Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 07:10 am BST

PDB ID	:	8OIC
Title	:	Trichomonas vaginalis riboside hydrolase (His-tagged)
Authors	:	Patrone, M.; Stockman, B.J.; Degano, M.
Deposited on	:	2023-03-22
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

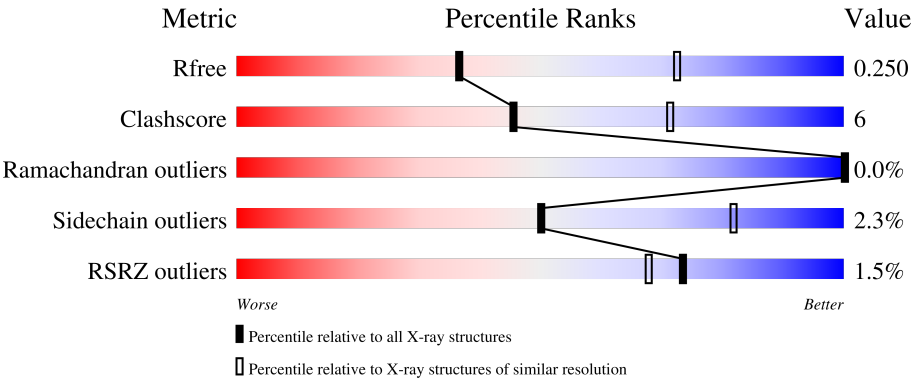
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 >=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	367	81% 11% 7%
1	B	367	79% 11% • 9%
1	C	367	80% 12% • 8%
1	D	367	78% 10% • 11%
1	E	367	78% 13% • 7%

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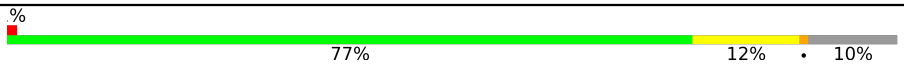
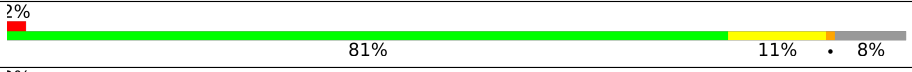
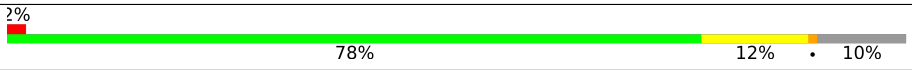
Mol	Chain	Length	Quality of chain
1	F	367	
1	G	367	
1	H	367	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21659 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 Inosine-uridine preferring nucleoside hydrolase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	1	0
			2705	1736	446	506	17			
1	B	333	Total	C	N	O	S	0	1	0
			2650	1700	437	496	17			
1	C	338	Total	C	N	O	S	0	1	0
			2693	1728	444	504	17			
1	D	326	Total	C	N	O	S	0	1	0
			2600	1669	428	486	17			
1	E	340	Total	C	N	O	S	0	1	0
			2705	1736	446	506	17			
1	F	330	Total	C	N	O	S	0	1	0
			2632	1690	435	490	17			
1	G	339	Total	C	N	O	S	0	1	0
			2696	1731	445	503	17			
1	H	332	Total	C	N	O	S	0	1	0
			2644	1698	437	492	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A2FTT0
A	-18	GLY	-	expression tag	UNP A2FTT0
A	-17	SER	-	expression tag	UNP A2FTT0
A	-16	SER	-	expression tag	UNP A2FTT0
A	-15	HIS	-	expression tag	UNP A2FTT0
A	-14	HIS	-	expression tag	UNP A2FTT0
A	-13	HIS	-	expression tag	UNP A2FTT0
A	-12	HIS	-	expression tag	UNP A2FTT0
A	-11	HIS	-	expression tag	UNP A2FTT0
A	-10	HIS	-	expression tag	UNP A2FTT0
A	-9	SER	-	expression tag	UNP A2FTT0
A	-8	SER	-	expression tag	UNP A2FTT0
A	-7	GLY	-	expression tag	UNP A2FTT0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A2FTT0
A	-5	VAL	-	expression tag	UNP A2FTT0
A	-4	PRO	-	expression tag	UNP A2FTT0
A	-3	ARG	-	expression tag	UNP A2FTT0
A	-2	GLY	-	expression tag	UNP A2FTT0
A	-1	SER	-	expression tag	UNP A2FTT0
A	0	HIS	-	expression tag	UNP A2FTT0
B	-19	MET	-	initiating methionine	UNP A2FTT0
B	-18	GLY	-	expression tag	UNP A2FTT0
B	-17	SER	-	expression tag	UNP A2FTT0
B	-16	SER	-	expression tag	UNP A2FTT0
B	-15	HIS	-	expression tag	UNP A2FTT0
B	-14	HIS	-	expression tag	UNP A2FTT0
B	-13	HIS	-	expression tag	UNP A2FTT0
B	-12	HIS	-	expression tag	UNP A2FTT0
B	-11	HIS	-	expression tag	UNP A2FTT0
B	-10	HIS	-	expression tag	UNP A2FTT0
B	-9	SER	-	expression tag	UNP A2FTT0
B	-8	SER	-	expression tag	UNP A2FTT0
B	-7	GLY	-	expression tag	UNP A2FTT0
B	-6	LEU	-	expression tag	UNP A2FTT0
B	-5	VAL	-	expression tag	UNP A2FTT0
B	-4	PRO	-	expression tag	UNP A2FTT0
B	-3	ARG	-	expression tag	UNP A2FTT0
B	-2	GLY	-	expression tag	UNP A2FTT0
B	-1	SER	-	expression tag	UNP A2FTT0
B	0	HIS	-	expression tag	UNP A2FTT0
C	-19	MET	-	initiating methionine	UNP A2FTT0
C	-18	GLY	-	expression tag	UNP A2FTT0
C	-17	SER	-	expression tag	UNP A2FTT0
C	-16	SER	-	expression tag	UNP A2FTT0
C	-15	HIS	-	expression tag	UNP A2FTT0
C	-14	HIS	-	expression tag	UNP A2FTT0
C	-13	HIS	-	expression tag	UNP A2FTT0
C	-12	HIS	-	expression tag	UNP A2FTT0
C	-11	HIS	-	expression tag	UNP A2FTT0
C	-10	HIS	-	expression tag	UNP A2FTT0
C	-9	SER	-	expression tag	UNP A2FTT0
C	-8	SER	-	expression tag	UNP A2FTT0
C	-7	GLY	-	expression tag	UNP A2FTT0
C	-6	LEU	-	expression tag	UNP A2FTT0
C	-5	VAL	-	expression tag	UNP A2FTT0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A2FTT0
C	-3	ARG	-	expression tag	UNP A2FTT0
C	-2	GLY	-	expression tag	UNP A2FTT0
C	-1	SER	-	expression tag	UNP A2FTT0
C	0	HIS	-	expression tag	UNP A2FTT0
D	-19	MET	-	initiating methionine	UNP A2FTT0
D	-18	GLY	-	expression tag	UNP A2FTT0
D	-17	SER	-	expression tag	UNP A2FTT0
D	-16	SER	-	expression tag	UNP A2FTT0
D	-15	HIS	-	expression tag	UNP A2FTT0
D	-14	HIS	-	expression tag	UNP A2FTT0
D	-13	HIS	-	expression tag	UNP A2FTT0
D	-12	HIS	-	expression tag	UNP A2FTT0
D	-11	HIS	-	expression tag	UNP A2FTT0
D	-10	HIS	-	expression tag	UNP A2FTT0
D	-9	SER	-	expression tag	UNP A2FTT0
D	-8	SER	-	expression tag	UNP A2FTT0
D	-7	GLY	-	expression tag	UNP A2FTT0
D	-6	LEU	-	expression tag	UNP A2FTT0
D	-5	VAL	-	expression tag	UNP A2FTT0
D	-4	PRO	-	expression tag	UNP A2FTT0
D	-3	ARG	-	expression tag	UNP A2FTT0
D	-2	GLY	-	expression tag	UNP A2FTT0
D	-1	SER	-	expression tag	UNP A2FTT0
D	0	HIS	-	expression tag	UNP A2FTT0
E	-19	MET	-	initiating methionine	UNP A2FTT0
E	-18	GLY	-	expression tag	UNP A2FTT0
E	-17	SER	-	expression tag	UNP A2FTT0
E	-16	SER	-	expression tag	UNP A2FTT0
E	-15	HIS	-	expression tag	UNP A2FTT0
E	-14	HIS	-	expression tag	UNP A2FTT0
E	-13	HIS	-	expression tag	UNP A2FTT0
E	-12	HIS	-	expression tag	UNP A2FTT0
E	-11	HIS	-	expression tag	UNP A2FTT0
E	-10	HIS	-	expression tag	UNP A2FTT0
E	-9	SER	-	expression tag	UNP A2FTT0
E	-8	SER	-	expression tag	UNP A2FTT0
E	-7	GLY	-	expression tag	UNP A2FTT0
E	-6	LEU	-	expression tag	UNP A2FTT0
E	-5	VAL	-	expression tag	UNP A2FTT0
E	-4	PRO	-	expression tag	UNP A2FTT0
E	-3	ARG	-	expression tag	UNP A2FTT0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A2FTT0
E	-1	SER	-	expression tag	UNP A2FTT0
E	0	HIS	-	expression tag	UNP A2FTT0
F	-19	MET	-	initiating methionine	UNP A2FTT0
F	-18	GLY	-	expression tag	UNP A2FTT0
F	-17	SER	-	expression tag	UNP A2FTT0
F	-16	SER	-	expression tag	UNP A2FTT0
F	-15	HIS	-	expression tag	UNP A2FTT0
F	-14	HIS	-	expression tag	UNP A2FTT0
F	-13	HIS	-	expression tag	UNP A2FTT0
F	-12	HIS	-	expression tag	UNP A2FTT0
F	-11	HIS	-	expression tag	UNP A2FTT0
F	-10	HIS	-	expression tag	UNP A2FTT0
F	-9	SER	-	expression tag	UNP A2FTT0
F	-8	SER	-	expression tag	UNP A2FTT0
F	-7	GLY	-	expression tag	UNP A2FTT0
F	-6	LEU	-	expression tag	UNP A2FTT0
F	-5	VAL	-	expression tag	UNP A2FTT0
F	-4	PRO	-	expression tag	UNP A2FTT0
F	-3	ARG	-	expression tag	UNP A2FTT0
F	-2	GLY	-	expression tag	UNP A2FTT0
F	-1	SER	-	expression tag	UNP A2FTT0
F	0	HIS	-	expression tag	UNP A2FTT0
G	-19	MET	-	initiating methionine	UNP A2FTT0
G	-18	GLY	-	expression tag	UNP A2FTT0
G	-17	SER	-	expression tag	UNP A2FTT0
G	-16	SER	-	expression tag	UNP A2FTT0
G	-15	HIS	-	expression tag	UNP A2FTT0
G	-14	HIS	-	expression tag	UNP A2FTT0
G	-13	HIS	-	expression tag	UNP A2FTT0
G	-12	HIS	-	expression tag	UNP A2FTT0
G	-11	HIS	-	expression tag	UNP A2FTT0
G	-10	HIS	-	expression tag	UNP A2FTT0
G	-9	SER	-	expression tag	UNP A2FTT0
G	-8	SER	-	expression tag	UNP A2FTT0
G	-7	GLY	-	expression tag	UNP A2FTT0
G	-6	LEU	-	expression tag	UNP A2FTT0
G	-5	VAL	-	expression tag	UNP A2FTT0
G	-4	PRO	-	expression tag	UNP A2FTT0
G	-3	ARG	-	expression tag	UNP A2FTT0
G	-2	GLY	-	expression tag	UNP A2FTT0
G	-1	SER	-	expression tag	UNP A2FTT0

