wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 12:08 AM EDT

PDB ID	:	5WOB
Title	:	Crystal Structure Analysis of Fab1-Bound Human Insulin Degrading Enzyme (IDE) in Complex with Insulin
Authors	:	McCord, L.A.; Liang, W.G.; Farcasanu, M.; Wang, A.G.; Koide, S.; Tang, W.J.
Deposited on	:	2017-08-01
Resolution	:	3.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

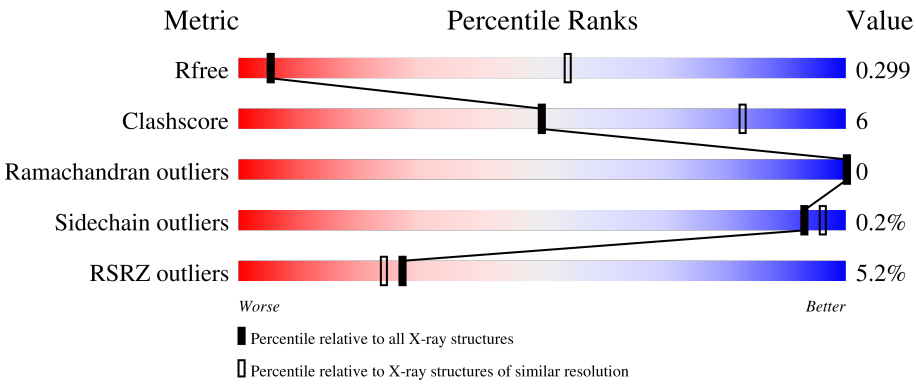
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.95 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	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	%, 81%, 14%, 5%
1	B	990	%, 81%, 14%, •
1	C	990	5%, 81%, 15%, •
1	D	990	6%, 80%, 16%, •
1	E	990	5%, 81%, 15%, 5%

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Mol	Chain	Length	Quality of chain
1	F	990	6% 82% 13% 5%
1	G	990	2% 81% 14% 5%
1	H	990	3% 81% 13% 5%
2	a	20	5% 100%
2	b	20	5% 25% 75%
2	c	20	5% 100%
2	d	20	15% 85%
2	e	20	5% 40% 5% 55%
2	f	20	90% 10%
2	g	20	70% 5% 25%
2	h	20	30% 70%
3	I	263	2% 71% 11% 18%
3	K	263	7% 64% 14% 21%
3	M	263	4% 67% 14% 19%
3	O	263	11% 68% 11% 21%
3	Q	263	12% 65% 11% 24%
3	S	263	5% 66% 16% 18%
3	U	263	8% 61% 14% 24%
3	W	263	5% 64% 13% 22%
4	J	239	2% 67% 15% 17%
4	L	239	7% 62% 11% 26%
4	N	239	6% 71% 13% 16%
4	P	239	9% 67% 10% 23%
4	R	239	10% 63% 11% 26%
4	T	239	10% 68% 15% 17%

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Mol	Chain	Length	Quality of chain
4	V	239	5% 67% 11% 22%
4	X	239	5% 65% 18% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 86906 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	941	7708	4971	1294	1422	21	0	0	0
1	B	947	7758	4997	1302	1437	22	0	0	0
1	C	950	7772	5009	1304	1437	22	0	0	0
1	D	952	7790	5018	1307	1443	22	0	0	0
1	E	943	7713	4969	1294	1428	22	0	0	0
1	F	944	7735	4988	1301	1425	21	0	0	0
1	G	943	7722	4975	1298	1427	22	0	0	0
1	H	936	7663	4945	1288	1410	20	0	0	0

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	initiating methionine	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735
C	30	MET	-	initiating methionine	UNP P14735
C	31	HIS	-	expression tag	UNP P14735
C	32	HIS	-	expression tag	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
C	33	HIS	-	expression tag	UNP P14735
C	34	HIS	-	expression tag	UNP P14735
C	35	HIS	-	expression tag	UNP P14735
C	36	HIS	-	expression tag	UNP P14735
C	37	ALA	-	expression tag	UNP P14735
C	38	ALA	-	expression tag	UNP P14735
C	39	GLY	-	expression tag	UNP P14735
C	40	ILE	-	expression tag	UNP P14735
C	41	PRO	-	expression tag	UNP P14735
C	110	LEU	CYS	engineered mutation	UNP P14735
C	111	GLN	GLU	engineered mutation	UNP P14735
C	171	SER	CYS	engineered mutation	UNP P14735
C	178	ALA	CYS	engineered mutation	UNP P14735
C	257	VAL	CYS	engineered mutation	UNP P14735
C	414	LEU	CYS	engineered mutation	UNP P14735
C	573	ASN	CYS	engineered mutation	UNP P14735
C	590	SER	CYS	engineered mutation	UNP P14735
C	789	SER	CYS	engineered mutation	UNP P14735
C	812	ALA	CYS	engineered mutation	UNP P14735
C	819	ALA	CYS	engineered mutation	UNP P14735
C	904	SER	CYS	engineered mutation	UNP P14735
C	966	ASN	CYS	engineered mutation	UNP P14735
C	974	ALA	CYS	engineered mutation	UNP P14735
D	30	MET	-	initiating methionine	UNP P14735
D	31	HIS	-	expression tag	UNP P14735
D	32	HIS	-	expression tag	UNP P14735
D	33	HIS	-	expression tag	UNP P14735
D	34	HIS	-	expression tag	UNP P14735
D	35	HIS	-	expression tag	UNP P14735
D	36	HIS	-	expression tag	UNP P14735
D	37	ALA	-	expression tag	UNP P14735
D	38	ALA	-	expression tag	UNP P14735
D	39	GLY	-	expression tag	UNP P14735
D	40	ILE	-	expression tag	UNP P14735
D	41	PRO	-	expression tag	UNP P14735
D	110	LEU	CYS	engineered mutation	UNP P14735
D	111	GLN	GLU	engineered mutation	UNP P14735
D	171	SER	CYS	engineered mutation	UNP P14735
D	178	ALA	CYS	engineered mutation	UNP P14735
D	257	VAL	CYS	engineered mutation	UNP P14735
D	414	LEU	CYS	engineered mutation	UNP P14735
D	573	ASN	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
D	590	SER	CYS	engineered mutation	UNP P14735
D	789	SER	CYS	engineered mutation	UNP P14735
D	812	ALA	CYS	engineered mutation	UNP P14735
D	819	ALA	CYS	engineered mutation	UNP P14735
D	904	SER	CYS	engineered mutation	UNP P14735
D	966	ASN	CYS	engineered mutation	UNP P14735
D	974	ALA	CYS	engineered mutation	UNP P14735
E	30	MET	-	initiating methionine	UNP P14735
E	31	HIS	-	expression tag	UNP P14735
E	32	HIS	-	expression tag	UNP P14735
E	33	HIS	-	expression tag	UNP P14735
E	34	HIS	-	expression tag	UNP P14735
E	35	HIS	-	expression tag	UNP P14735
E	36	HIS	-	expression tag	UNP P14735
E	37	ALA	-	expression tag	UNP P14735
E	38	ALA	-	expression tag	UNP P14735
E	39	GLY	-	expression tag	UNP P14735
E	40	ILE	-	expression tag	UNP P14735
E	41	PRO	-	expression tag	UNP P14735
E	110	LEU	CYS	engineered mutation	UNP P14735
E	111	GLN	GLU	engineered mutation	UNP P14735
E	171	SER	CYS	engineered mutation	UNP P14735
E	178	ALA	CYS	engineered mutation	UNP P14735
E	257	VAL	CYS	engineered mutation	UNP P14735
E	414	LEU	CYS	engineered mutation	UNP P14735
E	573	ASN	CYS	engineered mutation	UNP P14735
E	590	SER	CYS	engineered mutation	UNP P14735
E	789	SER	CYS	engineered mutation	UNP P14735
E	812	ALA	CYS	engineered mutation	UNP P14735
E	819	ALA	CYS	engineered mutation	UNP P14735
E	904	SER	CYS	engineered mutation	UNP P14735
E	966	ASN	CYS	engineered mutation	UNP P14735
E	974	ALA	CYS	engineered mutation	UNP P14735
F	30	MET	-	initiating methionine	UNP P14735
F	31	HIS	-	expression tag	UNP P14735
F	32	HIS	-	expression tag	UNP P14735
F	33	HIS	-	expression tag	UNP P14735
F	34	HIS	-	expression tag	UNP P14735
F	35	HIS	-	expression tag	UNP P14735
F	36	HIS	-	expression tag	UNP P14735
F	37	ALA	-	expression tag	UNP P14735
F	38	ALA	-	expression tag	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
F	39	GLY	-	expression tag	UNP P14735
F	40	ILE	-	expression tag	UNP P14735
F	41	PRO	-	expression tag	UNP P14735
F	110	LEU	CYS	engineered mutation	UNP P14735
F	111	GLN	GLU	engineered mutation	UNP P14735
F	171	SER	CYS	engineered mutation	UNP P14735
F	178	ALA	CYS	engineered mutation	UNP P14735
F	257	VAL	CYS	engineered mutation	UNP P14735
F	414	LEU	CYS	engineered mutation	UNP P14735
F	573	ASN	CYS	engineered mutation	UNP P14735
F	590	SER	CYS	engineered mutation	UNP P14735
F	789	SER	CYS	engineered mutation	UNP P14735
F	812	ALA	CYS	engineered mutation	UNP P14735
F	819	ALA	CYS	engineered mutation	UNP P14735
F	904	SER	CYS	engineered mutation	UNP P14735
F	966	ASN	CYS	engineered mutation	UNP P14735
F	974	ALA	CYS	engineered mutation	UNP P14735
G	30	MET	-	initiating methionine	UNP P14735
G	31	HIS	-	expression tag	UNP P14735
G	32	HIS	-	expression tag	UNP P14735
G	33	HIS	-	expression tag	UNP P14735
G	34	HIS	-	expression tag	UNP P14735
G	35	HIS	-	expression tag	UNP P14735
G	36	HIS	-	expression tag	UNP P14735
G	37	ALA	-	expression tag	UNP P14735
G	38	ALA	-	expression tag	UNP P14735
G	39	GLY	-	expression tag	UNP P14735
G	40	ILE	-	expression tag	UNP P14735
G	41	PRO	-	expression tag	UNP P14735
G	110	LEU	CYS	engineered mutation	UNP P14735
G	111	GLN	GLU	engineered mutation	UNP P14735
G	171	SER	CYS	engineered mutation	UNP P14735
G	178	ALA	CYS	engineered mutation	UNP P14735
G	257	VAL	CYS	engineered mutation	UNP P14735
G	414	LEU	CYS	engineered mutation	UNP P14735
G	573	ASN	CYS	engineered mutation	UNP P14735
G	590	SER	CYS	engineered mutation	UNP P14735
G	789	SER	CYS	engineered mutation	UNP P14735
G	812	ALA	CYS	engineered mutation	UNP P14735
G	819	ALA	CYS	engineered mutation	UNP P14735
G	904	SER	CYS	engineered mutation	UNP P14735
G	966	ASN	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
G	974	ALA	CYS	engineered mutation	UNP P14735
H	30	MET	-	initiating methionine	UNP P14735
H	31	HIS	-	expression tag	UNP P14735
H	32	HIS	-	expression tag	UNP P14735
H	33	HIS	-	expression tag	UNP P14735
H	34	HIS	-	expression tag	UNP P14735
H	35	HIS	-	expression tag	UNP P14735
H	36	HIS	-	expression tag	UNP P14735
H	37	ALA	-	expression tag	UNP P14735
H	38	ALA	-	expression tag	UNP P14735
H	39	GLY	-	expression tag	UNP P14735
H	40	ILE	-	expression tag	UNP P14735
H	41	PRO	-	expression tag	UNP P14735
H	110	LEU	CYS	engineered mutation	UNP P14735
H	111	GLN	GLU	engineered mutation	UNP P14735
H	171	SER	CYS	engineered mutation	UNP P14735
H	178	ALA	CYS	engineered mutation	UNP P14735
H	257	VAL	CYS	engineered mutation	UNP P14735
H	414	LEU	CYS	engineered mutation	UNP P14735
H	573	ASN	CYS	engineered mutation	UNP P14735
H	590	SER	CYS	engineered mutation	UNP P14735
H	789	SER	CYS	engineered mutation	UNP P14735
H	812	ALA	CYS	engineered mutation	UNP P14735
H	819	ALA	CYS	engineered mutation	UNP P14735
H	904	SER	CYS	engineered mutation	UNP P14735
H	966	ASN	CYS	engineered mutation	UNP P14735
H	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	a	20	Total C N O S 154 95 23 32 4	0	0	0
2	b	5	Total C N O 37 23 6 8	0	0	0
2	c	20	Total C N O S 154 95 23 32 4	0	0	0
2	d	3	Total C N O 19 13 3 3	0	0	0
2	e	9	Total C N O 74 49 11 14	0	0	0
2	f	18	Total C N O S 134 80 21 29 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	g	15	121	76	18	25	2	0	0	0
			Total	C	N	O	S			
2	h	6	43	26	7	9	1	0	0	0

