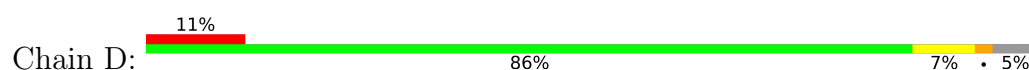
#### • Molecule 1: Fatty acid synthase

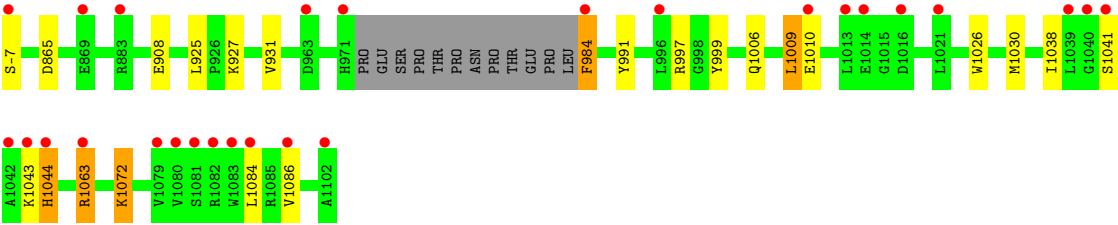


#### • Molecule 1: Fatty acid synthase



#### • Molecule 1: Fatty acid synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.13Å 108.13Å 221.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.21 – 1.80 31.21 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.21-1.80) 95.9 (31.21-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.207 , 0.228 0.207 , 0.227	Depositor DCC
$R_{free}$ test set	7117 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8510	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: IOD

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	0.43	0/2055	0.67	0/2806
1	B	0.37	0/1961	0.63	0/2670
1	C	0.45	0/2003	0.67	1/2729 (0.0%)
1	D	0.45	0/1952	0.66	0/2657
All	All	0.43	0/7971	0.66	1/10862 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	991	TYR	CB-CA-C	5.23	120.86	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1063	ARG	Sidechain

## 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	1995	0	1973	18	0
1	B	1910	0	1891	24	0
1	C	1947	0	1921	32	0
1	D	1904	0	1883	27	0
2	A	2	0	0	2	0
2	B	2	0	0	1	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	196	0	0	2	0
3	B	206	0	0	3	0
3	C	169	0	0	2	0
3	D	176	0	0	3	0
All	All	8510	0	7668	100	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 6.