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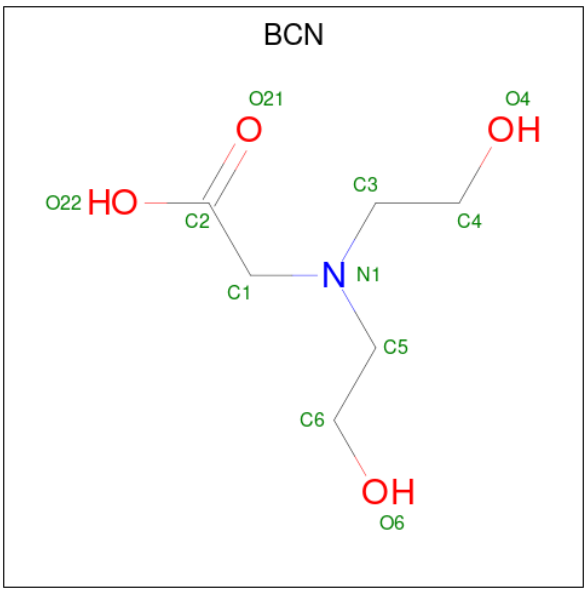
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A2FTT0
H	-19	MET	-	initiating methionine	UNP A2FTT0
H	-18	GLY	-	expression tag	UNP A2FTT0
H	-17	SER	-	expression tag	UNP A2FTT0
H	-16	SER	-	expression tag	UNP A2FTT0
H	-15	HIS	-	expression tag	UNP A2FTT0
H	-14	HIS	-	expression tag	UNP A2FTT0
H	-13	HIS	-	expression tag	UNP A2FTT0
H	-12	HIS	-	expression tag	UNP A2FTT0
H	-11	HIS	-	expression tag	UNP A2FTT0
H	-10	HIS	-	expression tag	UNP A2FTT0
H	-9	SER	-	expression tag	UNP A2FTT0
H	-8	SER	-	expression tag	UNP A2FTT0
H	-7	GLY	-	expression tag	UNP A2FTT0
H	-6	LEU	-	expression tag	UNP A2FTT0
H	-5	VAL	-	expression tag	UNP A2FTT0
H	-4	PRO	-	expression tag	UNP A2FTT0
H	-3	ARG	-	expression tag	UNP A2FTT0
H	-2	GLY	-	expression tag	UNP A2FTT0
H	-1	SER	-	expression tag	UNP A2FTT0
H	0	HIS	-	expression tag	UNP A2FTT0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 11 6 1 4	0	0
3	B	1	Total C N O 11 6 1 4	0	0
3	C	1	Total C N O 11 6 1 4	0	0
3	D	1	Total C N O 11 6 1 4	0	0
3	E	1	Total C N O 11 6 1 4	0	0
3	F	1	Total C N O 11 6 1 4	0	0
3	G	1	Total C N O 11 6 1 4	0	0
3	H	1	Total C N O 11 6 1 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0
4	B	29	Total O 29 29	0	0
4	C	25	Total O 25 25	0	0

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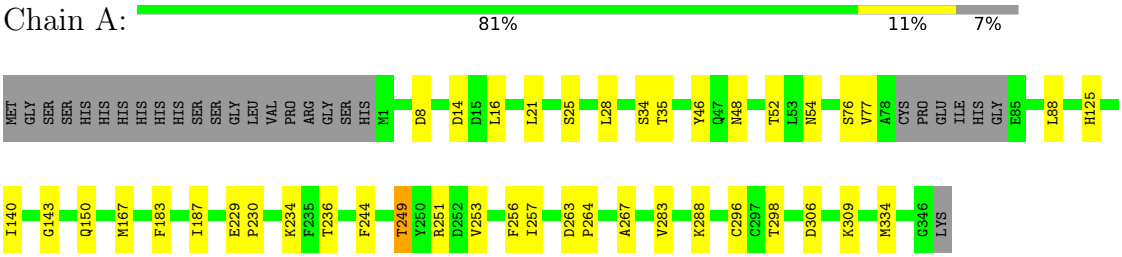
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	25	Total O 25 25	0	0
4	E	32	Total O 32 32	0	0
4	F	36	Total O 36 36	0	0
4	G	24	Total O 24 24	0	0
4	H	26	Total O 26 26	0	0

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.

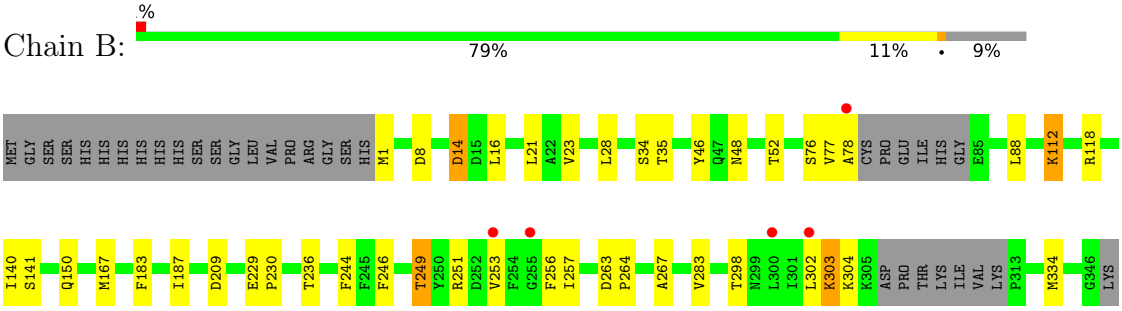
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain A:



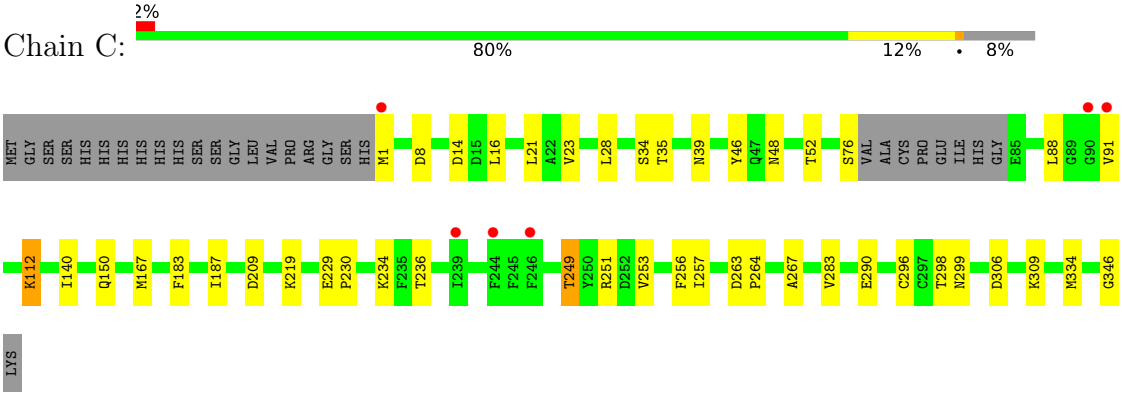
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain B:



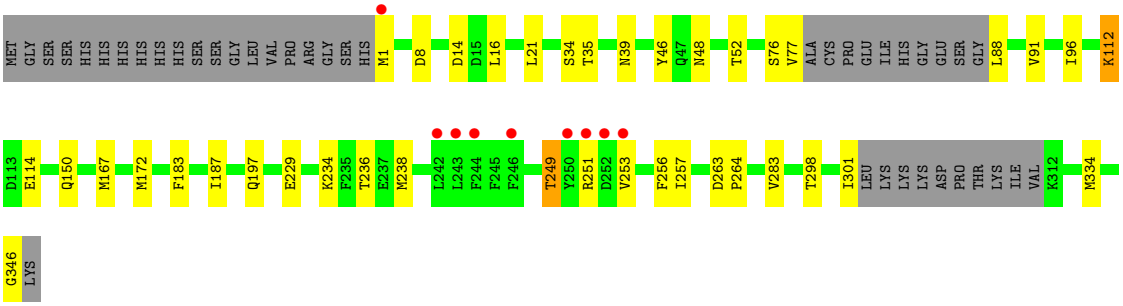
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain C:



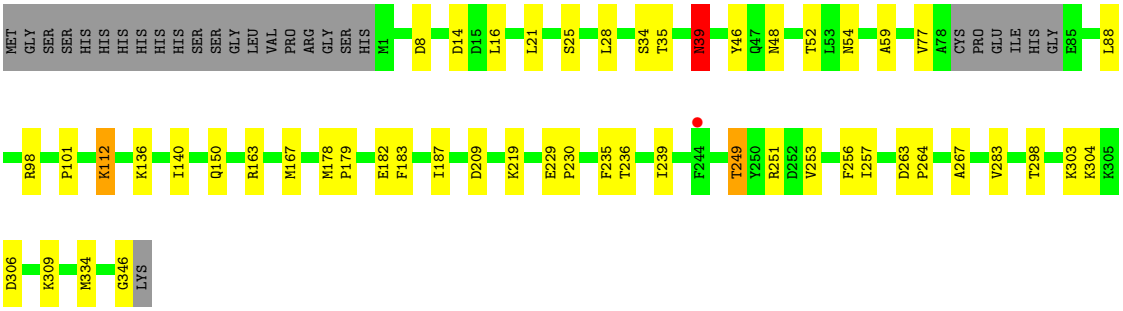
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain D:



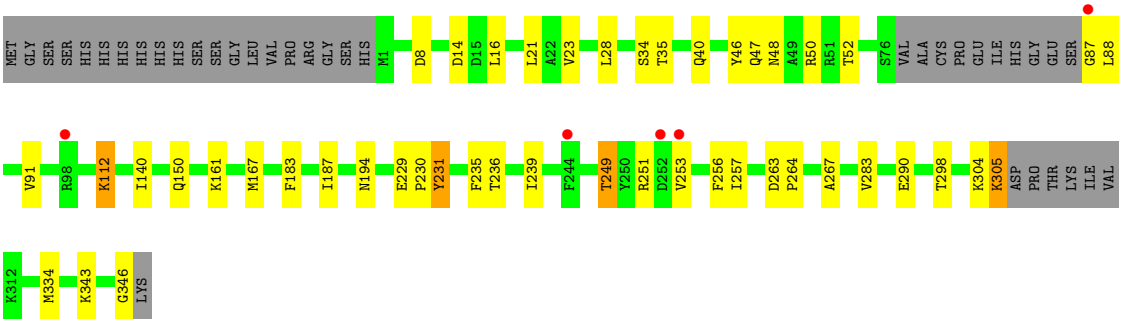
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain E:



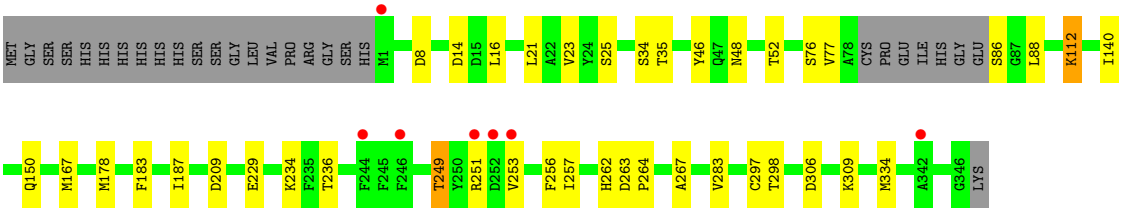
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain F:



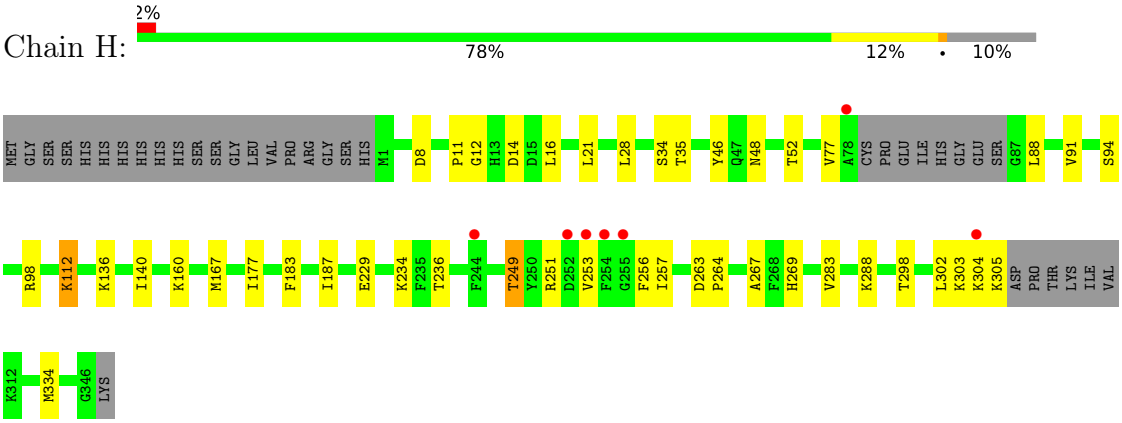
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain G:



• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain H:


2%
78%
12%
10%
MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M1 D8 P11 G12 H13 D14 D15 L16 L21 L28 S34 T35 Y46 Q47 N48 T52 V77 A78 CYS PRO GLU ILE HIS GLY GLU SER G87 L88 V91 S94
R98 K112 K136 I140 K160 M167 I177 F183 I187 E229 K234 F235 T236 F244 T249 Y250 R251 D252 V253 F254 G255 F256 I257 D263 P264 A267 F268 H269 V283 K288 T298 L302 K303 K304 K305 ASP PRO THR LYS ILE VAL
K312 M334 G346 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.06Å 94.67Å 120.59Å 105.08° 89.96° 93.83°	Depositor
Resolution (Å)	116.42 – 2.80 116.42 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.6 (116.42-2.80) 98.4 (116.42-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.209 , 0.251 0.212 , 0.250	Depositor DCC
R_{free} test set	5261 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21659	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/2772	0.62	0/3761
1	B	0.37	0/2715	0.62	0/3681
1	C	0.35	0/2760	0.60	0/3744
1	D	0.34	0/2665	0.60	0/3617
1	E	0.36	0/2772	0.63	1/3761 (0.0%)
1	F	0.35	0/2697	0.61	1/3656 (0.0%)
1	G	0.36	0/2763	0.60	0/3749
1	H	0.35	0/2709	0.60	0/3673
All	All	0.36	0/21853	0.61	2/29642 (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
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	39	ASN	CB-CA-C	7.37	125.14	110.40
1	F	231	TYR	CB-CG-CD1	-5.03	117.98	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	118	ARG	Sidechain
1	E	98	ARG	Sidechain
1	G	86	SER	Peptide
1	H	304	LYS	Peptide