- Molecule 3 is a protein called IDE-bound Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	215	1632	1041	267	317	7	0	0	0
			Total	C	N	O	S			
3	K	207	1582	1009	259	307	7	0	0	0
			Total	C	N	O	S			
3	M	214	1623	1035	265	316	7	0	0	0
			Total	C	N	O	S			
3	O	209	1587	1011	261	309	6	0	0	0
			Total	C	N	O	S			
3	Q	201	1539	984	252	297	6	0	0	0
			Total	C	N	O	S			
3	S	215	1632	1041	267	317	7	0	0	0
			Total	C	N	O	S			
3	U	199	1518	970	248	293	7	0	0	0
			Total	C	N	O	S			
3	W	204	1546	986	252	302	6	0	0	0

- Molecule 4 is a protein called IDE-bound Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	198	1523	959	254	305	5	0	0	0
			Total	C	N	O	S			
4	L	176	1356	854	226	272	4	0	0	0
			Total	C	N	O	S			
4	N	200	1532	964	256	307	5	0	0	0
			Total	C	N	O	S			
4	P	184	1416	891	239	281	5	0	0	0
			Total	C	N	O	S			
4	R	177	1350	846	224	276	4	0	0	0
			Total	C	N	O	S			
4	T	198	1518	952	255	306	5	0	0	0
			Total	C	N	O	S			
4	V	186	1432	900	239	289	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	X	198	1515	949	255	307	4	0	0	0

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

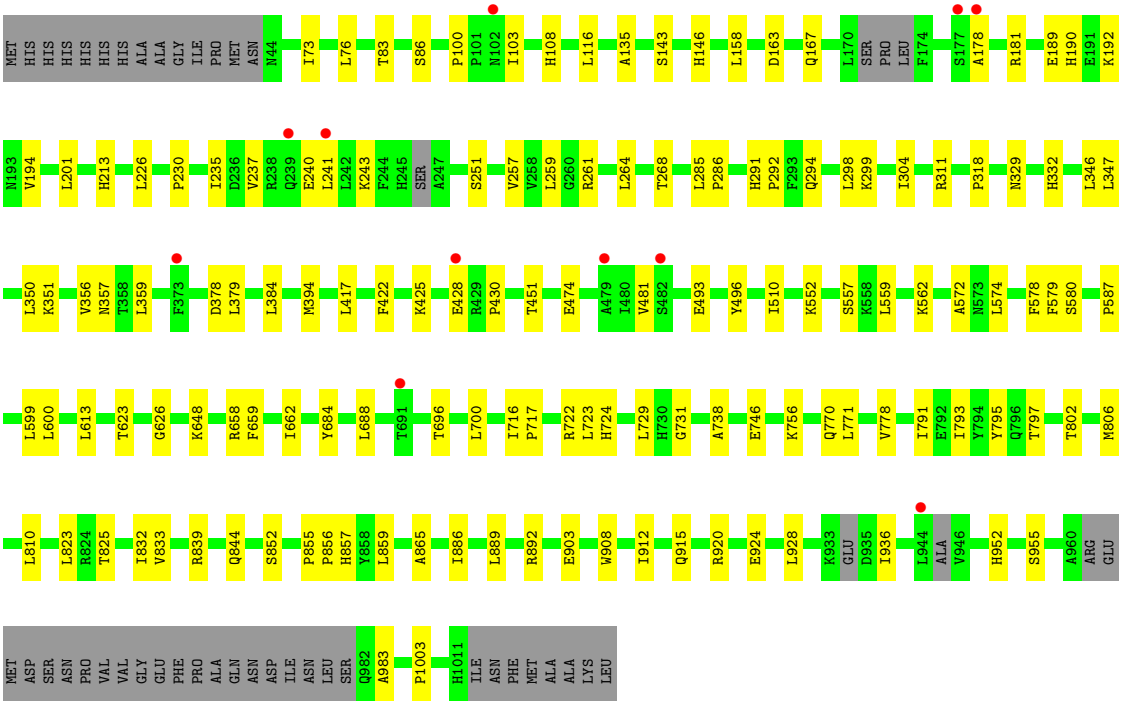
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0
5	E	1	1	1	0	0
5	F	1	1	1	0	0
5	G	1	1	1	0	0
5	H	1	1	1	0	0

3 Residue-property plots (i)

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

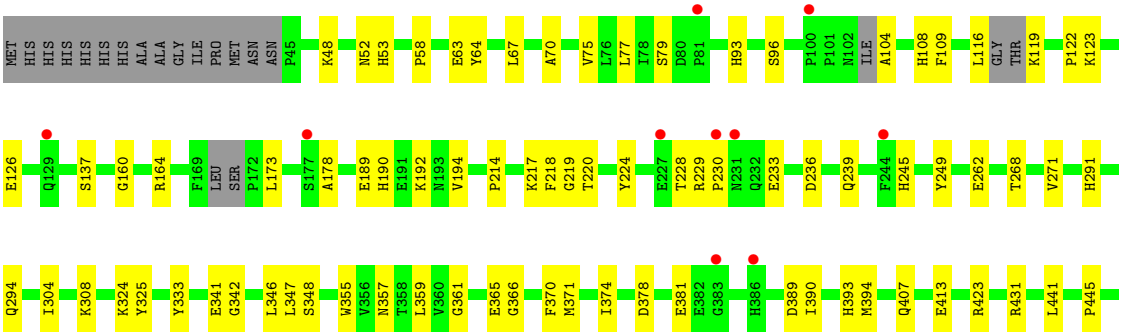
• Molecule 1: Insulin-degrading enzyme

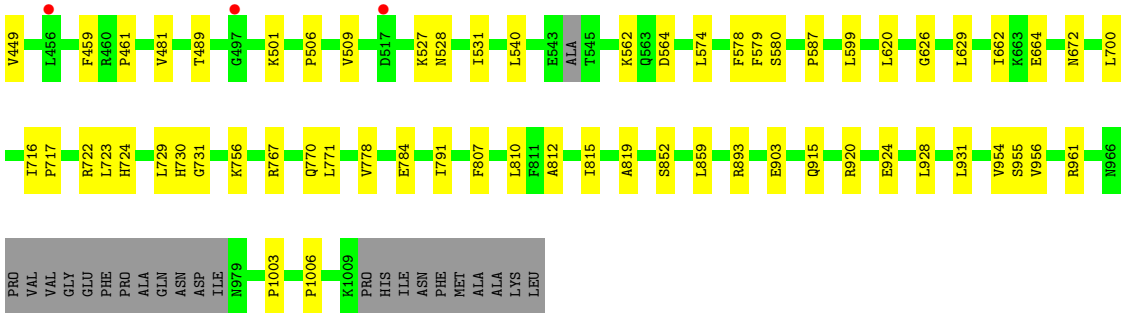
Chain A:



• Molecule 1: Insulin-degrading enzyme

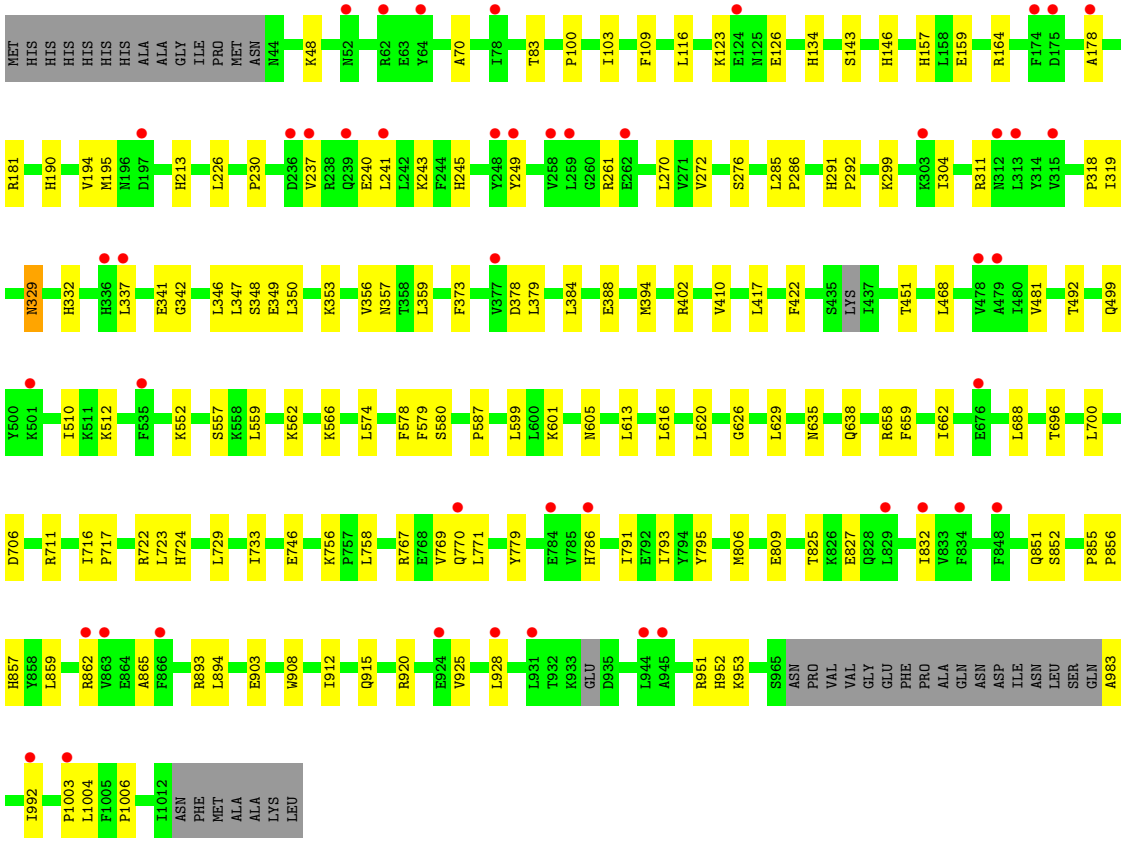
Chain B:





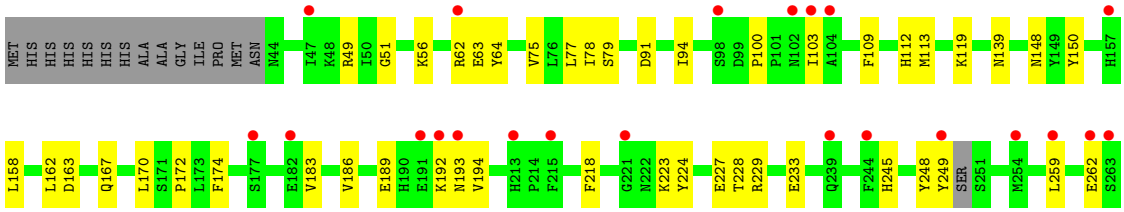
• Molecule 1: Insulin-degrading enzyme

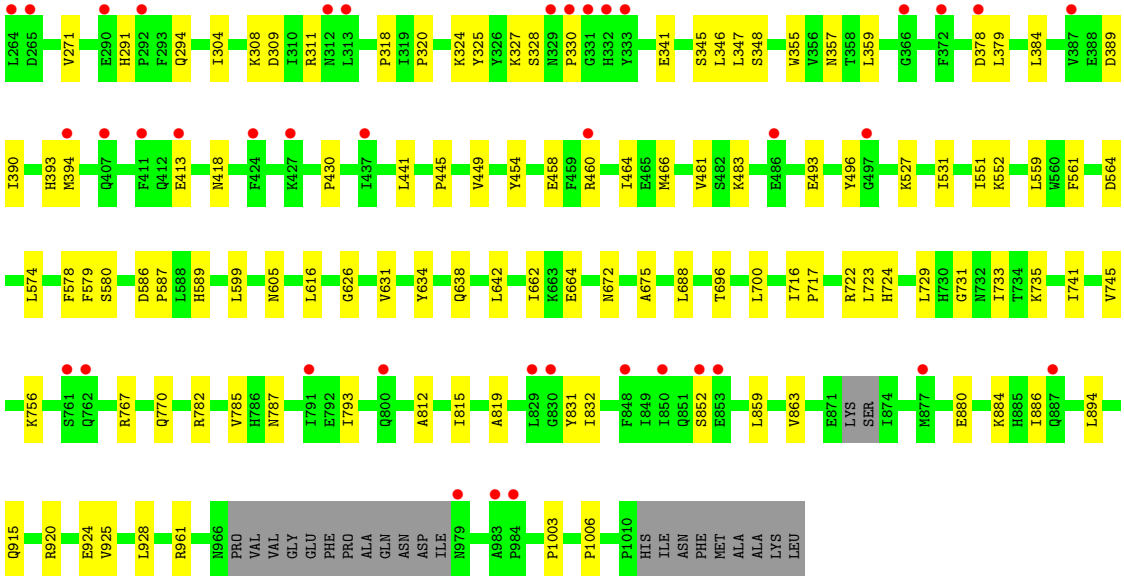
Chain C:



• Molecule 1: Insulin-degrading enzyme

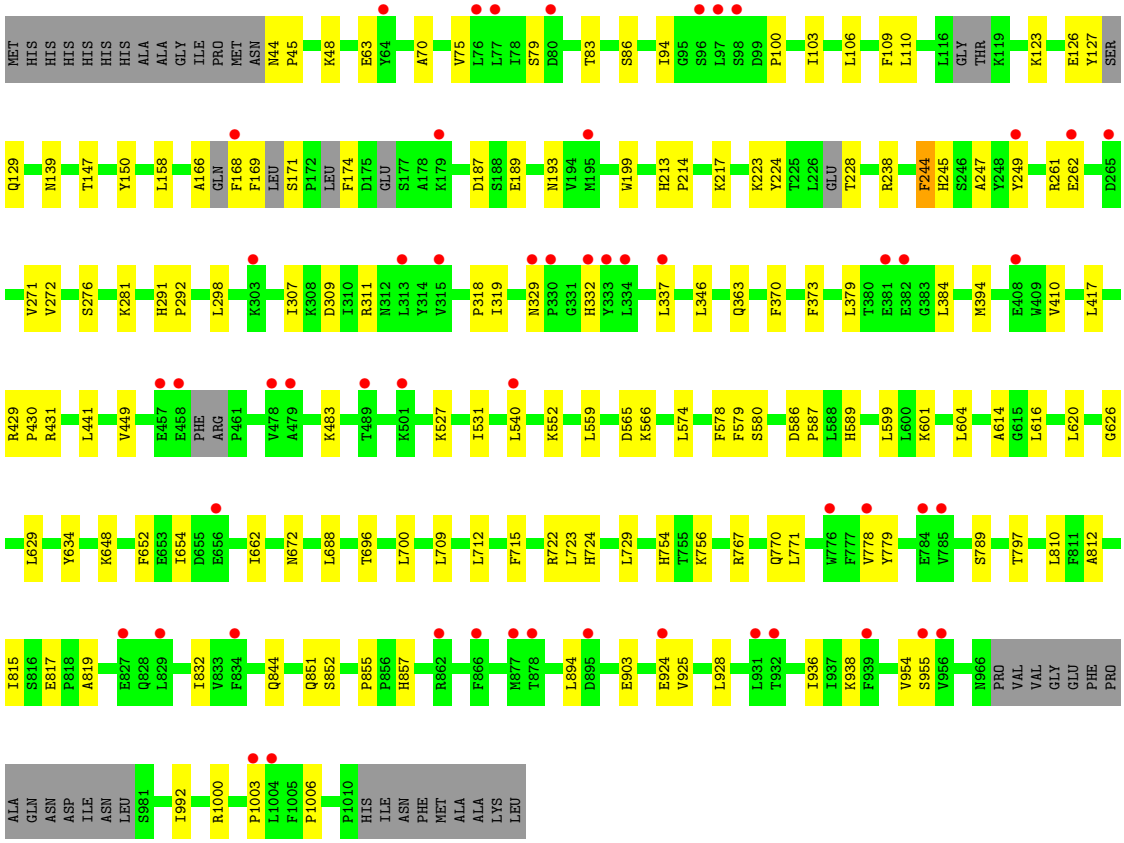
Chain D:





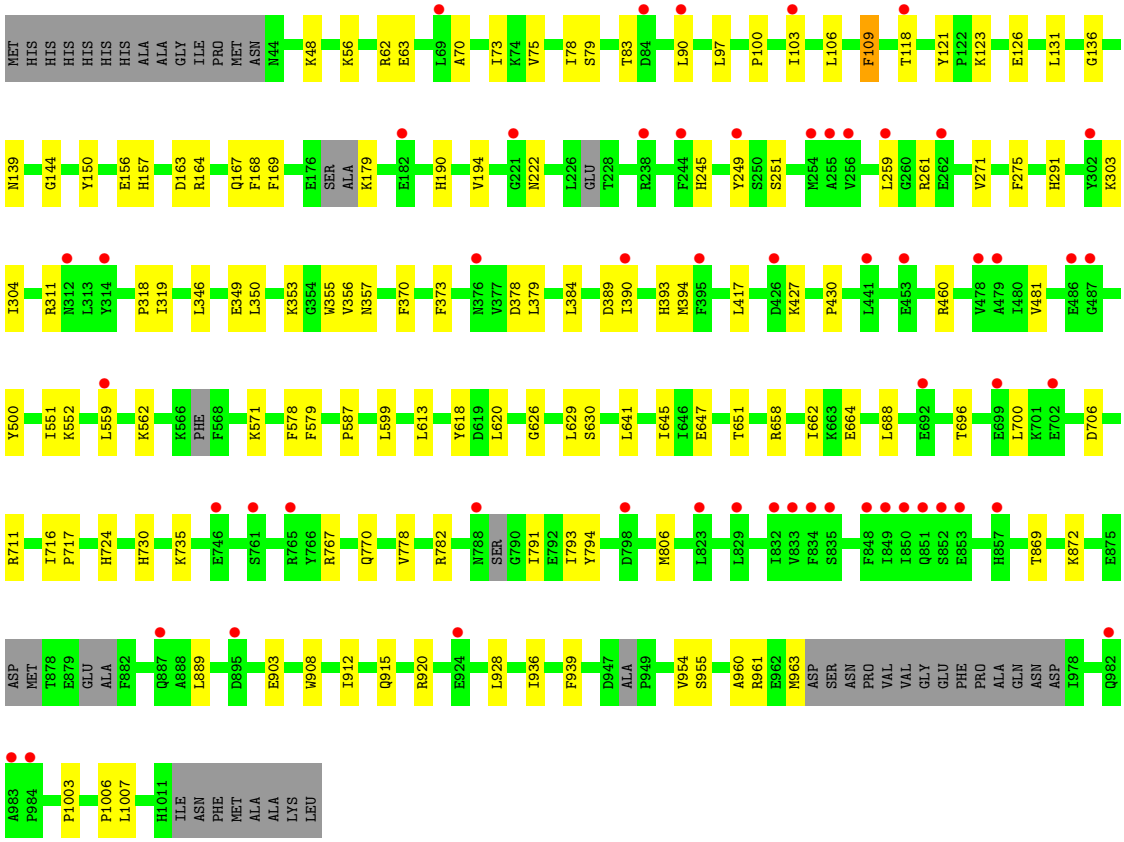
- Molecule 1: Insulin-degrading enzyme

Chain E:



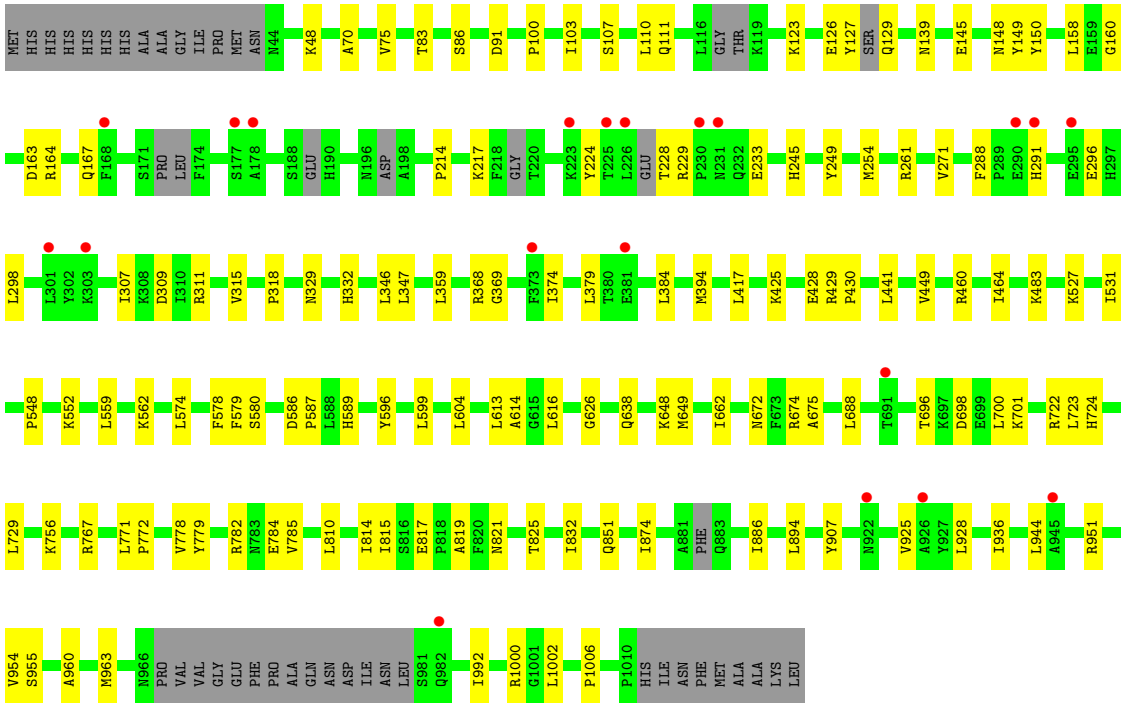
- Molecule 1: Insulin-degrading enzyme

Chain F:



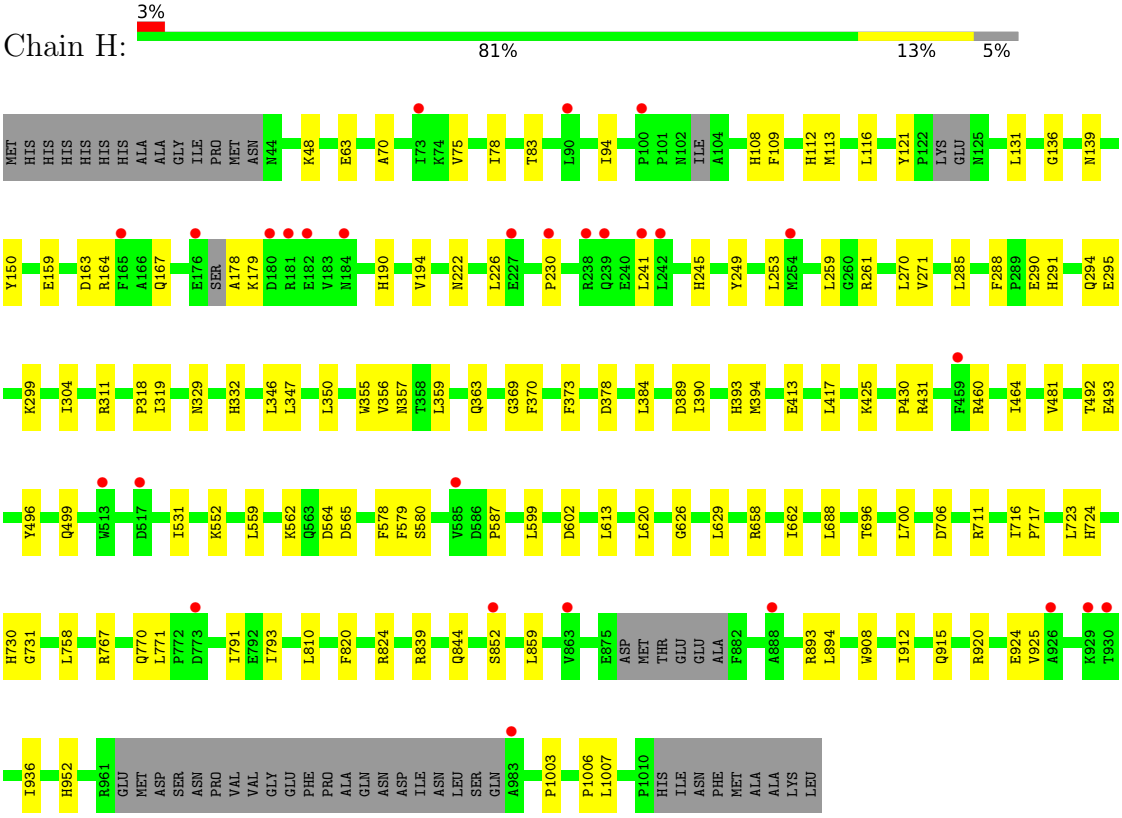
- Molecule 1: Insulin-degrading enzyme

Chain G:



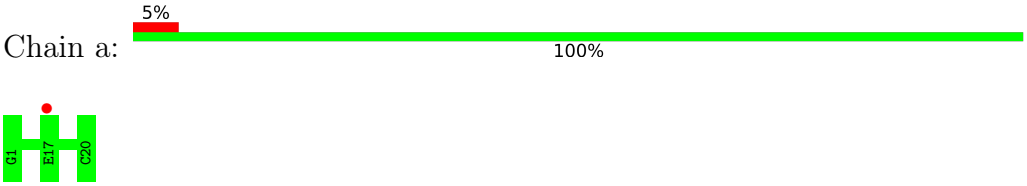
- Molecule 1: Insulin-degrading enzyme

Chain H:



- Molecule 2: Insulin

Chain a:

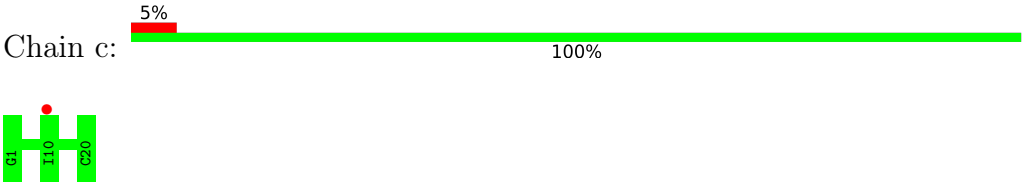


- Molecule 2: Insulin

Chain b:

- Molecule 2: Insulin

Chain c:

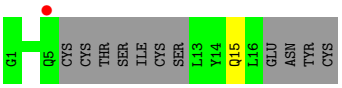


- Molecule 2: Insulin

Chain d:

• Molecule 2: Insulin

Chain e:

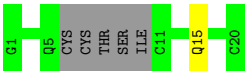


• Molecule 2: Insulin

Chain f:

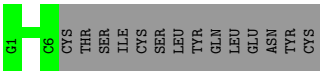
• Molecule 2: Insulin

Chain g:



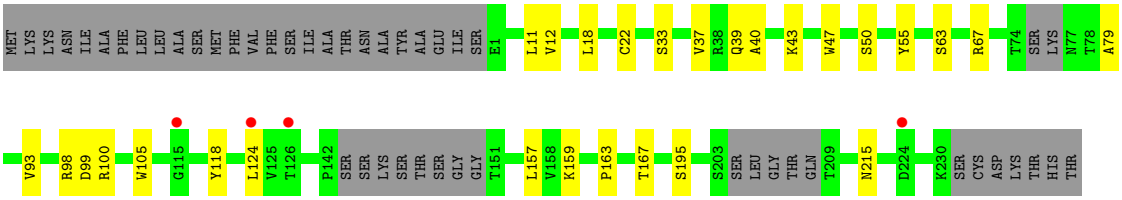
• Molecule 2: Insulin

Chain h:



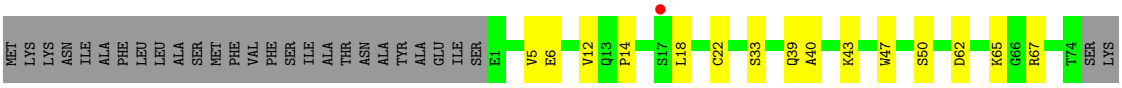
• Molecule 3: IDE-bound Fab heavy chain

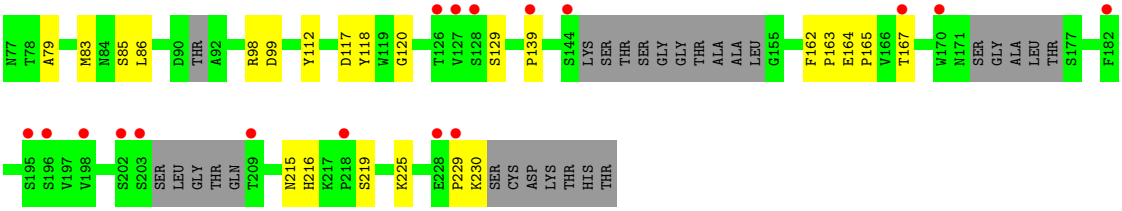
Chain I:



• Molecule 3: IDE-bound Fab heavy chain

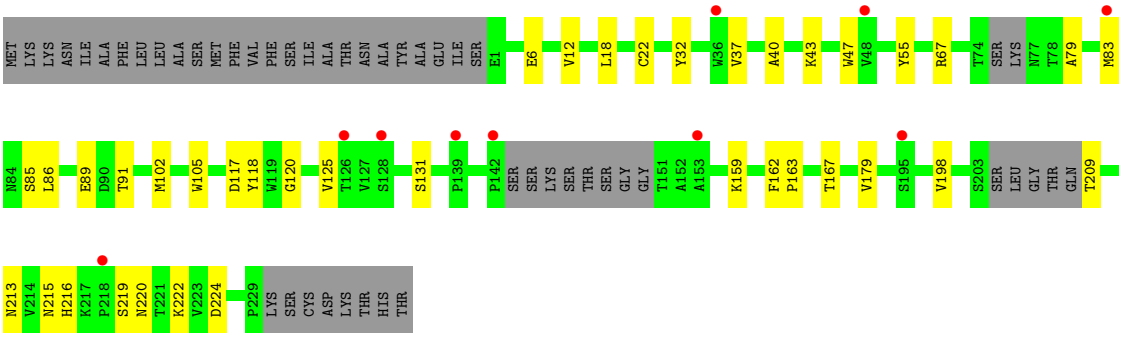
Chain K:





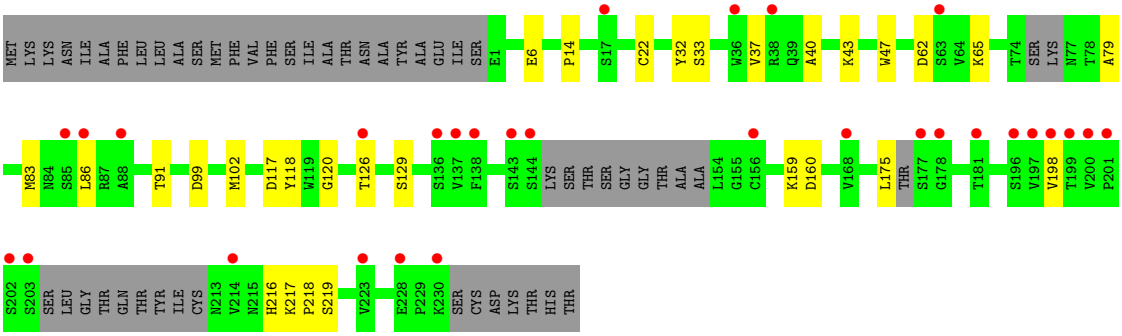
- Molecule 3: IDE-bound Fab heavy chain

Chain M:



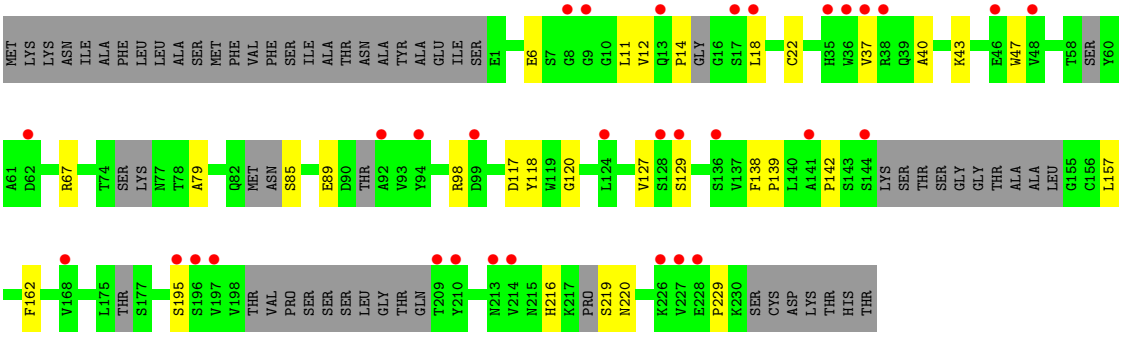
- Molecule 3: IDE-bound Fab heavy chain

Chain O:



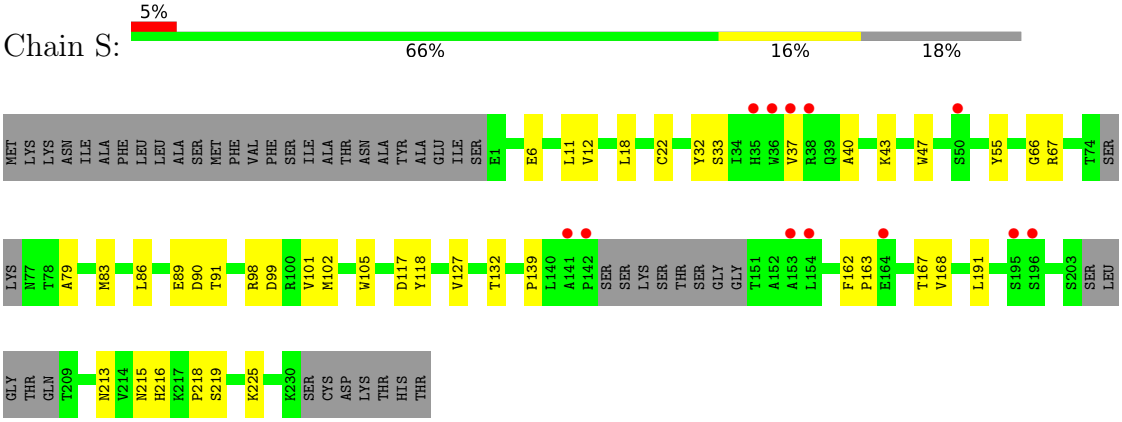
- Molecule 3: IDE-bound Fab heavy chain

Chain Q:



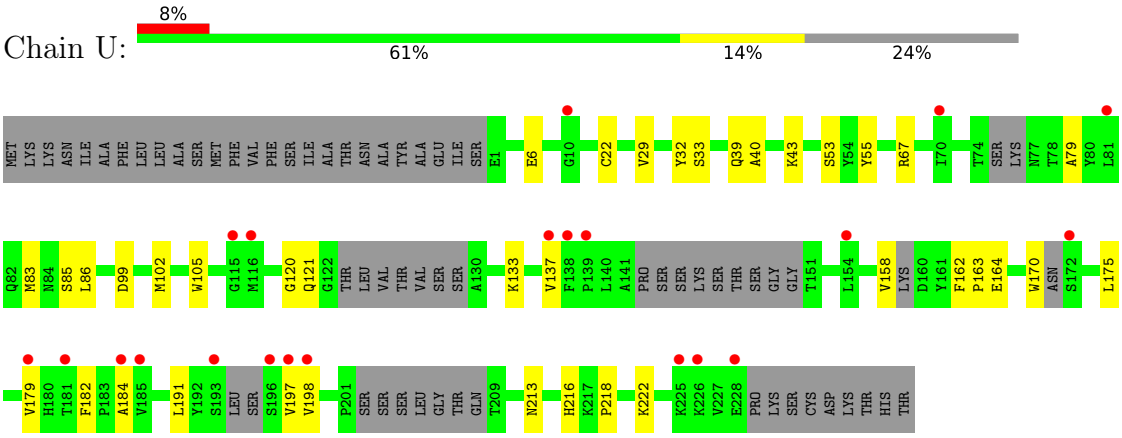
• Molecule 3: IDE-bound Fab heavy chain

Chain S:



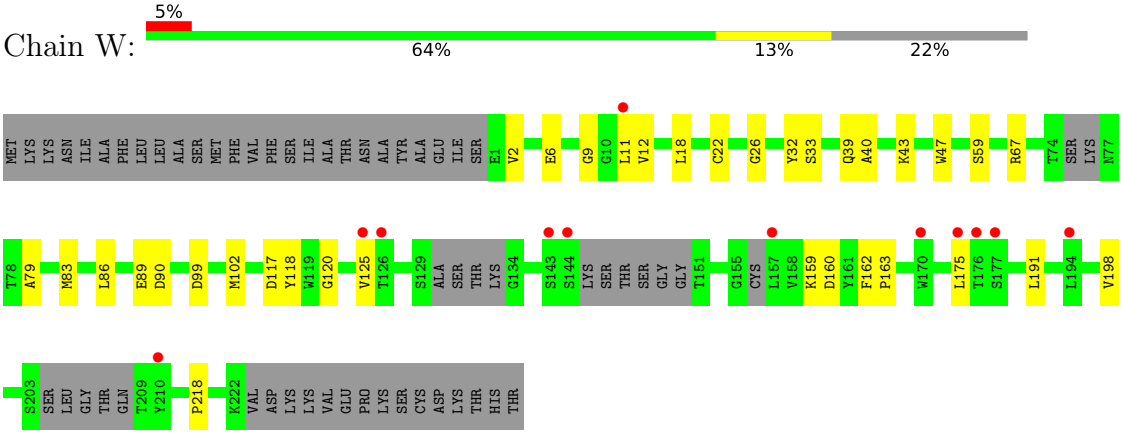
• Molecule 3: IDE-bound Fab heavy chain

Chain U:



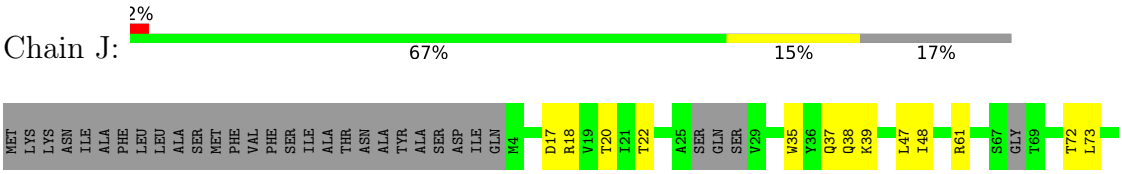
• Molecule 3: IDE-bound Fab heavy chain

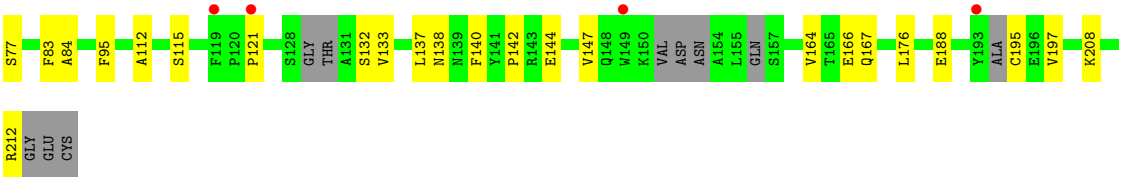
Chain W:



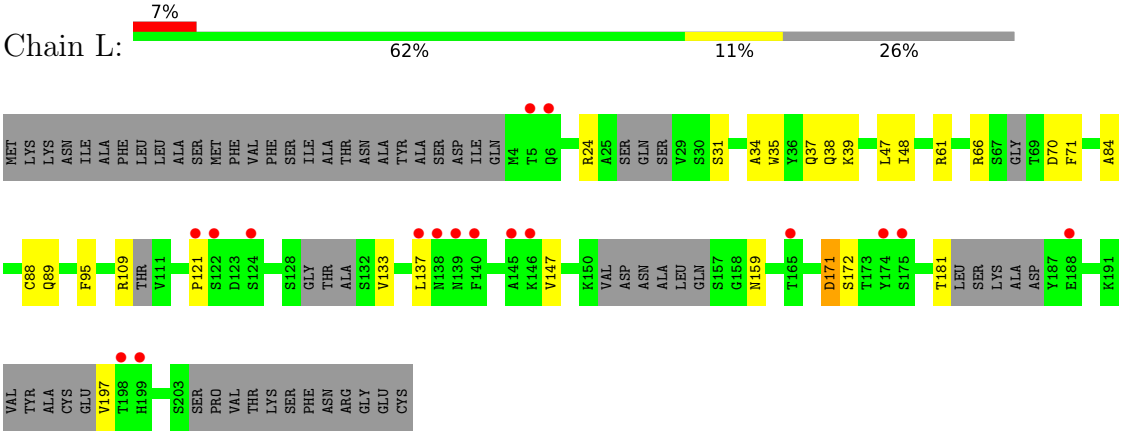
• Molecule 4: IDE-bound Fab light chain

Chain J:

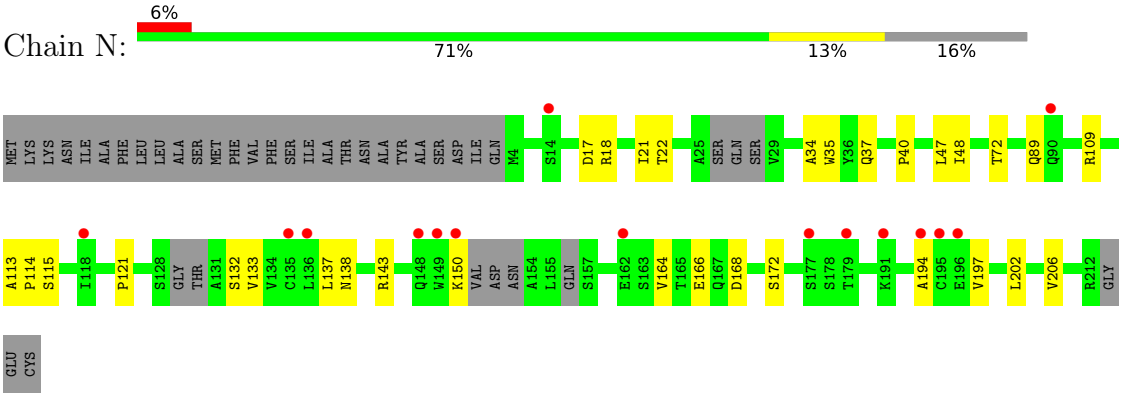




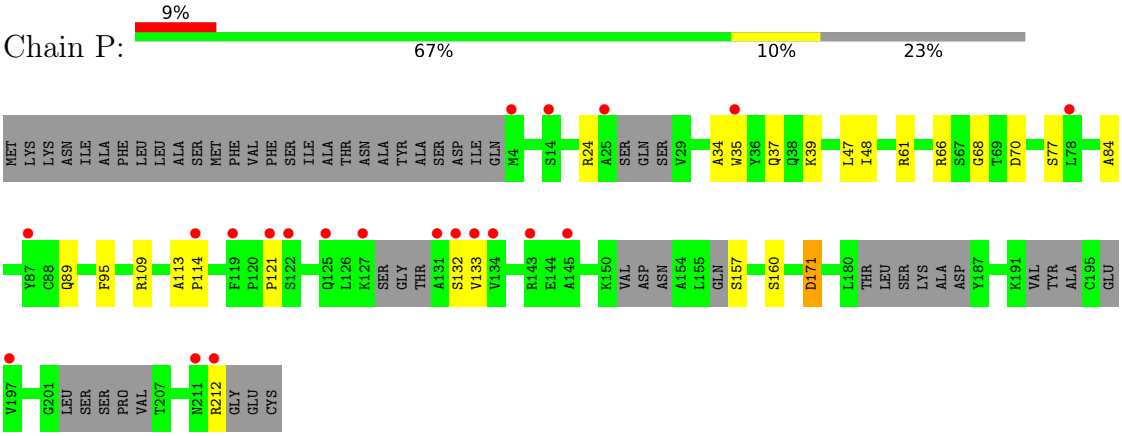
• Molecule 4: IDE-bound Fab light chain



• Molecule 4: IDE-bound Fab light chain

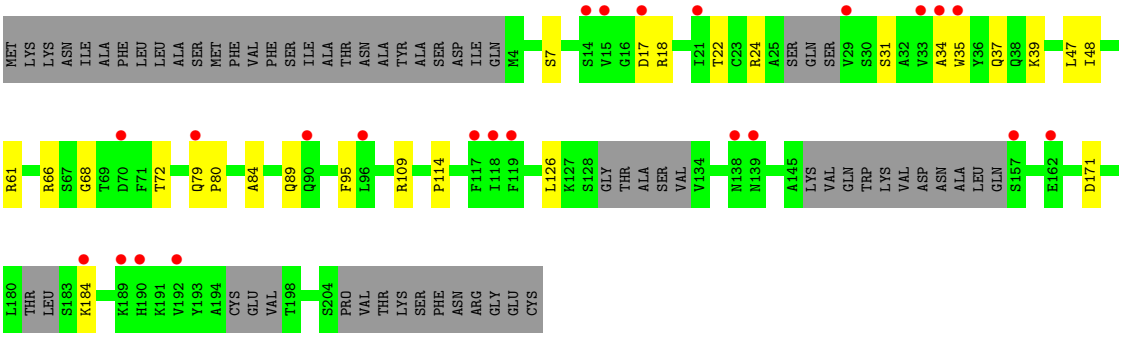


• Molecule 4: IDE-bound Fab light chain



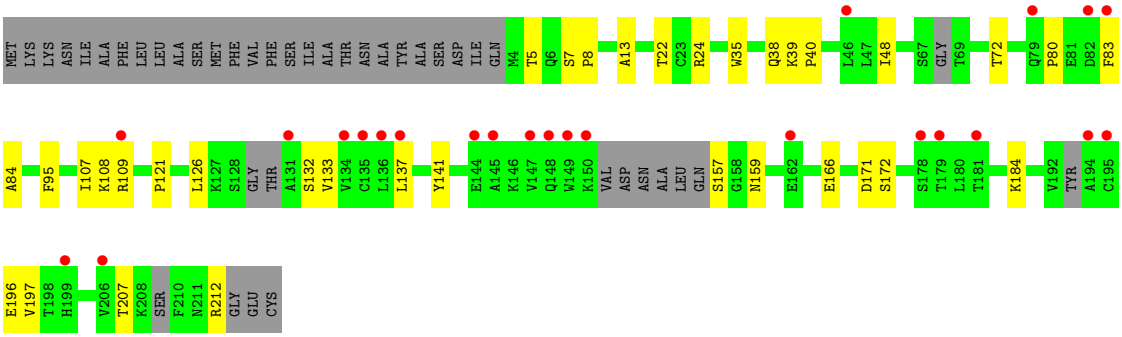
• Molecule 4: IDE-bound Fab light chain

Chain R:



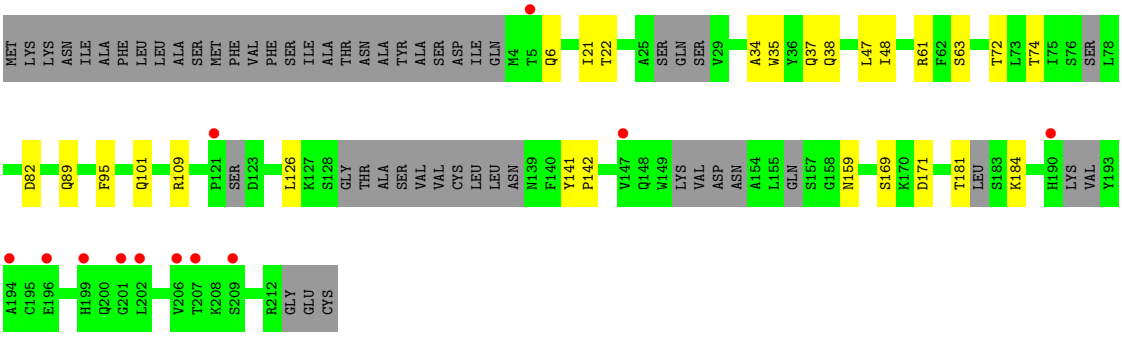
- Molecule 4: IDE-bound Fab light chain

Chain T:



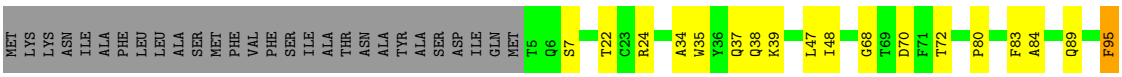
- Molecule 4: IDE-bound Fab light chain

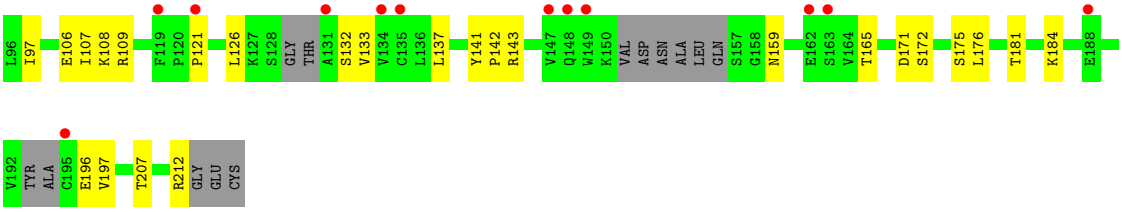
Chain V:



- Molecule 4: IDE-bound Fab light chain

Chain X:




L96
I97
E106
I107
K108
R109
F119
P120
P121
L126
K127
S128
GLY
THR
A131
S132
V133
V134
C135
L136
L137
Y141
P142
R143
V147
Q148
W149
K150
VAL
ASP
ASN
ALA
LEU
GLN
S157
G158
N159
E162
S163
V164
T165
D171
S172
S175
L176
T181
K184
E188
V192
TYR
ALA
C195
E196
V197
T207
R212
GLY
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.59Å 138.19Å 376.51Å 90.00° 99.36° 90.00°	Depositor
Resolution (Å)	49.54 – 3.95 49.54 – 3.93	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.54-3.95) 93.6 (49.54-3.93)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.243 , 0.291 0.252 , 0.299	Depositor DCC
R_{free} test set	1990 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.379 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	86906	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1507e-03.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.24	0/7898	0.39	0/10677
1	B	0.25	0/7947	0.40	0/10739
1	C	0.25	0/7965	0.39	0/10772
1	D	0.25	0/7982	0.39	0/10795
1	E	0.24	0/7898	0.40	0/10670
1	F	0.24	0/7922	0.40	0/10704
1	G	0.24	0/7906	0.40	0/10680
1	H	0.24	0/7853	0.39	0/10618
2	a	0.26	0/155	0.59	0/209
2	b	0.24	0/36	0.44	0/47
2	c	0.32	0/155	0.62	0/209
2	d	0.19	0/18	0.39	0/23
2	e	0.23	0/73	0.53	0/96
2	f	0.26	0/133	0.59	0/177
2	g	0.25	0/121	0.49	0/161
2	h	0.25	0/42	0.50	0/55
3	I	0.24	0/1675	0.44	0/2282
3	K	0.24	0/1623	0.42	0/2206
3	M	0.24	0/1666	0.43	0/2271
3	O	0.24	0/1628	0.42	0/2214
3	Q	0.24	0/1574	0.42	0/2131
3	S	0.24	0/1675	0.43	0/2282
3	U	0.24	0/1555	0.44	0/2111
3	W	0.25	0/1586	0.44	0/2160
4	J	0.24	0/1551	0.41	0/2096
4	L	0.25	0/1380	0.45	0/1862
4	N	0.24	0/1562	0.42	0/2114
4	P	0.24	0/1440	0.42	0/1940
4	R	0.24	0/1375	0.42	0/1858
4	T	0.24	0/1546	0.44	0/2090
4	V	0.24	0/1458	0.42	0/1967
4	X	0.24	0/1545	0.43	0/2092