All (100) 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:984:PHE:CE2	1:D:1010:GLU:HG2	1.72	1.25
1:D:984:PHE:CD2	1:D:1010:GLU:HG2	1.74	1.21
1:D:984:PHE:CD2	1:D:1010:GLU:CG	2.35	1.09
1:C:885:LEU:HD11	1:C:922:ALA:HB1	1.46	0.95
1:C:1050:THR:HG21	1:C:1100:GLU:HG3	1.51	0.92
1:D:984:PHE:HD2	1:D:1010:GLU:CG	1.79	0.91
1:A:1009:LEU:HD21	1:A:1021:LEU:HG	1.58	0.85
1:D:984:PHE:HE2	1:D:1010:GLU:HG2	1.40	0.82
1:C:957:LYS:HE3	3:C:2125:HOH:O	1.79	0.81
1:D:984:PHE:CE2	1:D:1010:GLU:CG	2.59	0.78
1:A:881:ASP:HB2	1:A:1046:LEU:HD22	1.66	0.77
1:C:1050:THR:HG21	1:C:1100:GLU:CG	2.15	0.75
2:A:2001:IOD:I	3:A:2260:HOH:O	2.77	0.71
1:B:880:LEU:HD22	1:B:999:TYR:HA	1.73	0.71
1:D:984:PHE:HD2	1:D:1010:GLU:HG3	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:997:ARG:HH12	1:D:1041:SER:HB3	1.57	0.70
1:B:858[B]:SER:OG	1:B:937:LEU:HD12	1.91	0.69
1:B:879:THR:O	1:B:880:LEU:HD23	1.92	0.69
1:B:1009:LEU:CD2	1:B:1021:LEU:HD23	2.25	0.65
1:B:1082:ARG:NH2	3:B:2105:HOH:O	2.31	0.64
1:D:927:LYS:HD2	3:D:2173:HOH:O	1.98	0.63
1:B:858[A]:SER:HB2	3:B:2183:HOH:O	1.98	0.63
1:B:1009:LEU:HD21	1:B:1021:LEU:HD23	1.82	0.62
1:B:885:LEU:HD12	1:B:924:ILE:HD11	1.82	0.61
1:B:1071:ASP:O	1:B:1072:LYS:HB2	1.99	0.60
1:D:984:PHE:CE2	1:D:1010:GLU:OE2	2.55	0.60
1:C:1071:ASP:O	1:C:1072:LYS:HB2	2.02	0.59
1:D:1084:LEU:O	1:D:1086:VAL:HG23	2.04	0.57
1:D:991:TYR:CZ	1:D:1006:GLN:HA	2.40	0.56
1:B:1101:SER:O	1:B:1102:ALA:HB2	2.06	0.56
1:B:858[B]:SER:HB3	3:B:2183:HOH:O	2.06	0.55
1:A:1037[A]:SER:OG	2:A:2001:IOD:I	2.95	0.54
1:C:927:LYS:HG3	1:C:928:THR:H	1.74	0.54
1:B:885:LEU:HD12	1:B:924:ILE:CD1	2.37	0.53
1:D:984:PHE:CD2	1:D:1010:GLU:CD	2.81	0.53
1:A:864:ILE:HB	1:A:931[A]:VAL:HG22	1.89	0.53
1:A:963:ASP:OD1	1:A:963:ASP:N	2.40	0.53
1:C:1082:ARG:NH2	3:C:2103:HOH:O	2.42	0.53
1:A:864:ILE:HB	1:A:931[A]:VAL:CG2	2.38	0.53
1:A:1009:LEU:HD21	1:A:1021:LEU:CG	2.36	0.52
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.45	0.52
1:B:1043:LYS:HB3	1:B:1047:TYR:OH	2.10	0.52
1:B:1084:LEU:HD21	1:C:1024:ASP:HB3	1.91	0.51
1:C:927:LYS:HG3	1:C:928:THR:N	2.25	0.51
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.46	0.50
1:C:991:TYR:CZ	1:C:1006:GLN:HA	2.46	0.50
1:A:1050:THR:HG21	1:A:1100:GLU:HB2	1.92	0.50
1:A:858:SER:OG	1:A:937:LEU:HD12	2.11	0.50
1:B:881:ASP:HB2	1:B:1046:LEU:HD21	1.94	0.50
1:C:885:LEU:HD12	1:C:924:ILE:HD13	1.93	0.50
1:D:1072:LYS:O	3:D:2101:HOH:O	2.20	0.50
1:C:885:LEU:CD1	1:C:924:ILE:HD13	2.42	0.49
1:D:999:TYR:CE2	1:D:1038:ILE:HD13	2.47	0.49
1:B:1021:LEU:HD22	1:B:1075:VAL:HG12	1.95	0.49
1:C:1070:GLN:H	1:C:1070:GLN:CD	2.16	0.49
1:B:858[B]:SER:HG	1:B:937:LEU:HD12	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1044:HIS:CD2	1:D:1044:HIS:N	2.80	0.48
1:C:864:ILE:O	1:C:930:THR:HA	2.13	0.48
1:A:879:THR:O	1:A:880:LEU:HD23	2.13	0.48
1:B:1037:SER:OG	2:B:2001:IOD:I	3.00	0.47
1:C:1061:THR:HA	1:C:1064:GLN:HE21	1.79	0.47
1:D:908:GLU:HB3	1:D:1063[B]:ARG:NH2	2.29	0.47
1:B:883:ARG:HH11	1:B:924:ILE:HG21	1.79	0.47
1:A:883:ARG:NH2	3:A:2103:HOH:O	2.33	0.46
1:C:985:LEU:CD1	1:C:1013:LEU:HD12	2.45	0.46
1:A:879:THR:C	1:A:880:LEU:HD23	2.36	0.45
1:D:984:PHE:CD2	1:D:1010:GLU:OE2	2.69	0.45
1:C:1099:THR:C	1:C:1100:GLU:HG2	2.35	0.45
1:A:1009:LEU:CD2	1:A:1021:LEU:HG	2.38	0.45
1:A:1022:TRP:CZ2	1:A:1024:ASP:HA	2.52	0.45
1:D:925:LEU:HD22	1:D:931:VAL:HB	2.00	0.44
1:B:1059:PRO:O	1:B:1063:ARG:HG3	2.18	0.44
1:C:985:LEU:HD12	1:C:1013:LEU:HD12	2.00	0.44
1:C:1048:LEU:HD12	1:C:1048:LEU:HA	1.85	0.44
1:D:1044:HIS:CD2	1:D:1044:HIS:H	2.35	0.44
1:C:985:LEU:CD1	1:C:1013:LEU:HA	2.48	0.44
1:C:880:LEU:O	1:C:881:ASP:HB2	2.19	0.43
1:C:1022:TRP:CZ2	1:C:1024:ASP:HA	2.54	0.43
1:D:1026:TRP:O	1:D:1030:MET:HG3	2.19	0.43
1:C:864:ILE:HD13	1:D:-7:SER:HB3	1.99	0.43
1:C:991:TYR:O	1:C:995:ARG:HB2	2.18	0.43
1:D:999:TYR:CD1	1:D:999:TYR:N	2.85	0.43
1:C:1082:ARG:O	1:C:1085:ARG:HD2	2.19	0.42
1:A:984:PHE:HD2	1:A:1010:GLU:HB3	1.83	0.42
1:C:920:HIS:C	1:C:921[B]:GLN:HG2	2.40	0.42
1:B:858[B]:SER:OG	1:B:937:LEU:HB2	2.20	0.42
1:C:967:ARG:NE	1:C:967:ARG:HA	2.35	0.42
1:C:999:TYR:HB3	1:C:1001:TYR:CE2	2.54	0.42
1:C:911:PRO:HB2	1:C:961:TRP:HB3	2.02	0.42
1:C:1070:GLN:CD	1:C:1070:GLN:N	2.73	0.42
1:A:978:ASN:HA	1:A:979:PRO:HD3	1.89	0.41
1:C:-7:SER:HA	3:D:2114:HOH:O	2.20	0.41
1:D:997:ARG:NH1	1:D:1038:ILE:O	2.53	0.41
1:D:1041:SER:C	1:D:1043:LYS:H	2.24	0.41
1:A:-2:PHE:CD1	1:A:936:ARG:HB3	2.55	0.41
1:B:879:THR:HA	1:B:883:ARG:O	2.20	0.41
1:B:925:LEU:N	1:B:925:LEU:HD23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1044:HIS:H	1:D:1044:HIS:HD2	1.66	0.40
1:C:992:LYS:O	1:C:996:LEU:HG	2.21	0.40
1:D:1009:LEU:HD23	1:D:1009:LEU:HA	1.85	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	253/252 (100%)	250 (99%)	3 (1%)	0	100	100
1	B	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
1	C	244/252 (97%)	238 (98%)	6 (2%)	0	100	100
1	D	237/252 (94%)	237 (100%)	0	0	100	100
All	All	973/1008 (96%)	962 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	220/217 (101%)	216 (98%)	4 (2%)	54	45
1	B	208/217 (96%)	201 (97%)	7 (3%)	32	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	213/217 (98%)	207 (97%)	6 (3%)	38	27
1	D	206/217 (95%)	199 (97%)	7 (3%)	32	20
All	All	847/868 (98%)	823 (97%)	24 (3%)	40	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	869	GLU
1	A	907	VAL
1	A	1013	LEU
1	A	1072	LYS
1	B	864	ILE
1	B	885	LEU
1	B	909	GLN
1	B	925	LEU
1	B	1009	LEU
1	B	1010	GLU
1	B	1021	LEU
1	C	881	ASP
1	C	963	ASP
1	C	1016	ASP
1	C	1038	ILE
1	C	1048	LEU
1	C	1072	LYS
1	D	865	ASP
1	D	984	PHE
1	D	1009	LEU
1	D	1044	HIS
1	D	1063[A]	ARG
1	D	1063[B]	ARG
1	D	1072	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	971	HIS
1	B	1098	HIS
1	C	1064	GLN
1	D	-1	GLN
1	D	878	HIS