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	2705	0	2692	31	0
1	B	2650	0	2628	32	0
1	C	2693	0	2678	29	0
1	D	2600	0	2571	34	0
1	E	2705	0	2692	38	0
1	F	2632	0	2615	35	0
1	G	2696	0	2686	28	0
1	H	2644	0	2629	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	11	0	11	2	0
3	B	11	0	11	3	0
3	C	11	0	11	4	0
3	D	11	0	11	1	0
3	E	11	0	11	5	0
3	F	11	0	11	2	0
3	G	11	0	11	2	0
3	H	11	0	11	3	0
4	A	41	0	0	8	0
4	B	29	0	0	5	0
4	C	25	0	0	7	0
4	D	25	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	32	0	0	12	0
4	F	36	0	0	10	0
4	G	24	0	0	5	0
4	H	26	0	0	11	0
All	All	21659	0	21279	274	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 (274) 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:346:GLY:C	4:D:511:HOH:O	1.99	0.99
1:F:47:GLN:HG3	4:F:535:HOH:O	1.63	0.98
1:A:25:SER:O	4:A:501:HOH:O	1.82	0.97
1:E:178:MET:CE	4:E:509:HOH:O	2.11	0.96
1:H:98:ARG:HD2	4:H:519:HOH:O	1.72	0.89
1:A:309:LYS:HB2	4:A:519:HOH:O	1.74	0.86
1:G:178:MET:CE	4:G:515:HOH:O	2.25	0.85
1:G:178:MET:HE3	4:G:515:HOH:O	1.77	0.84
1:E:25:SER:O	4:E:501:HOH:O	1.95	0.82
3:A:401:BCN:H42	3:A:401:BCN:H62	1.62	0.80
1:H:28:LEU:O	4:H:501:HOH:O	1.99	0.79
1:H:305:LYS:N	4:H:502:HOH:O	2.15	0.78
1:D:197:GLN:HB2	4:D:523:HOH:O	1.83	0.78
1:E:136:LYS:HE2	4:E:503:HOH:O	1.82	0.77
1:E:178:MET:HE3	4:E:509:HOH:O	1.75	0.77
1:G:23:VAL:O	4:G:501:HOH:O	2.02	0.75
1:E:59:ALA:CB	4:E:532:HOH:O	2.35	0.75
1:B:28:LEU:O	4:B:501:HOH:O	2.04	0.74
1:A:28:LEU:O	4:A:501:HOH:O	2.08	0.72
1:F:290:GLU:HB2	1:H:288:LYS:HE3	1.72	0.72
3:H:401:BCN:H42	3:H:401:BCN:H62	1.72	0.71
1:E:28:LEU:O	4:E:501:HOH:O	2.11	0.69
3:F:401:BCN:H42	3:F:401:BCN:H62	1.75	0.69
1:F:229:GLU:HG3	1:F:236:THR:HG21	1.75	0.68
3:G:401:BCN:H31	4:G:505:HOH:O	1.93	0.68
1:D:96:ILE:HG12	4:D:524:HOH:O	1.93	0.68
1:C:39:ASN:HA	4:C:518:HOH:O	1.93	0.68
1:B:141:SER:OG	4:B:502:HOH:O	2.11	0.68
1:C:23:VAL:O	4:C:501:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:LEU:HD22	1:F:334:MET:HE1	1.76	0.68
1:B:21:LEU:HD22	1:B:334:MET:HE1	1.76	0.67
1:A:296:CYS:O	4:A:502:HOH:O	2.11	0.67
1:H:94:SER:HA	4:H:523:HOH:O	1.95	0.67
1:F:40:GLN:NE2	4:F:502:HOH:O	2.23	0.67
1:B:229:GLU:HG3	1:B:236:THR:HG21	1.77	0.67
1:C:283:VAL:HG22	1:C:298:THR:HG22	1.78	0.66
1:C:296:CYS:O	4:C:502:HOH:O	2.14	0.66
1:G:21:LEU:HD22	1:G:334:MET:HE1	1.75	0.66
1:E:229:GLU:HG3	1:E:236:THR:HG21	1.78	0.66
1:D:21:LEU:HD22	1:D:334:MET:HE1	1.76	0.66
1:E:21:LEU:HD22	1:E:334:MET:HE1	1.77	0.66
1:D:229:GLU:HG3	1:D:236:THR:HG21	1.77	0.65
1:G:283:VAL:HG22	1:G:298:THR:HG22	1.79	0.65
3:H:401:BCN:H62	3:H:401:BCN:C4	2.27	0.65
1:H:21:LEU:HD22	1:H:334:MET:HE1	1.77	0.65
1:H:269:HIS:ND1	4:H:505:HOH:O	2.30	0.65
1:C:346:GLY:C	4:C:517:HOH:O	2.35	0.65
1:E:283:VAL:HG22	1:E:298:THR:HG22	1.79	0.65
1:F:283:VAL:HG22	1:F:298:THR:HG22	1.79	0.64
1:A:21:LEU:HD22	1:A:334:MET:HE1	1.78	0.64
1:C:229:GLU:HG3	1:C:236:THR:HG21	1.78	0.64
1:F:87:GLY:N	4:F:503:HOH:O	2.30	0.64
1:B:283:VAL:HG22	1:B:298:THR:HG22	1.80	0.64
1:E:303:LYS:HE2	4:E:531:HOH:O	1.98	0.64
1:G:229:GLU:HG3	1:G:236:THR:HG21	1.78	0.63
1:A:283:VAL:HG22	1:A:298:THR:HG22	1.80	0.63
1:D:283:VAL:HG22	1:D:298:THR:HG22	1.80	0.63
1:H:283:VAL:HG22	1:H:298:THR:HG22	1.81	0.62
1:C:21:LEU:HD22	1:C:334:MET:HE1	1.79	0.62
1:E:59:ALA:HB1	4:E:532:HOH:O	1.98	0.62
1:B:304:LYS:HE3	1:D:253:VAL:HG13	1.81	0.62
1:A:288:LYS:NZ	1:C:290:GLU:OE1	2.33	0.62
1:H:253:VAL:O	4:H:503:HOH:O	2.16	0.61
1:E:101:PRO:HD2	4:E:532:HOH:O	1.99	0.61
3:A:401:BCN:H62	3:A:401:BCN:C4	2.30	0.61
1:E:35:THR:HG21	1:E:46:TYR:HA	1.83	0.61
1:C:35:THR:HG21	1:C:46:TYR:HA	1.83	0.60
1:G:35:THR:HG21	1:G:46:TYR:HA	1.83	0.60
1:F:35:THR:HG21	1:F:46:TYR:HA	1.84	0.60
1:B:35:THR:HG21	1:B:46:TYR:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HG21	1:A:46:TYR:HA	1.84	0.60
1:D:91:VAL:HG21	1:D:238:MET:CE	2.31	0.59
3:C:401:BCN:H42	3:C:401:BCN:H62	1.83	0.59
1:D:114:GLU:HG3	4:D:516:HOH:O	2.03	0.59
1:G:234:LYS:HA	1:G:234:LYS:HE2	1.85	0.59
1:D:35:THR:HG21	1:D:46:TYR:HA	1.84	0.59
1:H:35:THR:HG21	1:H:46:TYR:HA	1.83	0.58
1:E:77:VAL:HG22	1:E:187:ILE:HG13	1.86	0.58
1:G:25:SER:O	4:G:501:HOH:O	2.17	0.58
1:F:28:LEU:O	4:F:501:HOH:O	2.17	0.58
1:B:304:LYS:CE	1:D:253:VAL:HG13	2.35	0.57
1:F:290:GLU:HB2	1:H:288:LYS:CE	2.34	0.57
1:D:91:VAL:HG21	1:D:238:MET:HE3	1.86	0.56
3:C:401:BCN:H42	3:C:401:BCN:C6	2.35	0.56
3:F:401:BCN:H62	3:F:401:BCN:C4	2.35	0.56
1:H:302:LEU:O	1:H:305:LYS:HB2	2.06	0.55
1:B:14:ASP:OD2	3:B:401:BCN:H42	2.07	0.55
1:D:183:PHE:CZ	1:D:187:ILE:HD12	2.42	0.55
1:H:303:LYS:HD2	4:H:525:HOH:O	2.06	0.55
1:D:150[A]:GLN:OE1	1:D:150[A]:GLN:HA	2.07	0.55
1:B:229:GLU:CG	1:B:236:THR:HG21	2.36	0.54
1:B:246:PHE:O	1:B:249:THR:HG23	2.08	0.54
3:B:401:BCN:C6	3:B:401:BCN:H41	2.38	0.54
1:C:263:ASP:N	1:C:264:PRO:HD2	2.23	0.54
1:F:263:ASP:N	1:F:264:PRO:HD2	2.23	0.54
1:B:263:ASP:N	1:B:264:PRO:HD2	2.23	0.54
1:H:305:LYS:HG3	4:H:502:HOH:O	2.08	0.54
1:A:263:ASP:N	1:A:264:PRO:HD2	2.23	0.54
1:G:263:ASP:N	1:G:264:PRO:HD2	2.23	0.54
3:H:401:BCN:C4	3:H:401:BCN:C6	2.85	0.54
1:E:263:ASP:N	1:E:264:PRO:HD2	2.23	0.53
1:D:263:ASP:N	1:D:264:PRO:HD2	2.23	0.53
1:B:77:VAL:HG22	1:B:187:ILE:HG13	1.89	0.53
1:H:183:PHE:CZ	1:H:187:ILE:HD12	2.44	0.53
1:H:263:ASP:N	1:H:264:PRO:HD2	2.23	0.53
1:B:257:ILE:HD12	1:B:257:ILE:H	1.73	0.53
3:D:401:BCN:H41	4:D:501:HOH:O	2.09	0.53
1:A:229:GLU:CG	1:A:236:THR:HG21	2.38	0.53
1:B:78:ALA:HB3	4:B:520:HOH:O	2.09	0.53
1:C:183:PHE:CZ	1:C:187:ILE:HD12	2.44	0.53
1:G:262:HIS:CD2	3:G:401:BCN:H52	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:GLU:HG3	1:H:236:THR:HG21	1.90	0.53
1:E:183:PHE:CZ	1:E:187:ILE:HD12	2.44	0.52
1:B:150[A]:GLN:HA	1:B:150[A]:GLN:OE1	2.10	0.52
1:B:183:PHE:CZ	1:B:187:ILE:HD12	2.44	0.52
1:E:229:GLU:CG	1:E:236:THR:HG21	2.39	0.52
1:H:136:LYS:HE3	1:H:160:LYS:O	2.10	0.52
1:A:257:ILE:HD12	1:A:257:ILE:H	1.74	0.52
1:F:183:PHE:CZ	1:F:187:ILE:HD12	2.43	0.52
1:G:183:PHE:CZ	1:G:187:ILE:HD12	2.45	0.52
1:H:229:GLU:CG	1:H:236:THR:HG21	2.39	0.52
1:G:229:GLU:CG	1:G:236:THR:HG21	2.40	0.52
1:H:77:VAL:HG22	1:H:187:ILE:HG13	1.91	0.52
3:B:401:BCN:H41	3:B:401:BCN:H62	1.93	0.51
1:G:8:ASP:HA	1:G:34:SER:O	2.11	0.51
1:D:8:ASP:HA	1:D:34:SER:O	2.11	0.51
1:H:8:ASP:HA	1:H:34:SER:O	2.11	0.51
1:C:8:ASP:HA	1:C:34:SER:O	2.11	0.51
1:B:302:LEU:O	1:B:304:LYS:N	2.44	0.51
1:A:183:PHE:CZ	1:A:187:ILE:HD12	2.47	0.50
1:C:229:GLU:CG	1:C:236:THR:HG21	2.41	0.50
1:D:39:ASN:ND2	4:D:501:HOH:O	2.16	0.50
1:A:8:ASP:HA	1:A:34:SER:O	2.11	0.50
1:B:23:VAL:O	4:B:501:HOH:O	2.19	0.50
1:B:303:LYS:O	1:B:304:LYS:HD3	2.11	0.50
1:E:8:ASP:HA	1:E:34:SER:O	2.11	0.50
3:E:401:BCN:C6	3:E:401:BCN:C4	2.90	0.50
1:F:150[A]:GLN:OE1	1:F:150[A]:GLN:HA	2.12	0.50
1:F:231:TYR:CD1	1:F:343:LYS:HG2	2.47	0.50
1:A:150[A]:GLN:OE1	1:A:150[A]:GLN:HA	2.11	0.50
1:B:8:ASP:HA	1:B:34:SER:O	2.10	0.50