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.24	0/88943	0.41	0/120308

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	7708	0	7652	81	0
1	B	7758	0	7696	83	0
1	C	7772	0	7714	84	0
1	D	7790	0	7728	95	0
1	E	7713	0	7650	86	1
1	F	7735	0	7691	76	0
1	G	7722	0	7667	81	0
1	H	7663	0	7617	77	0
2	a	154	0	145	0	0
2	b	37	0	39	0	0
2	c	154	0	145	0	0
2	d	19	0	25	0	0
2	e	74	0	77	0	0
2	f	134	0	124	0	0
2	g	121	0	113	0	0
2	h	43	0	44	0	0
3	I	1632	0	1575	18	0
3	K	1582	0	1517	22	0
3	M	1623	0	1562	24	0
3	O	1587	0	1530	15	0
3	Q	1539	0	1474	19	0
3	S	1632	0	1575	29	0
3	U	1518	0	1446	24	0
3	W	1546	0	1476	21	0
4	J	1523	0	1495	20	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1356	0	1327	17	0
4	N	1532	0	1505	19	0
4	P	1416	0	1385	14	0
4	R	1350	0	1311	14	0
4	T	1518	0	1489	20	0
4	V	1432	0	1386	14	0
4	X	1515	0	1485	27	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	86906	0	85665	958	1

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.

The worst 5 of 958 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)
4:T:121:PRO:HB3	4:T:132:SER:H	1.51	0.76
4:R:34:ALA:HB3	4:R:89:GLN:HB3	1.68	0.75
3:I:22:CYS:HB3	3:I:79:ALA:HB3	1.69	0.74
4:L:34:ALA:HB3	4:L:89:GLN:HB3	1.70	0.73
1:F:123:LYS:HB3	1:F:126:GLU:HB2	1.70	0.73

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:LYS:NZ	4:J:188:GLU:O[1_654]	2.08	0.12

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	929/990 (94%)	919 (99%)	10 (1%)	0	100	100
1	B	935/990 (94%)	926 (99%)	9 (1%)	0	100	100
1	C	942/990 (95%)	932 (99%)	10 (1%)	0	100	100
1	D	944/990 (95%)	932 (99%)	12 (1%)	0	100	100
1	E	923/990 (93%)	906 (98%)	17 (2%)	0	100	100
1	F	926/990 (94%)	914 (99%)	12 (1%)	0	100	100
1	G	923/990 (93%)	911 (99%)	12 (1%)	0	100	100
1	H	924/990 (93%)	912 (99%)	12 (1%)	0	100	100
2	a	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
2	b	3/20 (15%)	2 (67%)	1 (33%)	0	100	100
2	c	18/20 (90%)	18 (100%)	0	0	100	100
2	d	1/20 (5%)	0	1 (100%)	0	100	100
2	e	5/20 (25%)	5 (100%)	0	0	100	100
2	f	14/20 (70%)	14 (100%)	0	0	100	100
2	g	11/20 (55%)	10 (91%)	1 (9%)	0	100	100
2	h	4/20 (20%)	3 (75%)	1 (25%)	0	100	100
3	I	207/263 (79%)	200 (97%)	7 (3%)	0	100	100
3	K	195/263 (74%)	189 (97%)	6 (3%)	0	100	100
3	M	206/263 (78%)	195 (95%)	11 (5%)	0	100	100
3	O	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
3	Q	181/263 (69%)	175 (97%)	6 (3%)	0	100	100
3	S	207/263 (79%)	201 (97%)	6 (3%)	0	100	100
3	U	183/263 (70%)	174 (95%)	9 (5%)	0	100	100
3	W	192/263 (73%)	186 (97%)	6 (3%)	0	100	100
4	J	184/239 (77%)	175 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	160/239 (67%)	156 (98%)	4 (2%)	0	100	100
4	N	190/239 (80%)	183 (96%)	7 (4%)	0	100	100
4	P	167/239 (70%)	162 (97%)	5 (3%)	0	100	100
4	R	165/239 (69%)	160 (97%)	5 (3%)	0	100	100
4	T	186/239 (78%)	179 (96%)	7 (4%)	0	100	100
4	V	168/239 (70%)	167 (99%)	1 (1%)	0	100	100
4	X	190/239 (80%)	183 (96%)	7 (4%)	0	100	100
All	All	10500/12096 (87%)	10299 (98%)	201 (2%)	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	838/879 (95%)	838 (100%)	0	100	100
1	B	845/879 (96%)	844 (100%)	1 (0%)	93	96
1	C	846/879 (96%)	844 (100%)	2 (0%)	93	96
1	D	848/879 (96%)	846 (100%)	2 (0%)	93	96
1	E	840/879 (96%)	838 (100%)	2 (0%)	93	96
1	F	843/879 (96%)	842 (100%)	1 (0%)	93	96
1	G	841/879 (96%)	841 (100%)	0	100	100
1	H	833/879 (95%)	833 (100%)	0	100	100
2	a	19/19 (100%)	19 (100%)	0	100	100
2	b	4/19 (21%)	4 (100%)	0	100	100
2	c	19/19 (100%)	19 (100%)	0	100	100
2	d	2/19 (10%)	2 (100%)	0	100	100
2	e	8/19 (42%)	7 (88%)	1 (12%)	4	23
2	f	17/19 (90%)	17 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	g	14/19 (74%)	13 (93%)	1 (7%)	14	42
2	h	5/19 (26%)	5 (100%)	0	100	100
3	I	180/220 (82%)	180 (100%)	0	100	100
3	K	176/220 (80%)	176 (100%)	0	100	100
3	M	179/220 (81%)	179 (100%)	0	100	100
3	O	176/220 (80%)	176 (100%)	0	100	100
3	Q	169/220 (77%)	169 (100%)	0	100	100
3	S	180/220 (82%)	180 (100%)	0	100	100
3	U	164/220 (74%)	164 (100%)	0	100	100
3	W	170/220 (77%)	170 (100%)	0	100	100
4	J	178/210 (85%)	177 (99%)	1 (1%)	86	91
4	L	159/210 (76%)	157 (99%)	2 (1%)	69	81
4	N	178/210 (85%)	178 (100%)	0	100	100
4	P	164/210 (78%)	162 (99%)	2 (1%)	71	83
4	R	157/210 (75%)	155 (99%)	2 (1%)	69	81
4	T	178/210 (85%)	177 (99%)	1 (1%)	86	91
4	V	165/210 (79%)	164 (99%)	1 (1%)	86	91
4	X	178/210 (85%)	177 (99%)	1 (1%)	86	91
All	All	9573/10624 (90%)	9553 (100%)	20 (0%)	93	96

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P	171	ASP
4	T	95	PHE
4	X	95	PHE
4	V	95	PHE
1	E	244	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	e	15	GLN
2	h	5	GLN
4	V	6	GLN

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Mol	Chain	Res	Type
1	H	184	ASN
1	H	332	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	941/990 (95%)	-0.09	11 (1%)	79	70	53, 77, 99, 113	0
1	B	947/990 (95%)	-0.04	13 (1%)	75	66	54, 77, 97, 116	0
1	C	950/990 (95%)	0.21	47 (4%)	29	25	100, 118, 135, 148	0
1	D	952/990 (96%)	0.35	62 (6%)	18	15	116, 136, 150, 161	0
1	E	943/990 (95%)	0.35	53 (5%)	24	21	106, 133, 147, 160	0
1	F	944/990 (95%)	0.29	56 (5%)	22	18	105, 128, 146, 158	0
1	G	943/990 (95%)	0.08	20 (2%)	63	54	66, 88, 106, 131	0
1	H	936/990 (94%)	0.08	28 (2%)	50	39	65, 91, 115, 135	0
2	a	20/20 (100%)	0.13	1 (5%)	28	25	70, 108, 127, 129	0
2	b	5/20 (25%)	0.19	1 (20%)	1	1	74, 83, 103, 114	0
2	c	20/20 (100%)	0.28	1 (5%)	28	25	106, 124, 132, 136	0
2	d	3/20 (15%)	0.03	0	100	100	118, 118, 121, 121	0
2	e	9/20 (45%)	0.60	1 (11%)	5	5	117, 123, 128, 132	0
2	f	18/20 (90%)	0.11	0	100	100	111, 128, 136, 138	0
2	g	15/20 (75%)	0.26	0	100	100	88, 105, 122, 130	0
2	h	6/20 (30%)	0.19	0	100	100	79, 102, 126, 126	0
3	I	215/263 (81%)	0.20	4 (1%)	66	58	73, 103, 126, 140	0
3	K	207/263 (78%)	0.39	18 (8%)	10	9	74, 106, 136, 155	0
3	M	214/263 (81%)	0.30	10 (4%)	31	26	107, 123, 135, 138	0
3	O	209/263 (79%)	0.70	30 (14%)	2	3	128, 153, 170, 180	0
3	Q	201/263 (76%)	0.78	32 (15%)	1	2	140, 156, 170, 177	0
3	S	215/263 (81%)	0.30	12 (5%)	24	21	99, 124, 144, 151	0
3	U	199/263 (75%)	0.49	21 (10%)	6	6	77, 115, 146, 151	0
3	W	204/263 (77%)	0.25	12 (5%)	22	18	82, 106, 138, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
4	J	198/239 (82%)	0.06	4 (2%)	65	56	68, 102, 118, 130	0
4	L	176/239 (73%)	0.40	17 (9%)	7	7	72, 107, 130, 137	0
4	N	200/239 (83%)	0.40	15 (7%)	14	12	104, 125, 135, 145	0
4	P	184/239 (76%)	0.66	21 (11%)	5	5	131, 151, 172, 178	0
4	R	177/239 (74%)	0.75	23 (12%)	3	4	137, 154, 168, 177	0
4	T	198/239 (82%)	0.57	24 (12%)	4	5	108, 136, 154, 160	0
4	V	186/239 (77%)	0.43	12 (6%)	18	15	77, 107, 142, 155	0
4	X	198/239 (82%)	0.33	12 (6%)	21	17	83, 117, 135, 144	0
All	All	10833/12096 (89%)	0.24	561 (5%)	27	24	53, 116, 152, 180	0

The worst 5 of 561 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	852	SER	9.0
4	X	148	GLN	8.3
4	R	79	GLN	5.8
4	X	149	TRP	5.8
3	W	144	SER	5.7

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
5	ZN	F	1101	1/1	0.90	0.11	134,134,134,134	0
5	ZN	D	2001	1/1	0.91	0.10	139,139,139,139	0

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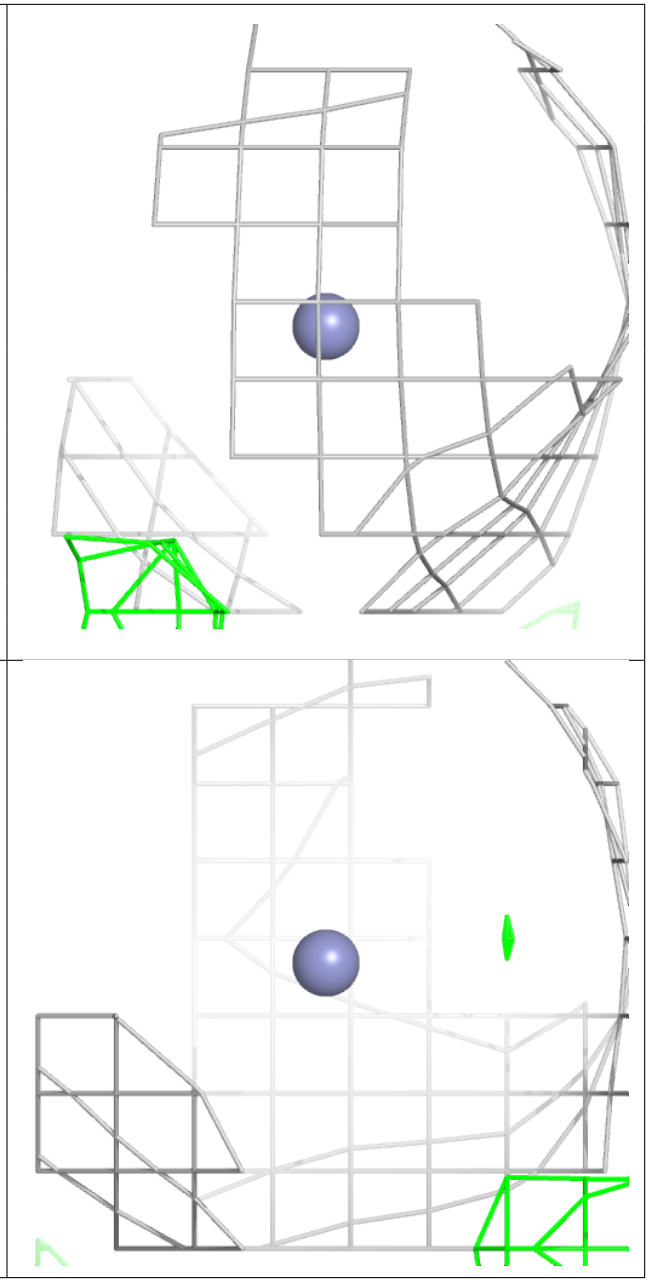
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	C	1101	1/1	0.94	0.12	110,110,110,110	0
5	ZN	E	2001	1/1	0.97	0.04	126,126,126,126	0
5	ZN	H	1101	1/1	0.97	0.15	97,97,97,97	0
5	ZN	B	2001	1/1	0.98	0.16	63,63,63,63	0
5	ZN	A	1101	1/1	0.98	0.17	65,65,65,65	0
5	ZN	G	2001	1/1	0.99	0.17	64,64,64,64	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.