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Mol	Chain	Res	Type
1	D	1044	HIS

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	252/252 (100%)	0.56	23 (9%)	16 14	22, 37, 65, 87	3 (1%)
1	B	241/252 (95%)	0.39	24 (9%)	14 11	20, 37, 57, 74	2 (0%)
1	C	245/252 (97%)	0.76	34 (13%)	7 6	21, 40, 68, 83	3 (1%)
1	D	240/252 (95%)	0.78	27 (11%)	11 9	25, 40, 70, 93	1 (0%)
All	All	978/1008 (97%)	0.62	108 (11%)	12 9	20, 39, 67, 93	9 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	983	LEU	7.5
1	A	980	THR	6.3
1	A	1013	LEU	6.0
1	B	880	LEU	5.9
1	D	984	PHE	5.9
1	A	979	PRO	5.4
1	D	1083	TRP	5.3
1	D	1084	LEU	5.3
1	B	1102	ALA	5.2
1	A	984	PHE	5.0
1	C	975	PRO	5.0
1	A	975	PRO	4.4
1	D	1042	ALA	4.4
1	D	971	HIS	4.3
1	B	881	ASP	4.3
1	C	976	THR	4.3
1	C	984	PHE	4.3
1	D	1081	SER	4.3
1	A	982	PRO	4.3
1	C	882	GLY	4.2
1	B	983	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	981	GLU	4.2
1	A	977	PRO	3.9
1	A	978	ASN	3.8
1	C	881	ASP	3.7
1	C	925	LEU	3.7
1	D	1013	LEU	3.7
1	C	1038	ILE	3.6
1	C	1102	ALA	3.6
1	D	-7	SER	3.5
1	A	930	THR	3.4
1	D	1102	ALA	3.4
1	B	1047	TYR	3.4
1	C	927	LYS	3.4
1	D	869	GLU	3.4
1	B	1083	TRP	3.3
1	D	1040	GLY	3.3
1	C	868	SER	3.3
1	C	928	THR	3.2
1	C	869	GLU	3.2
1	A	976	THR	3.2
1	D	1014	GLU	3.2
1	C	884	VAL	3.1
1	D	1039	LEU	3.1
1	C	929	GLY	3.0
1	B	984	PHE	3.0
1	D	963	ASP	3.0
1	D	1082	ARG	3.0
1	C	880	LEU	3.0
1	B	883	ARG	2.9
1	D	1086	VAL	2.9
1	C	1064	GLN	2.9
1	B	971	HIS	2.8
1	C	1070	GLN	2.8
1	B	884	VAL	2.8
1	C	930	THR	2.8
1	B	1013	LEU	2.7
1	B	925	LEU	2.7
1	C	883	ARG	2.7
1	D	1041	SER	2.7
1	B	882	GLY	2.7
1	D	1021	LEU	2.7
1	C	-7	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1037	SER	2.6
1	C	1083	TRP	2.5
1	D	1016	ASP	2.5
1	C	1013	LEU	2.5
1	D	1044	HIS	2.5
1	A	1102	ALA	2.5
1	B	1014	GLU	2.5
1	C	996	LEU	2.5
1	D	1010	GLU	2.5
1	D	1080	VAL	2.5
1	C	1082	ARG	2.4
1	C	885	LEU	2.4
1	A	868	SER	2.4
1	C	974	SER	2.4
1	A	1038	ILE	2.4
1	A	928	THR	2.3
1	A	1044	HIS	2.3
1	D	1063[A]	ARG	2.3
1	B	928	THR	2.3
1	B	1070	GLN	2.3
1	C	985	LEU	2.3
1	D	1043	LYS	2.2
1	B	1071	ASP	2.2
1	B	1081	SER	2.2
1	C	988	ALA	2.2
1	A	908	GLU	2.2
1	B	885	LEU	2.2
1	B	930	THR	2.1
1	A	1082	ARG	2.1
1	A	929	GLY	2.1
1	B	929	GLY	2.1
1	C	1009	LEU	2.1
1	C	1039	LEU	2.1
1	D	996	LEU	2.1
1	A	869	GLU	2.1
1	B	879	THR	2.1
1	C	963	ASP	2.0
1	D	1079	VAL	2.0
1	A	926	PRO	2.0
1	C	972	PRO	2.0
1	A	1014	GLU	2.0
1	B	1072	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	926	PRO	2.0
1	C	1085	ARG	2.0
1	D	883	ARG	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](#)