1:D:301:ILE:N	4:D:505:HOH:O	2.45	0.50
3:E:401:BCN:H62	3:E:401:BCN:H42	1.93	0.50
1:A:229:GLU:HG3	1:A:236:THR:HG21	1.93	0.50
1:F:8:ASP:HA	1:F:34:SER:O	2.11	0.50
1:A:234:LYS:HE2	1:A:234:LYS:HA	1.93	0.50
1:D:76:SER:O	1:D:77:VAL:HB	2.12	0.50
1:D:229:GLU:CG	1:D:236:THR:HG21	2.40	0.50
1:D:112:LYS:HE2	1:D:112:LYS:HA	1.93	0.49
1:H:257:ILE:HD12	1:H:257:ILE:H	1.77	0.49
1:E:150[A]:GLN:HA	1:E:150[A]:GLN:OE1	2.11	0.49
1:E:54:ASN:HB2	4:E:532:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150[A]:GLN:HA	1:G:150[A]:GLN:OE1	2.12	0.49
1:H:98:ARG:CD	4:H:519:HOH:O	2.45	0.49
1:C:257:ILE:HD12	1:C:257:ILE:H	1.77	0.49
1:H:112:LYS:HE2	1:H:112:LYS:HA	1.94	0.49
1:G:251:ARG:HA	1:G:256:PHE:O	2.13	0.49
1:A:306:ASP:OD2	1:A:309:LYS:HG2	2.13	0.49
1:F:251:ARG:HA	1:F:256:PHE:O	2.13	0.49
1:C:28:LEU:O	4:C:501:HOH:O	2.20	0.48
1:D:234:LYS:HE2	1:D:234:LYS:HA	1.95	0.48
1:A:251:ARG:HA	1:A:256:PHE:O	2.13	0.48
1:B:251:ARG:HA	1:B:256:PHE:O	2.13	0.48
1:F:112:LYS:HE2	1:F:112:LYS:HA	1.95	0.48
1:A:249:THR:HA	4:A:540:HOH:O	2.14	0.48
1:D:257:ILE:HD12	1:D:257:ILE:H	1.79	0.48
1:G:112:LYS:HE2	1:G:112:LYS:HA	1.95	0.48
1:B:112:LYS:HE2	1:B:112:LYS:HA	1.96	0.48
1:G:257:ILE:HD12	1:G:257:ILE:H	1.78	0.48
1:E:251:ARG:HA	1:E:256:PHE:O	2.13	0.48
1:C:251:ARG:HA	1:C:256:PHE:O	2.14	0.48
1:C:112:LYS:HA	1:C:112:LYS:HE2	1.95	0.47
1:F:305:LYS:HD3	4:F:534:HOH:O	2.14	0.47
1:F:161:LYS:HE3	4:F:533:HOH:O	2.13	0.47
1:C:21:LEU:HD22	1:C:334:MET:CE	2.45	0.47
1:E:112:LYS:HA	1:E:112:LYS:HE2	1.96	0.47
1:G:306:ASP:OD2	1:G:309:LYS:HG2	2.14	0.47
1:B:21:LEU:HD22	1:B:334:MET:CE	2.45	0.47
1:C:234:LYS:HE2	1:C:234:LYS:HA	1.96	0.47
1:D:251:ARG:HA	1:D:256:PHE:O	2.13	0.47
1:F:21:LEU:HD22	1:F:334:MET:CE	2.45	0.47
3:C:401:BCN:C6	3:C:401:BCN:C4	2.92	0.47
1:A:16:LEU:HG	1:A:52:THR:HG23	1.97	0.46
1:D:16:LEU:HG	1:D:52:THR:HG23	1.97	0.46
1:F:257:ILE:HD12	1:F:257:ILE:H	1.80	0.46
1:A:21:LEU:HD22	1:A:334:MET:CE	2.45	0.46
1:E:16:LEU:HG	1:E:52:THR:HG23	1.97	0.46
3:E:401:BCN:C4	3:E:401:BCN:H62	2.45	0.46
1:G:48:ASN:HB3	1:G:88:LEU:HD22	1.98	0.46
1:H:251:ARG:HA	1:H:256:PHE:O	2.14	0.46
1:F:229:GLU:CG	1:F:236:THR:HG21	2.43	0.46
1:G:140:ILE:HD13	1:G:267:ALA:HA	1.98	0.46
1:F:16:LEU:HG	1:F:52:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:GLY:C	4:F:521:HOH:O	2.54	0.46
1:D:21:LEU:HD22	1:D:334:MET:CE	2.45	0.46
1:D:48:ASN:HB3	1:D:88:LEU:HD22	1.97	0.46
1:E:182:GLU:OE2	3:E:401:BCN:O6	2.34	0.46
1:F:23:VAL:O	4:F:501:HOH:O	2.21	0.46
1:B:48:ASN:HB3	1:B:88:LEU:HD22	1.97	0.45
1:C:306:ASP:OD2	1:C:309:LYS:HG2	2.16	0.45
1:A:48:ASN:HB3	1:A:88:LEU:HD22	1.99	0.45
1:C:48:ASN:HB3	1:C:88:LEU:HD22	1.99	0.45
1:C:150[A]:GLN:HA	1:C:150[A]:GLN:OE1	2.16	0.45
1:E:48:ASN:HB3	1:E:88:LEU:HD22	1.99	0.45
1:B:249:THR:HA	4:B:511:HOH:O	2.17	0.45
1:C:234:LYS:N	1:C:234:LYS:HD2	2.32	0.45
1:E:257:ILE:H	1:E:257:ILE:HD12	1.81	0.45
1:B:16:LEU:HG	1:B:52:THR:HG23	1.98	0.45
1:H:21:LEU:HD22	1:H:334:MET:CE	2.45	0.45
1:H:16:LEU:HG	1:H:52:THR:HG23	1.99	0.44
1:A:77:VAL:HG22	1:A:187:ILE:HG13	1.98	0.44
1:G:16:LEU:HG	1:G:52:THR:HG23	1.99	0.44
1:A:143:GLY:HA2	4:A:505:HOH:O	2.18	0.44
1:C:16:LEU:HG	1:C:52:THR:HG23	1.99	0.44
1:C:16:LEU:C	1:C:16:LEU:HD23	2.39	0.44
1:D:172:MET:HE1	1:D:301:ILE:HG13	1.99	0.44
1:D:234:LYS:HD2	1:D:234:LYS:N	2.32	0.44
1:F:48:ASN:HB3	1:F:88:LEU:HD22	1.99	0.44
1:A:234:LYS:N	1:A:234:LYS:HD2	2.33	0.44
1:D:16:LEU:C	1:D:16:LEU:HD23	2.39	0.44
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.92	0.43
1:E:346:GLY:C	4:E:526:HOH:O	2.56	0.43
1:F:140:ILE:HD13	1:F:267:ALA:HA	2.00	0.43
1:B:16:LEU:HD23	1:B:16:LEU:C	2.38	0.43
1:G:16:LEU:HD23	1:G:16:LEU:C	2.39	0.43
1:E:16:LEU:HD23	1:E:16:LEU:C	2.38	0.43
1:H:16:LEU:C	1:H:16:LEU:HD23	2.39	0.43
1:E:21:LEU:HD22	1:E:334:MET:CE	2.46	0.43
1:G:21:LEU:HD22	1:G:334:MET:CE	2.45	0.43
3:C:401:BCN:H31	4:C:506:HOH:O	2.18	0.43
1:E:235:PHE:CZ	1:E:239:ILE:HG21	2.54	0.43
1:E:306:ASP:OD2	1:E:309:LYS:HE3	2.19	0.43
1:A:140:ILE:HD13	1:A:267:ALA:HA	2.01	0.43
1:F:16:LEU:C	1:F:16:LEU:HD23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:GLU:N	1:F:230:PRO:HD2	2.34	0.43
1:F:304:LYS:HB2	4:H:503:HOH:O	2.19	0.43
1:A:54:ASN:HA	4:A:529:HOH:O	2.19	0.42
1:A:229:GLU:N	1:A:230:PRO:HD2	2.34	0.42
1:C:140:ILE:HD13	1:C:267:ALA:HA	2.01	0.42
1:D:172:MET:CE	1:D:301:ILE:HG13	2.50	0.42
1:F:194:ASN:HB3	4:F:522:HOH:O	2.19	0.42
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.93	0.42
1:D:91:VAL:HG21	1:D:238:MET:HE2	2.01	0.42
1:A:16:LEU:C	1:A:16:LEU:HD23	2.38	0.42
1:G:234:LYS:HD2	1:G:234:LYS:N	2.35	0.42
1:F:249:THR:HA	1:F:253:VAL:HG23	2.02	0.42
1:H:305:LYS:C	4:H:522:HOH:O	2.58	0.42
1:H:48:ASN:HB3	1:H:88:LEU:HD22	2.01	0.42
1:B:140:ILE:HD13	1:B:267:ALA:HA	2.01	0.41
1:B:249:THR:HA	1:B:253:VAL:HG23	2.02	0.41
1:E:163:ARG:NH1	4:E:503:HOH:O	2.47	0.41
1:B:229:GLU:N	1:B:230:PRO:HD2	2.35	0.41
1:F:231:TYR:CE1	1:F:343:LYS:HG2	2.55	0.41
1:E:140:ILE:HD13	1:E:267:ALA:HA	2.03	0.41
1:A:249:THR:HA	1:A:253:VAL:HG23	2.02	0.41
1:D:249:THR:HA	1:D:253:VAL:HG23	2.03	0.41
1:F:50:ARG:HD3	4:F:514:HOH:O	2.19	0.41
1:F:235:PHE:CZ	1:F:239:ILE:HG21	2.56	0.41
1:G:77:VAL:HG22	1:G:187:ILE:HG13	2.01	0.41
1:A:125:HIS:HB2	4:A:526:HOH:O	2.21	0.41
1:C:299:ASN:HA	4:C:512:HOH:O	2.20	0.41
1:E:249:THR:HA	1:E:253:VAL:HG23	2.02	0.41
1:E:88:LEU:HD12	1:E:88:LEU:HA	1.93	0.41
1:C:229:GLU:N	1:C:230:PRO:HD2	2.36	0.41
1:H:249:THR:HA	1:H:253:VAL:HG23	2.03	0.41
1:C:249:THR:HA	1:C:253:VAL:HG23	2.03	0.41
1:E:179:PRO:HG2	1:G:297:CYS:HB3	2.03	0.41
1:H:88:LEU:HD12	1:H:88:LEU:HA	1.94	0.41
1:H:140:ILE:HD13	1:H:267:ALA:HA	2.02	0.41
1:G:249:THR:HA	1:G:253:VAL:HG23	2.03	0.40
1:H:11:PRO:HA	1:H:12:GLY:HA3	1.92	0.40
1:E:39:ASN:OD1	3:E:401:BCN:O22	2.40	0.40
1:E:229:GLU:N	1:E:230:PRO:HD2	2.36	0.40
1:H:177:ILE:HD13	1:H:177:ILE:HA	1.89	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	337/367 (92%)	318 (94%)	19 (6%)	0	100 100
1	B	328/367 (89%)	310 (94%)	17 (5%)	1 (0%)	41 72
1	C	335/367 (91%)	318 (95%)	17 (5%)	0	100 100
1	D	321/367 (88%)	305 (95%)	16 (5%)	0	100 100
1	E	337/367 (92%)	320 (95%)	17 (5%)	0	100 100
1	F	325/367 (89%)	309 (95%)	16 (5%)	0	100 100
1	G	336/367 (92%)	316 (94%)	20 (6%)	0	100 100
1	H	327/367 (89%)	310 (95%)	17 (5%)	0	100 100
All	All	2646/2936 (90%)	2506 (95%)	139 (5%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	298/320 (93%)	293 (98%)	5 (2%)	60 87
1	B	291/320 (91%)	283 (97%)	8 (3%)	44 78
1	C	297/320 (93%)	288 (97%)	9 (3%)	41 75
1	D	286/320 (89%)	281 (98%)	5 (2%)	60 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	298/320 (93%)	290 (97%)	8 (3%)	44 78
1	F	289/320 (90%)	283 (98%)	6 (2%)	53 84
1	G	297/320 (93%)	291 (98%)	6 (2%)	55 84
1	H	290/320 (91%)	284 (98%)	6 (2%)	53 84
All	All	2346/2560 (92%)	2293 (98%)	53 (2%)	50 82