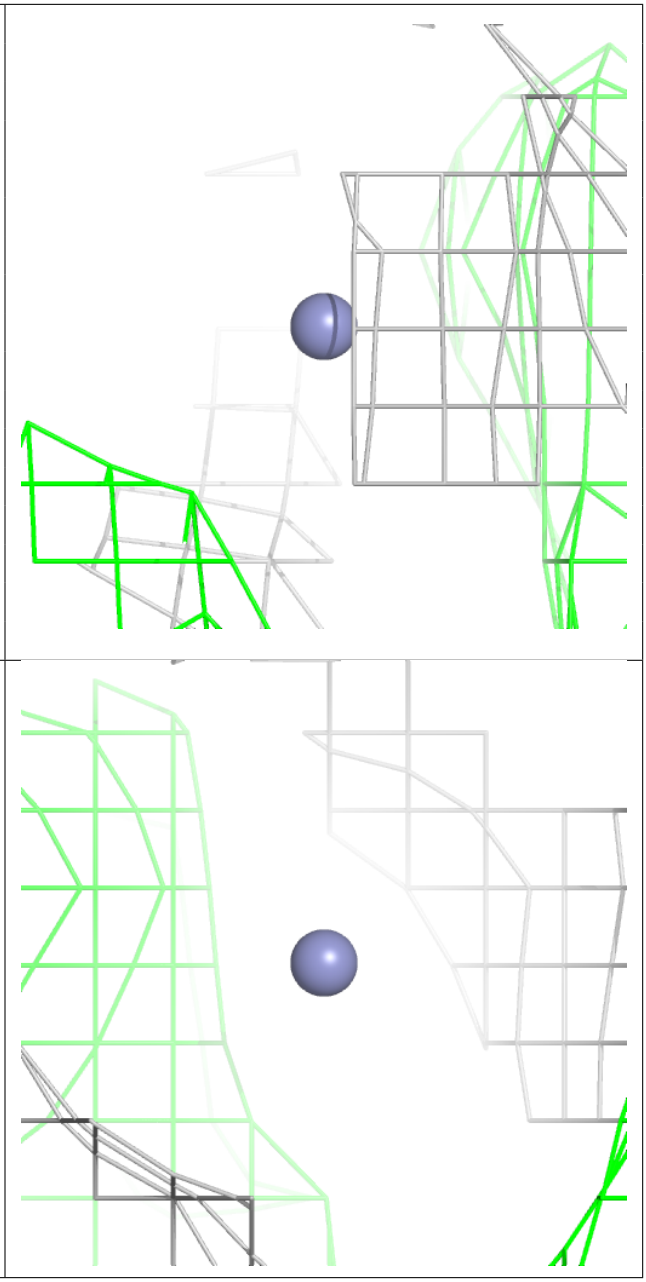
Electron density around ZN F 1101:

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



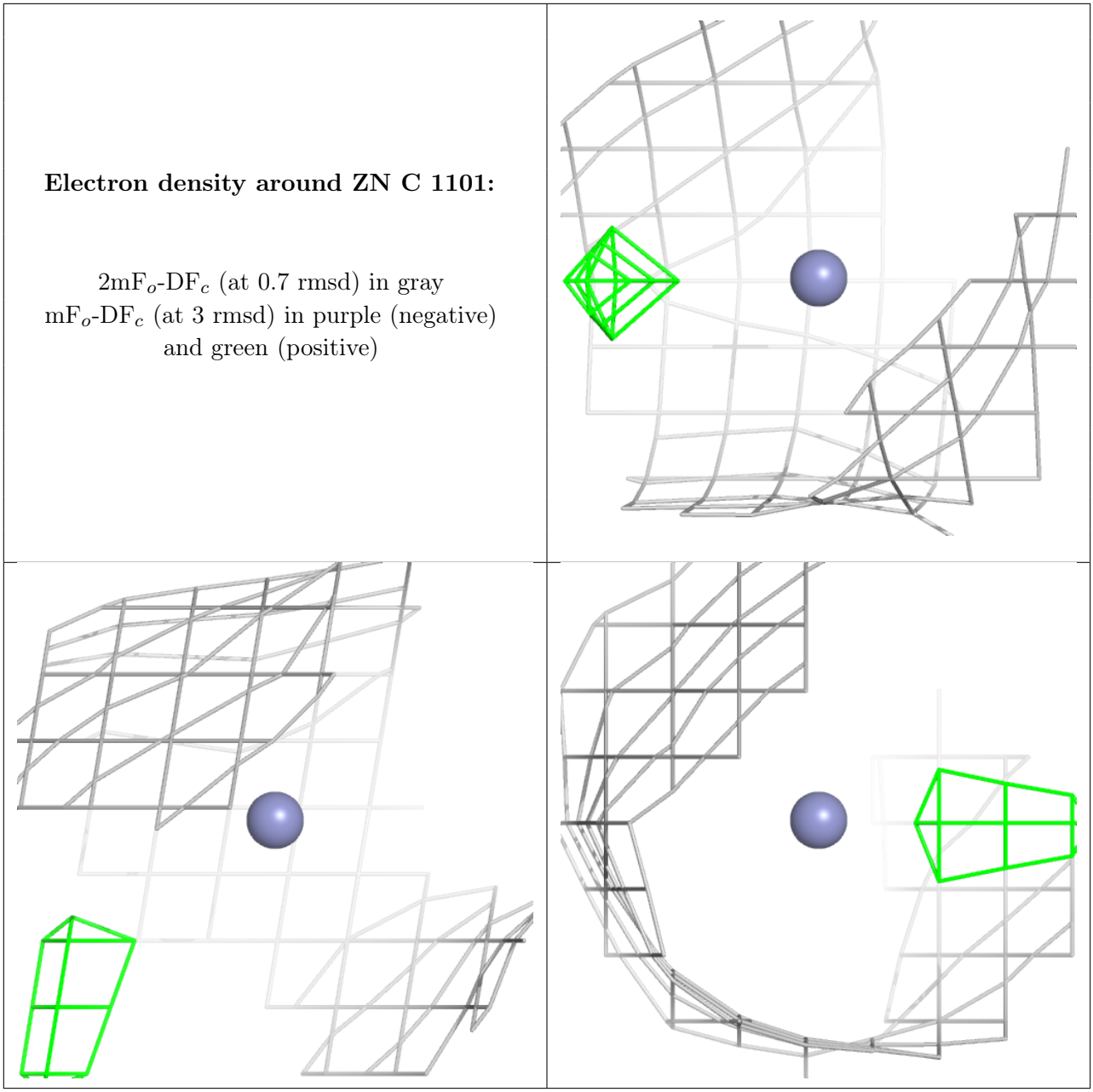
Electron density around ZN D 2001:

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



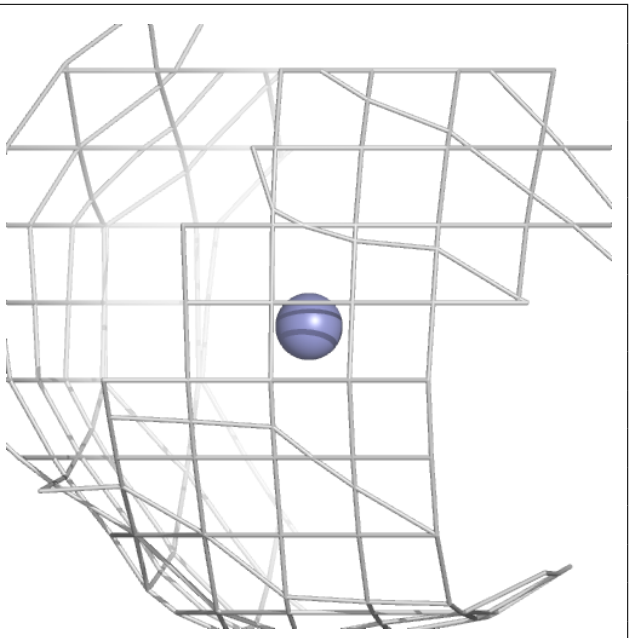
Electron density around ZN C 1101:

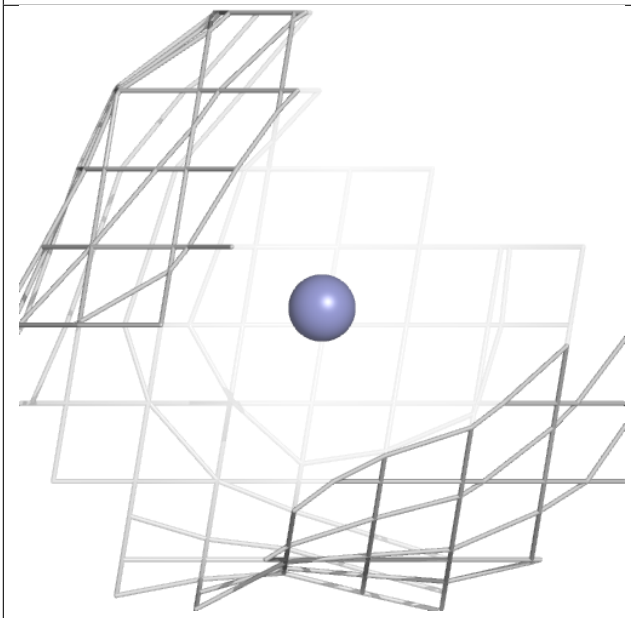
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

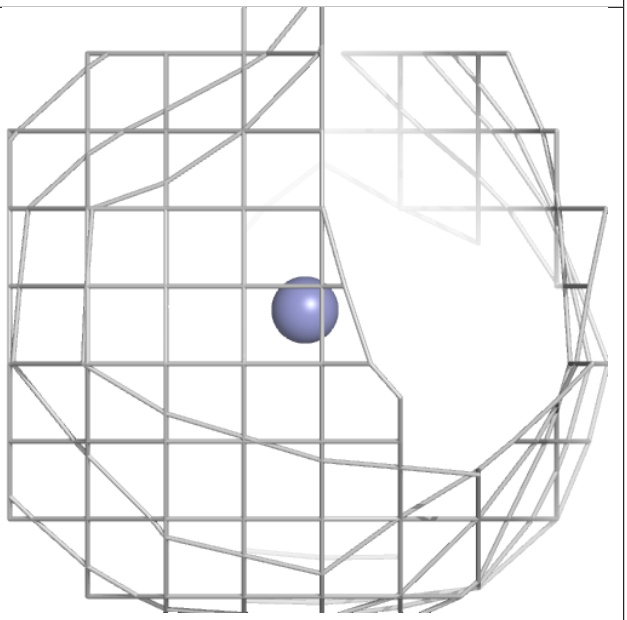


Electron density around ZN E 2001:

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

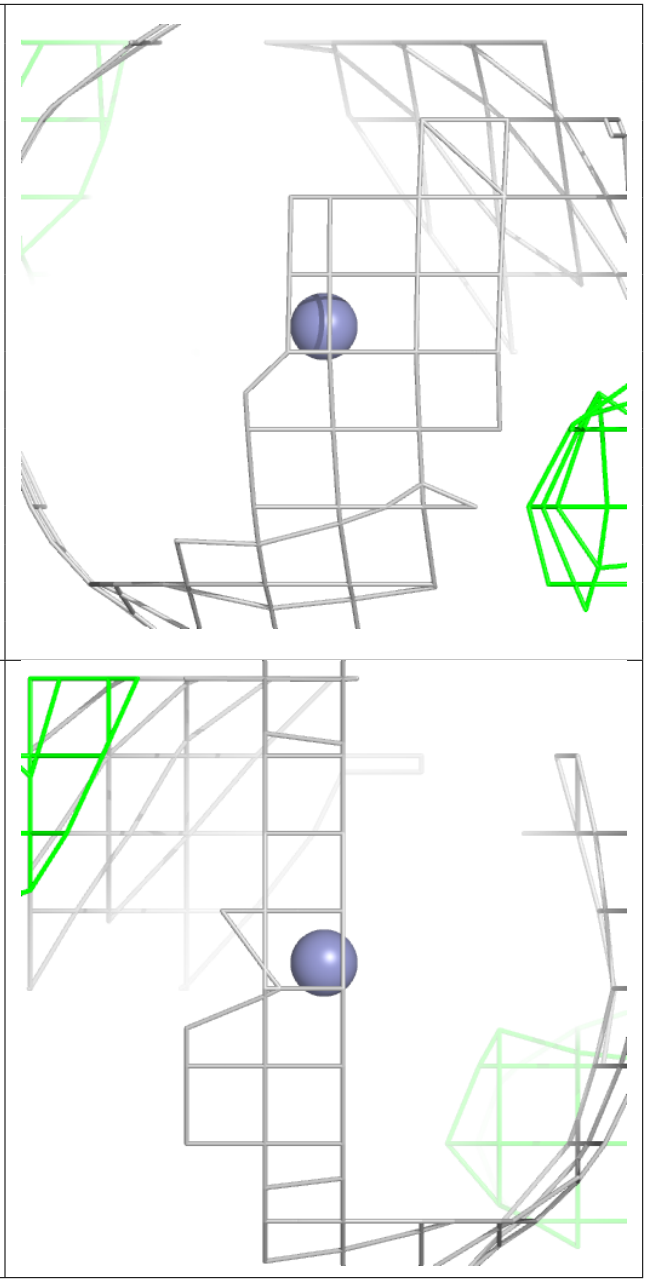






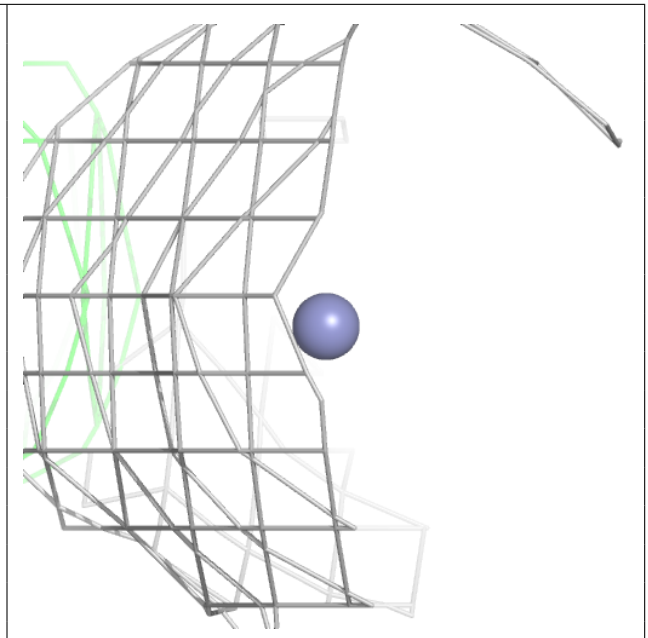
Electron density around ZN H 1101:

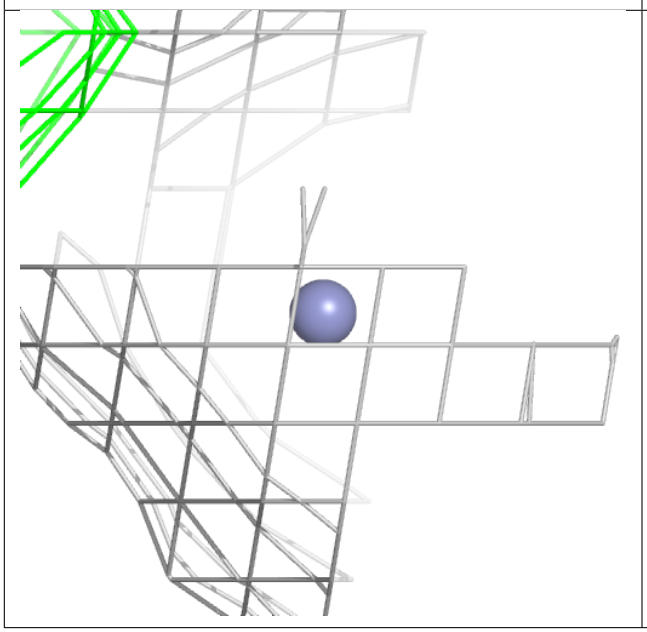
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

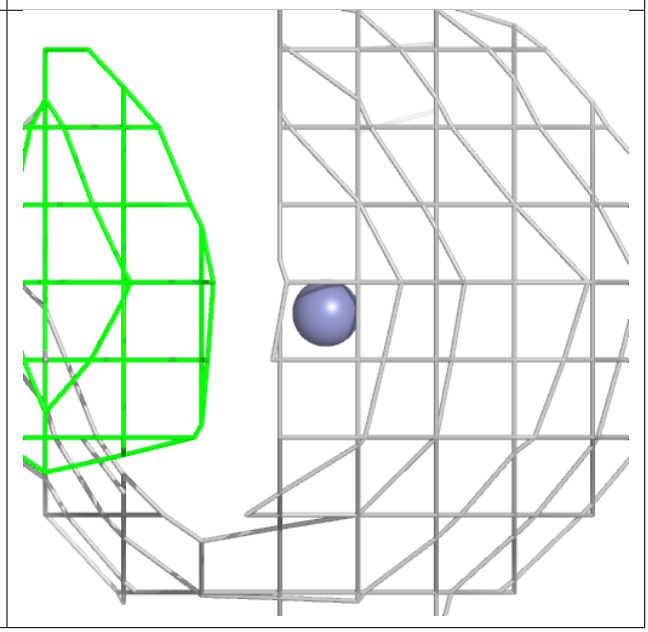


Electron density around ZN B 2001:

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

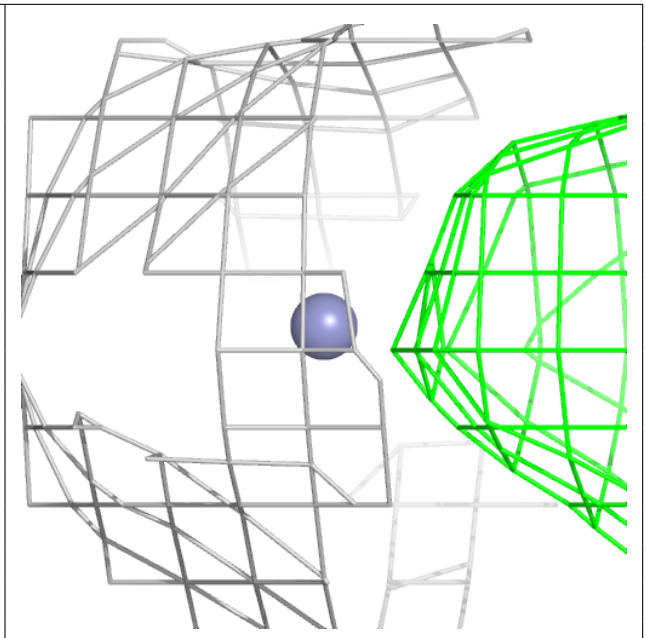


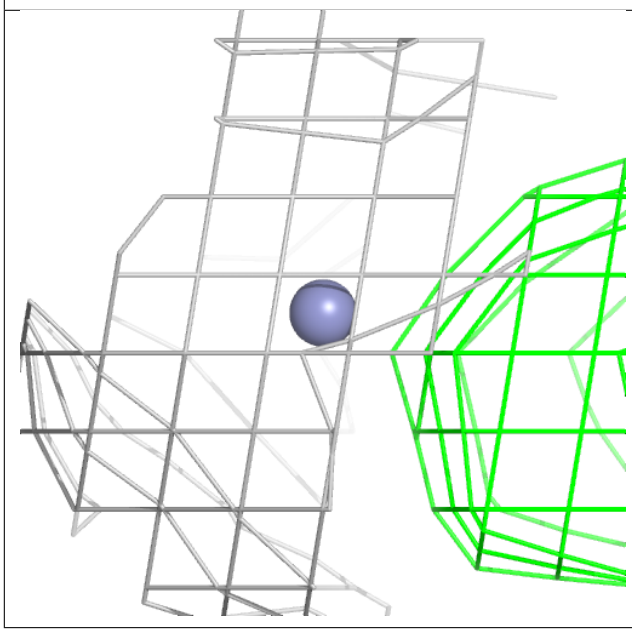


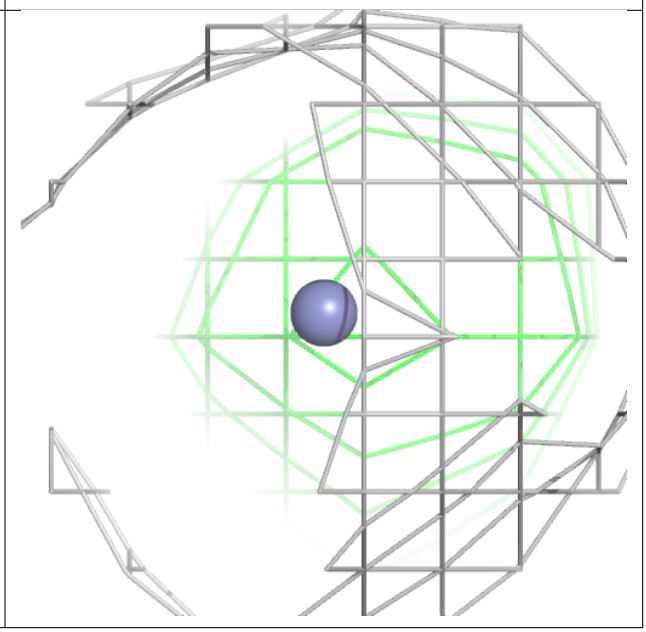


Electron density around ZN A 1101:

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

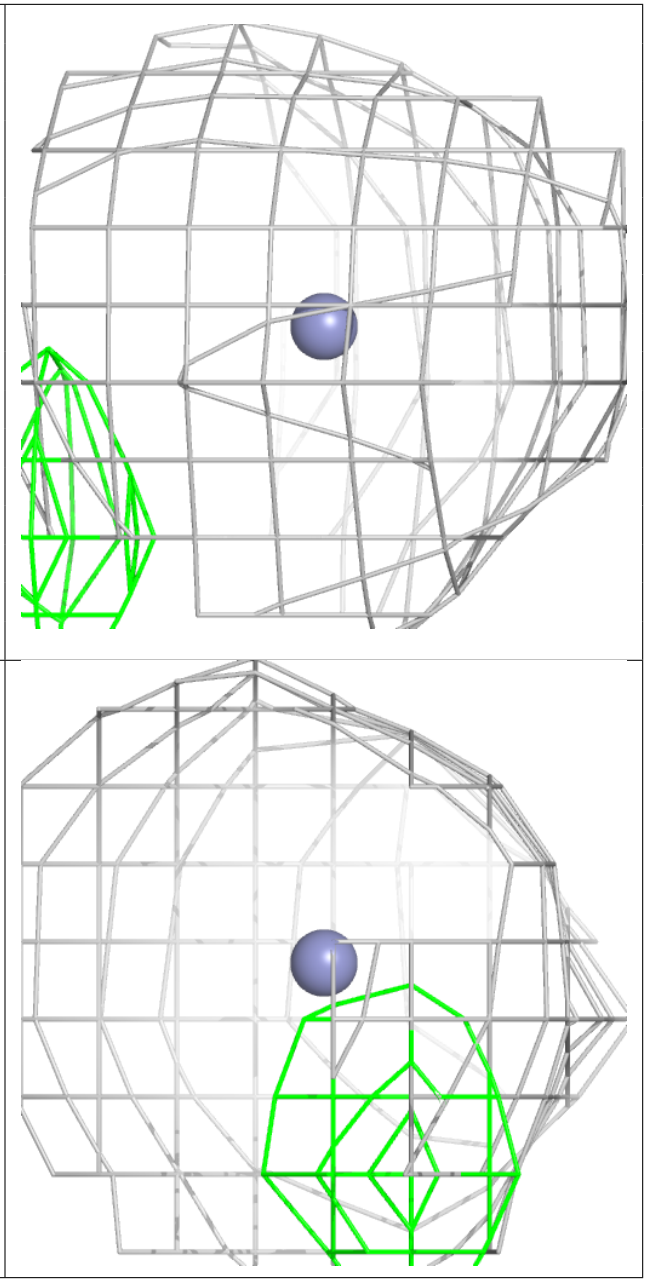






Electron density around ZN G 2001:

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



6.5 Other polymers (i)

There are no such residues in this entry.