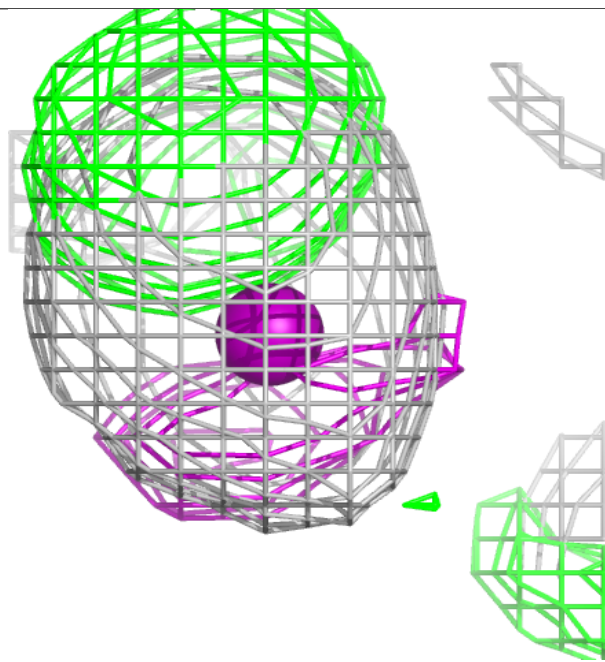
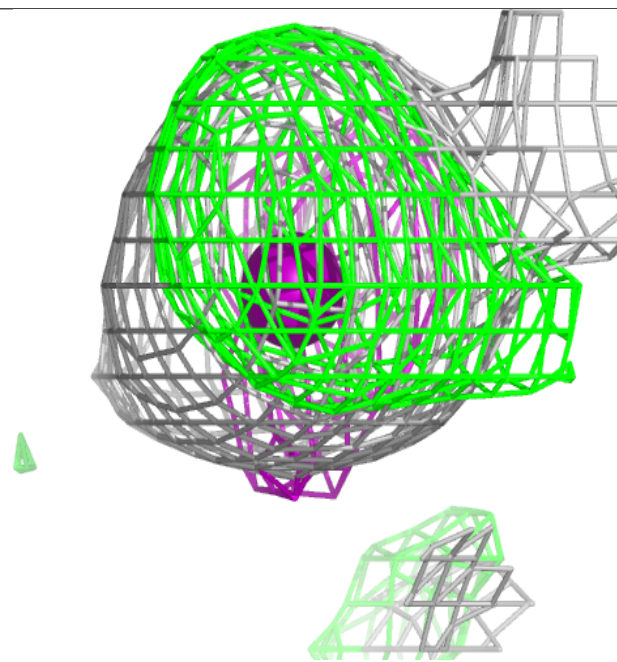
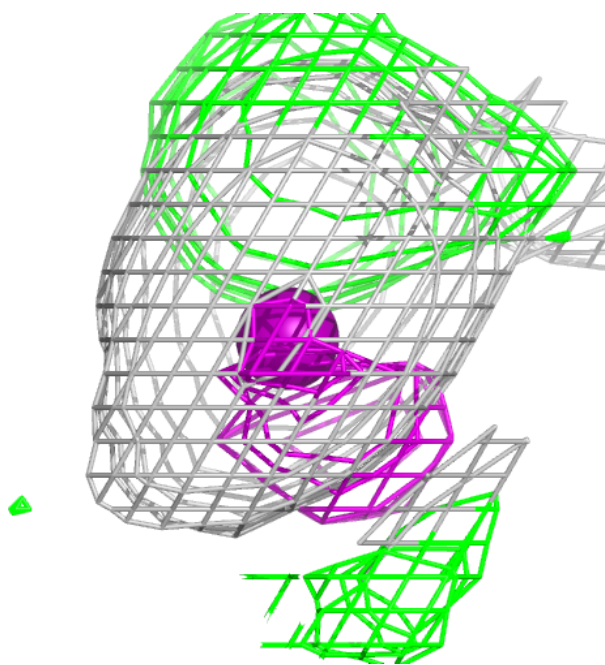
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	IOD	C	2001	1/1	0.80	0.17	53,53,53,53	1
2	IOD	A	2000	1/1	0.95	0.09	46,46,46,46	0
2	IOD	B	2000	1/1	0.97	0.09	40,40,40,40	0
2	IOD	C	2000	1/1	0.98	0.08	46,46,46,46	0
2	IOD	B	2001	1/1	0.98	0.05	49,49,49,49	1
2	IOD	D	2000	1/1	0.98	0.07	46,46,46,46	0
2	IOD	A	2001	1/1	0.99	0.03	42,42,42,42	1

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.