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	76	SER
1	A	167	MET
1	A	244	PHE
1	A	249	THR
1	B	1	MET
1	B	14	ASP
1	B	76	SER
1	B	112	LYS
1	B	167	MET
1	B	209	ASP
1	B	244	PHE
1	B	249	THR
1	C	1	MET
1	C	14	ASP
1	C	76	SER
1	C	91	VAL
1	C	112	LYS
1	C	167	MET
1	C	209	ASP
1	C	219	LYS
1	C	249	THR
1	D	1	MET
1	D	14	ASP
1	D	112	LYS
1	D	167	MET
1	D	249	THR
1	E	14	ASP
1	E	39	ASN
1	E	112	LYS
1	E	167	MET
1	E	209	ASP

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Mol	Chain	Res	Type
1	E	219	LYS
1	E	249	THR
1	E	304	LYS
1	F	14	ASP
1	F	91	VAL
1	F	112	LYS
1	F	167	MET
1	F	249	THR
1	F	305	LYS
1	G	14	ASP
1	G	76	SER
1	G	112	LYS
1	G	167	MET
1	G	209	ASP
1	G	249	THR
1	H	14	ASP
1	H	91	VAL
1	H	112	LYS
1	H	167	MET
1	H	234	LYS
1	H	249	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	39	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	BCN	E	401	2	10,10,10	0.74	0	11,11,11	0.57	0
3	BCN	A	401	2	10,10,10	0.78	0	11,11,11	0.79	0
3	BCN	F	401	2	10,10,10	0.97	0	11,11,11	0.99	1 (9%)
3	BCN	H	401	2	10,10,10	0.72	0	11,11,11	0.78	0
3	BCN	C	401	2	10,10,10	0.83	0	11,11,11	0.58	0
3	BCN	D	401	2	10,10,10	0.90	0	11,11,11	0.89	0
3	BCN	B	401	2	10,10,10	0.94	0	11,11,11	1.22	1 (9%)
3	BCN	G	401	2	10,10,10	0.71	0	11,11,11	1.01	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	BCN	E	401	2	-	5/10/10/10	-
3	BCN	A	401	2	-	5/10/10/10	-
3	BCN	F	401	2	-	4/10/10/10	-
3	BCN	H	401	2	-	6/10/10/10	-
3	BCN	C	401	2	-	6/10/10/10	-
3	BCN	D	401	2	-	6/10/10/10	-
3	BCN	B	401	2	-	4/10/10/10	-
3	BCN	G	401	2	-	8/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	BCN	C2-C1-N1	2.64	122.26	113.63
3	F	401	BCN	C2-C1-N1	2.21	120.85	113.63