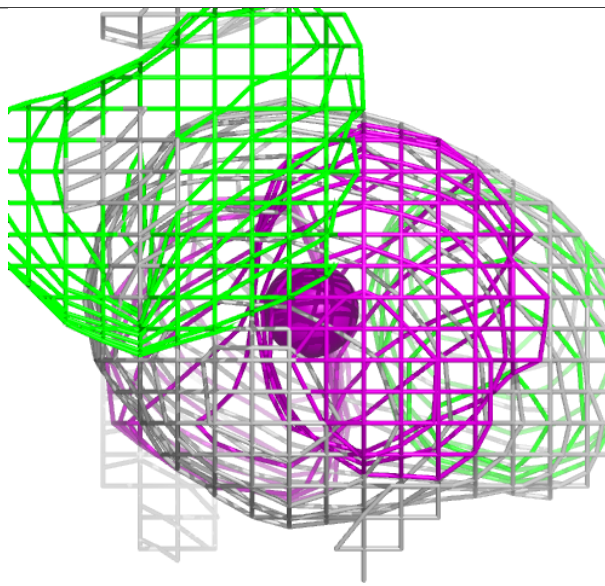
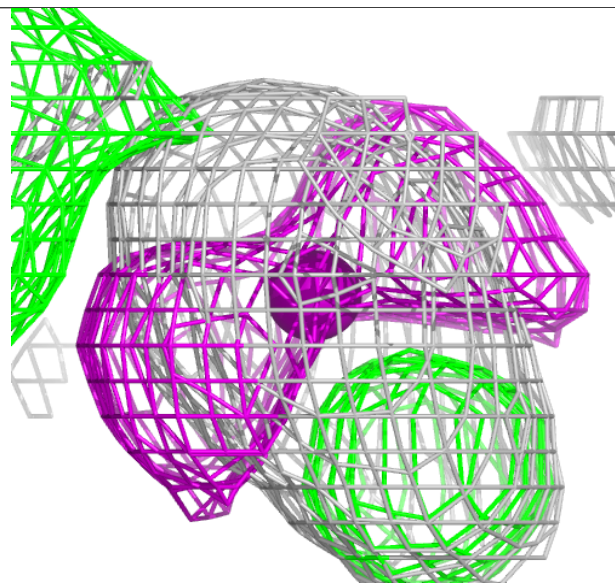
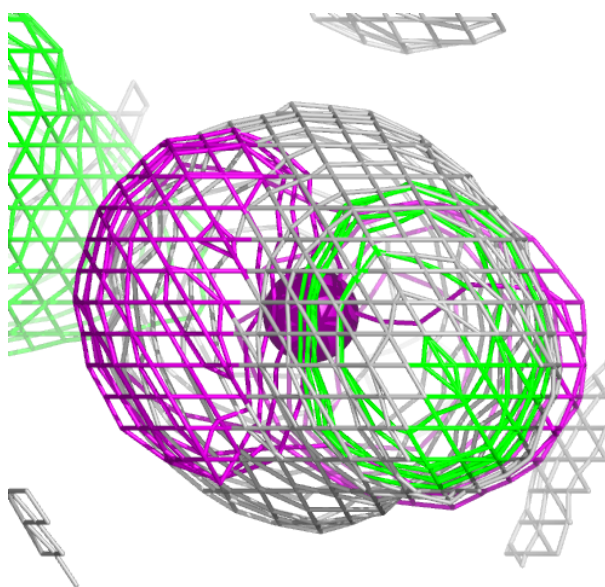
**Electron density around IOD C 2001:**

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



**Electron density around IOD A 2000:**

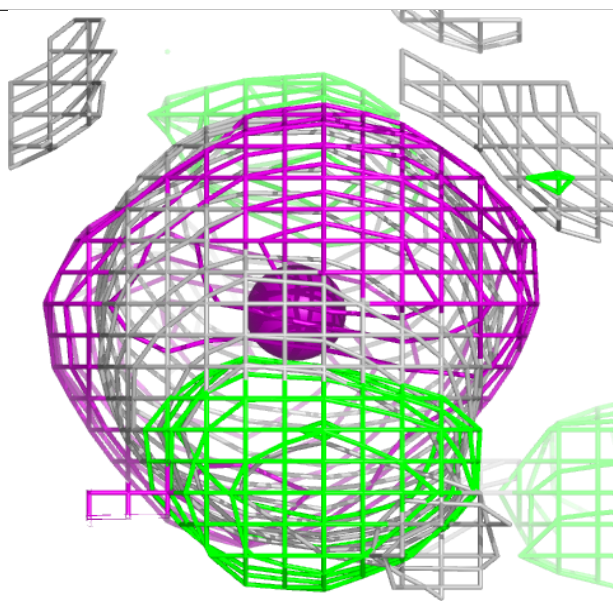
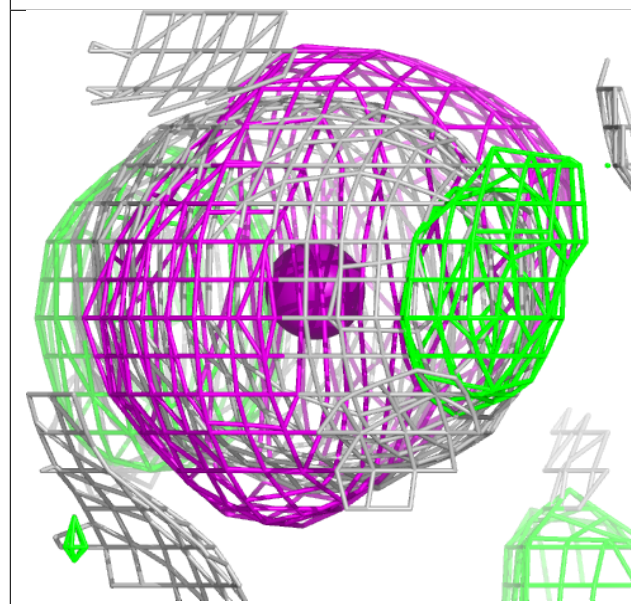
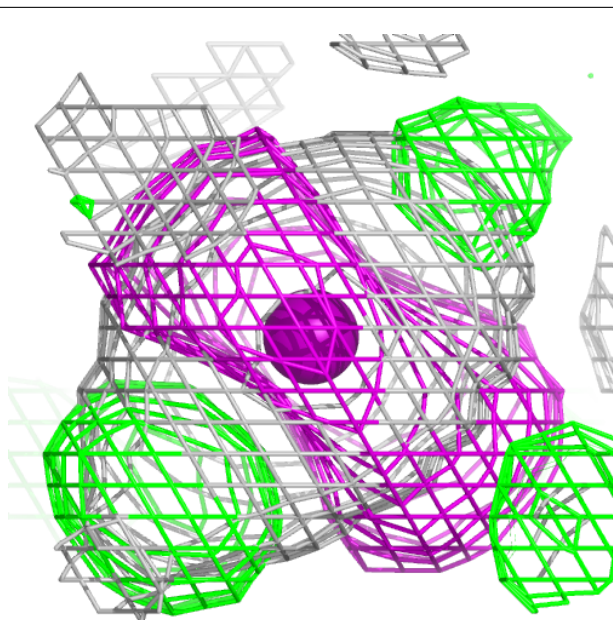
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





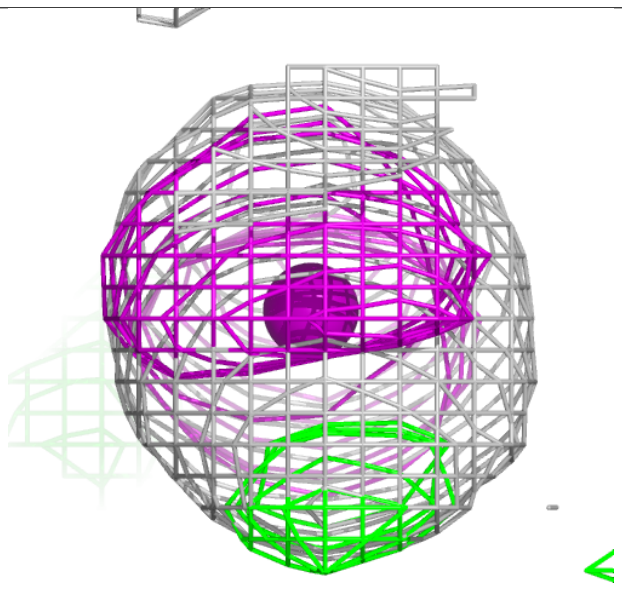
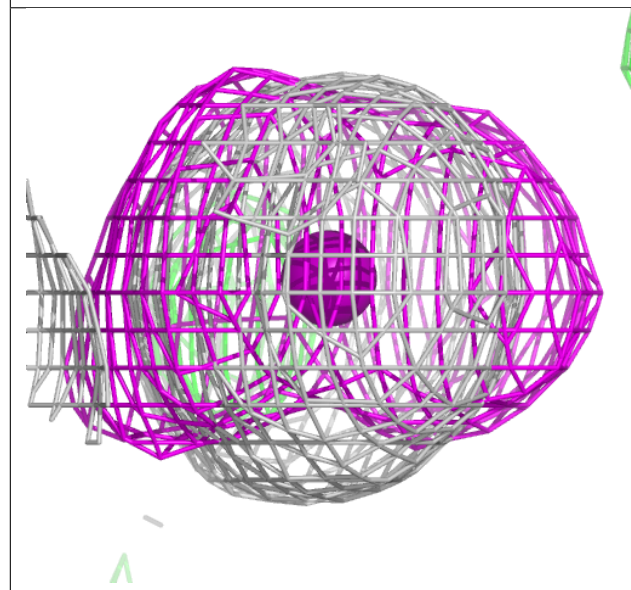
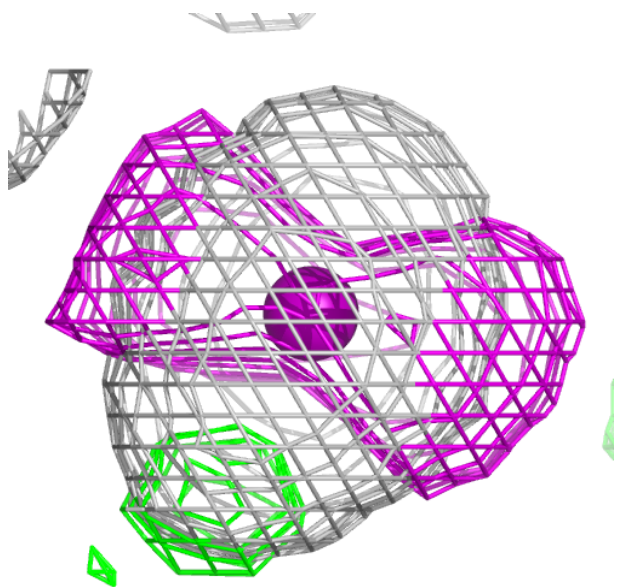
**Electron density around IOD B 2000:**