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	BCN	N1-C1-C2-O22
3	C	401	BCN	N1-C5-C6-O6
3	D	401	BCN	N1-C3-C4-O4
3	E	401	BCN	C2-C1-N1-C5
3	G	401	BCN	C2-C1-N1-C5
3	G	401	BCN	C6-C5-N1-C3
3	G	401	BCN	N1-C1-C2-O21
3	G	401	BCN	N1-C1-C2-O22
3	H	401	BCN	C4-C3-N1-C5
3	A	401	BCN	N1-C5-C6-O6
3	C	401	BCN	N1-C1-C2-O21
3	D	401	BCN	N1-C1-C2-O21
3	D	401	BCN	N1-C1-C2-O22
3	E	401	BCN	N1-C1-C2-O21
3	E	401	BCN	N1-C1-C2-O22
3	F	401	BCN	N1-C1-C2-O21
3	F	401	BCN	N1-C1-C2-O22
3	H	401	BCN	N1-C1-C2-O21
3	H	401	BCN	N1-C1-C2-O22
3	E	401	BCN	N1-C5-C6-O6
3	C	401	BCN	C2-C1-N1-C5
3	D	401	BCN	C2-C1-N1-C5
3	A	401	BCN	N1-C3-C4-O4
3	G	401	BCN	N1-C3-C4-O4
3	E	401	BCN	C4-C3-N1-C5
3	F	401	BCN	C4-C3-N1-C5
3	G	401	BCN	N1-C5-C6-O6
3	F	401	BCN	C2-C1-N1-C5
3	C	401	BCN	C4-C3-N1-C5
3	H	401	BCN	N1-C3-C4-O4
3	B	401	BCN	N1-C3-C4-O4
3	B	401	BCN	N1-C5-C6-O6
3	D	401	BCN	C6-C5-N1-C3
3	G	401	BCN	C2-C1-N1-C3
3	A	401	BCN	N1-C1-C2-O22
3	B	401	BCN	C4-C3-N1-C5

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Mol	Chain	Res	Type	Atoms
3	H	401	BCN	C6-C5-N1-C3
3	B	401	BCN	C2-C1-N1-C3
3	A	401	BCN	N1-C1-C2-O21
3	G	401	BCN	C6-C5-N1-C1
3	A	401	BCN	C6-C5-N1-C3
3	D	401	BCN	C4-C3-N1-C5
3	H	401	BCN	C4-C3-N1-C1
3	C	401	BCN	N1-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	BCN	5	0
3	A	401	BCN	2	0
3	F	401	BCN	2	0
3	H	401	BCN	3	0
3	C	401	BCN	4	0
3	D	401	BCN	1	0
3	B	401	BCN	3	0
3	G	401	BCN	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	340/367 (92%)	-0.14	0	100	100	36, 53, 82, 104	0
1	B	333/367 (90%)	-0.06	5 (1%)	73	68	41, 55, 93, 139	0
1	C	338/367 (92%)	0.08	6 (1%)	68	61	37, 69, 110, 142	0
1	D	326/367 (88%)	0.11	9 (2%)	53	43	45, 72, 116, 170	0
1	E	340/367 (92%)	-0.10	1 (0%)	94	93	36, 57, 88, 112	0
1	F	330/367 (89%)	0.03	5 (1%)	73	68	43, 60, 96, 136	0
1	G	339/367 (92%)	-0.03	7 (2%)	63	54	36, 62, 91, 122	0
1	H	332/367 (90%)	0.02	7 (2%)	63	54	44, 62, 103, 132	0
All	All	2678/2936 (91%)	-0.01	40 (1%)	73	68	36, 61, 99, 170	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	ASP	6.8
1	F	253	VAL	5.8
1	D	244	PHE	5.2
1	D	253	VAL	4.6
1	B	302	LEU	4.4
1	B	78	ALA	4.4
1	H	252	ASP	4.2
1	B	253	VAL	3.9
1	H	253	VAL	3.7
1	B	300	LEU	3.7
1	H	78	ALA	3.4
1	F	252	ASP	3.2
1	F	244	PHE	3.2
1	G	246	PHE	3.0
1	H	255	GLY	2.9
1	H	304	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	246	PHE	2.9
1	C	244	PHE	2.7
1	C	90	GLY	2.7
1	G	252	ASP	2.7
1	G	1	MET	2.6
1	H	254	PHE	2.6
1	G	244	PHE	2.5
1	G	251	ARG	2.5
1	D	251	ARG	2.4
1	B	255	GLY	2.4
1	D	242	LEU	2.4
1	H	244	PHE	2.4
1	F	87	GLY	2.3
1	C	246	PHE	2.3
1	C	1	MET	2.3
1	E	244	PHE	2.3
1	D	243	LEU	2.2
1	D	250	TYR	2.2
1	C	239	ILE	2.2
1	G	342	ALA	2.1
1	D	1	MET	2.1
1	C	91	VAL	2.1
1	F	98	ARG	2.1
1	G	253	VAL	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)

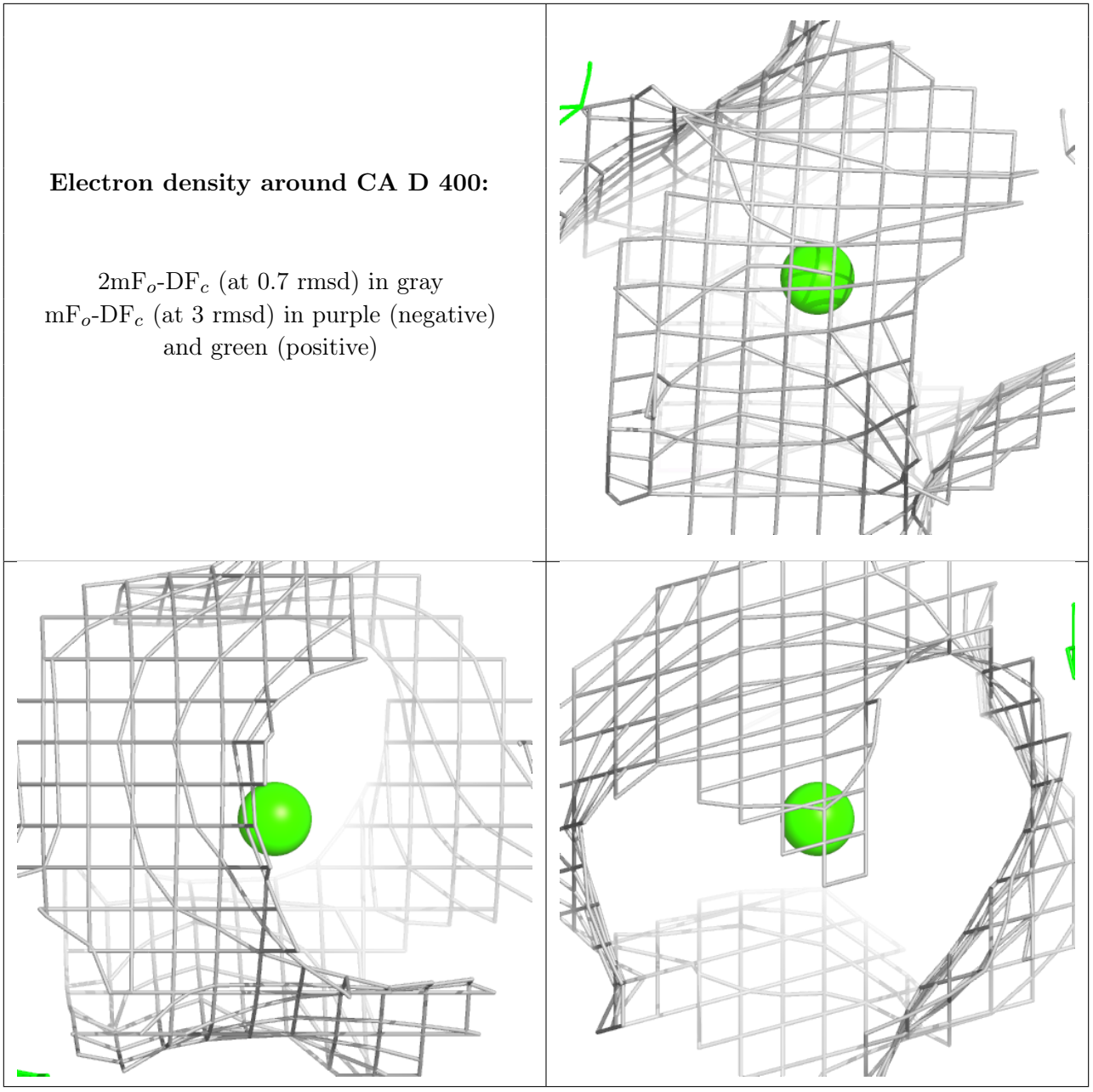
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BCN	D	401	11/11	0.81	0.18	66,81,90,92	0
3	BCN	A	401	11/11	0.82	0.18	56,62,68,68	0
3	BCN	H	401	11/11	0.83	0.17	67,85,90,90	0
3	BCN	G	401	11/11	0.85	0.19	64,68,74,77	0
3	BCN	C	401	11/11	0.86	0.18	71,85,103,104	0
3	BCN	B	401	11/11	0.86	0.18	60,71,81,81	0
3	BCN	E	401	11/11	0.89	0.21	62,81,85,87	0
3	BCN	F	401	11/11	0.91	0.17	61,67,78,82	0
2	CA	D	400	1/1	0.97	0.17	62,62,62,62	0
2	CA	G	400	1/1	0.98	0.12	49,49,49,49	0
2	CA	B	400	1/1	0.98	0.17	56,56,56,56	0
2	CA	E	400	1/1	0.98	0.13	55,55,55,55	0
2	CA	C	400	1/1	0.99	0.14	68,68,68,68	0
2	CA	F	400	1/1	0.99	0.16	55,55,55,55	0
2	CA	A	400	1/1	0.99	0.11	55,55,55,55	0
2	CA	H	400	1/1	0.99	0.15	58,58,58,58	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.