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



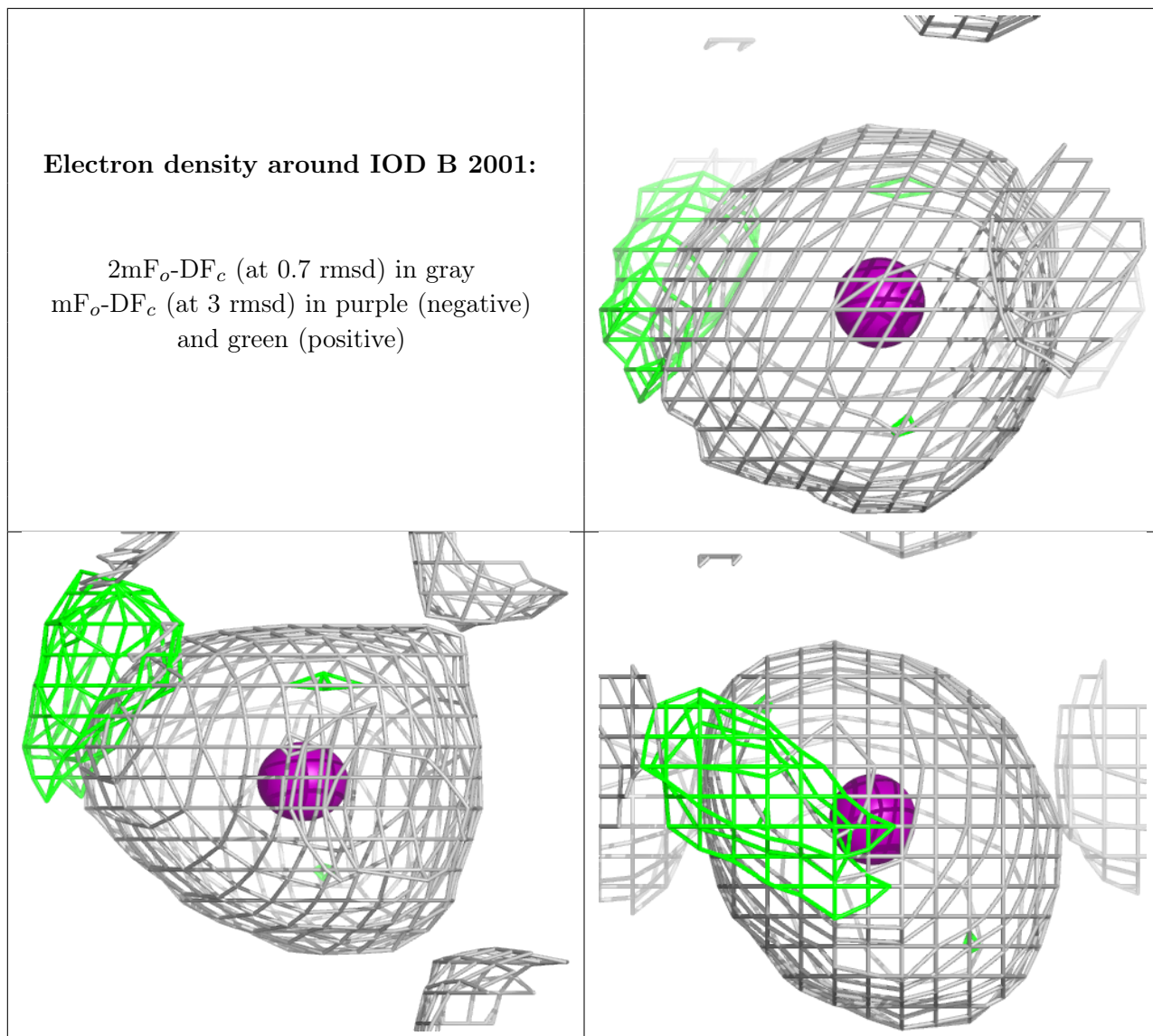
**Electron density around IOD C 2000:**

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



**Electron density around IOD B 2001:**

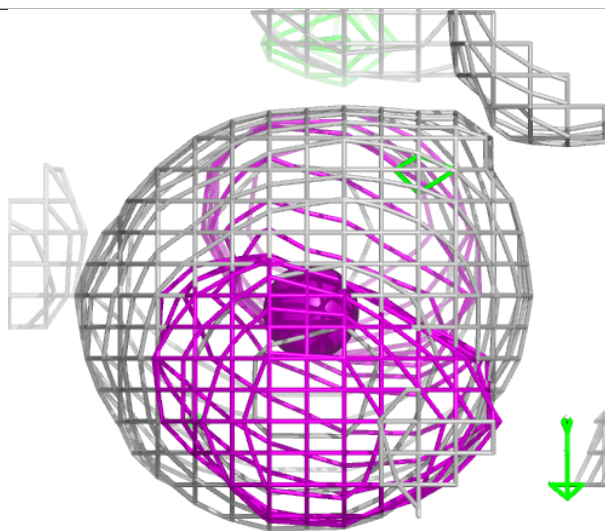
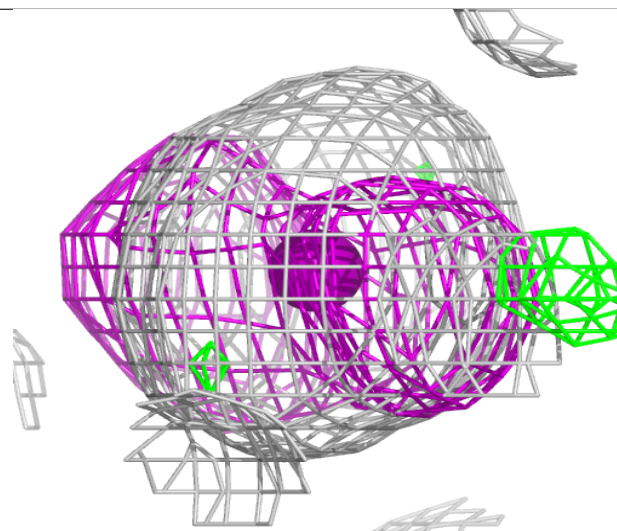
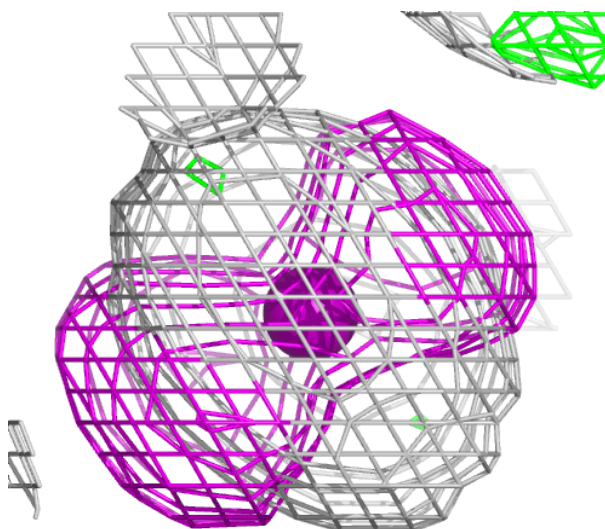
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

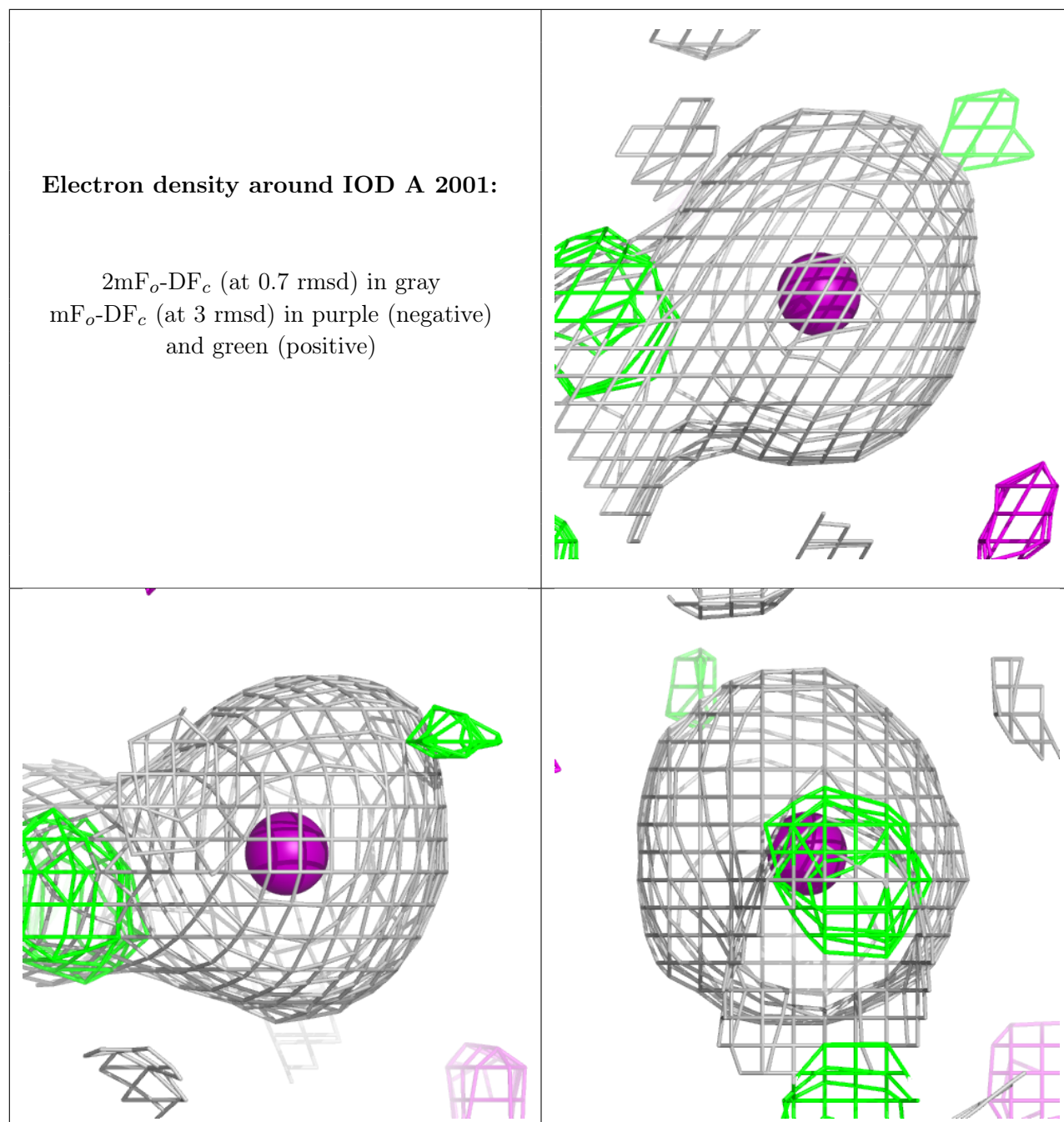




**Electron density around IOD D 2000:**

$2mF_o-DF_c$  (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.