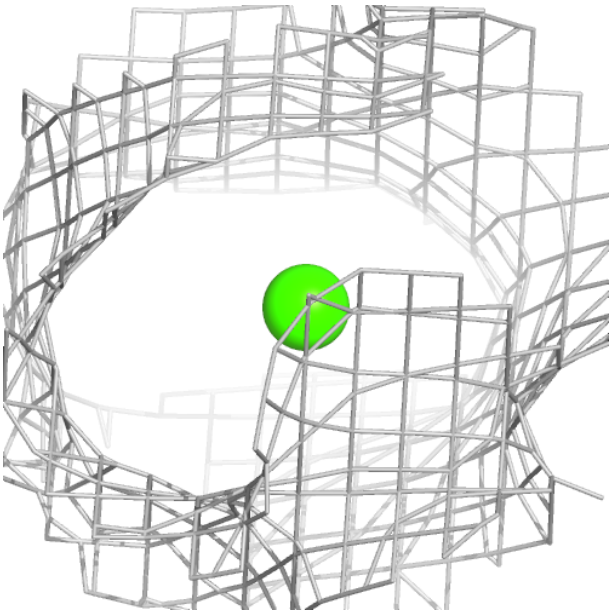
Electron density around CA D 400:

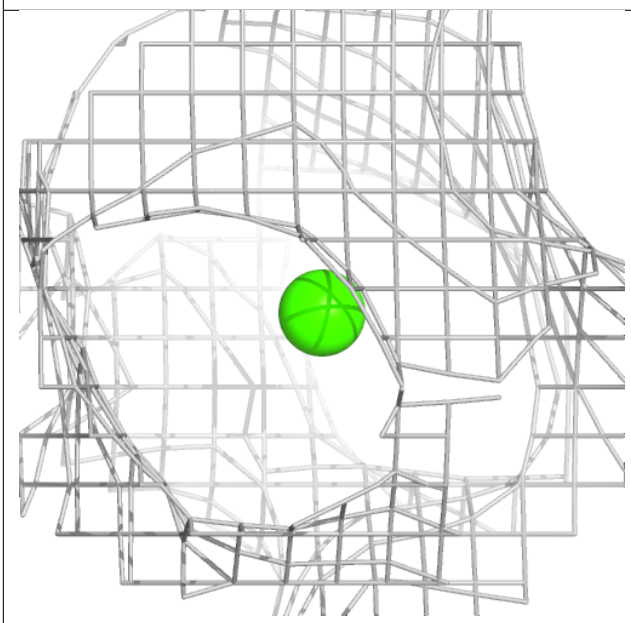
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

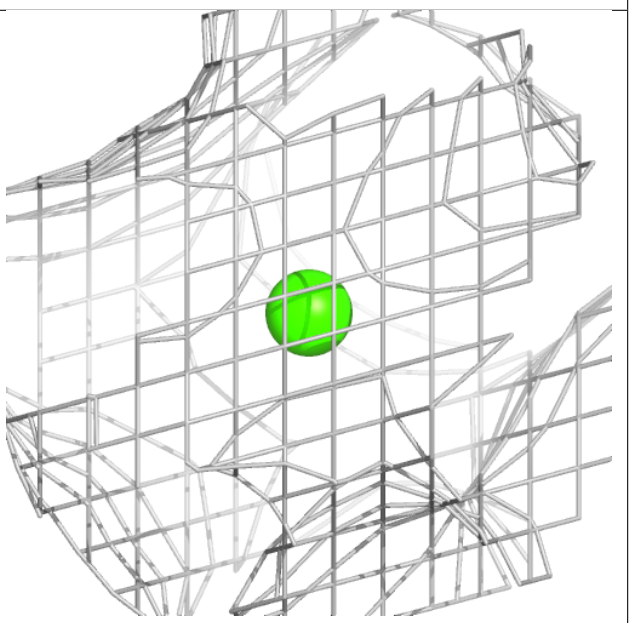


Electron density around CA G 400:

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

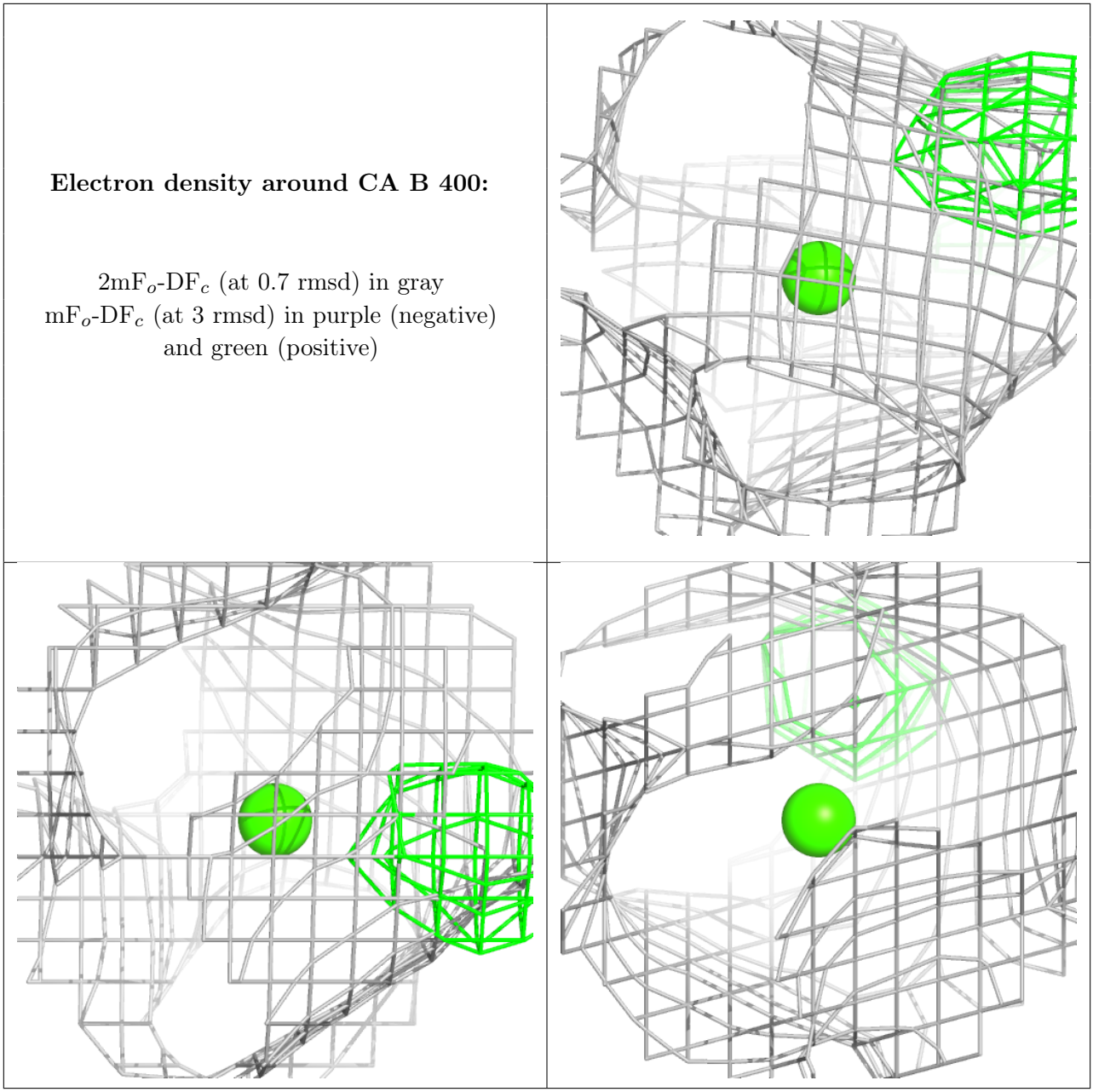






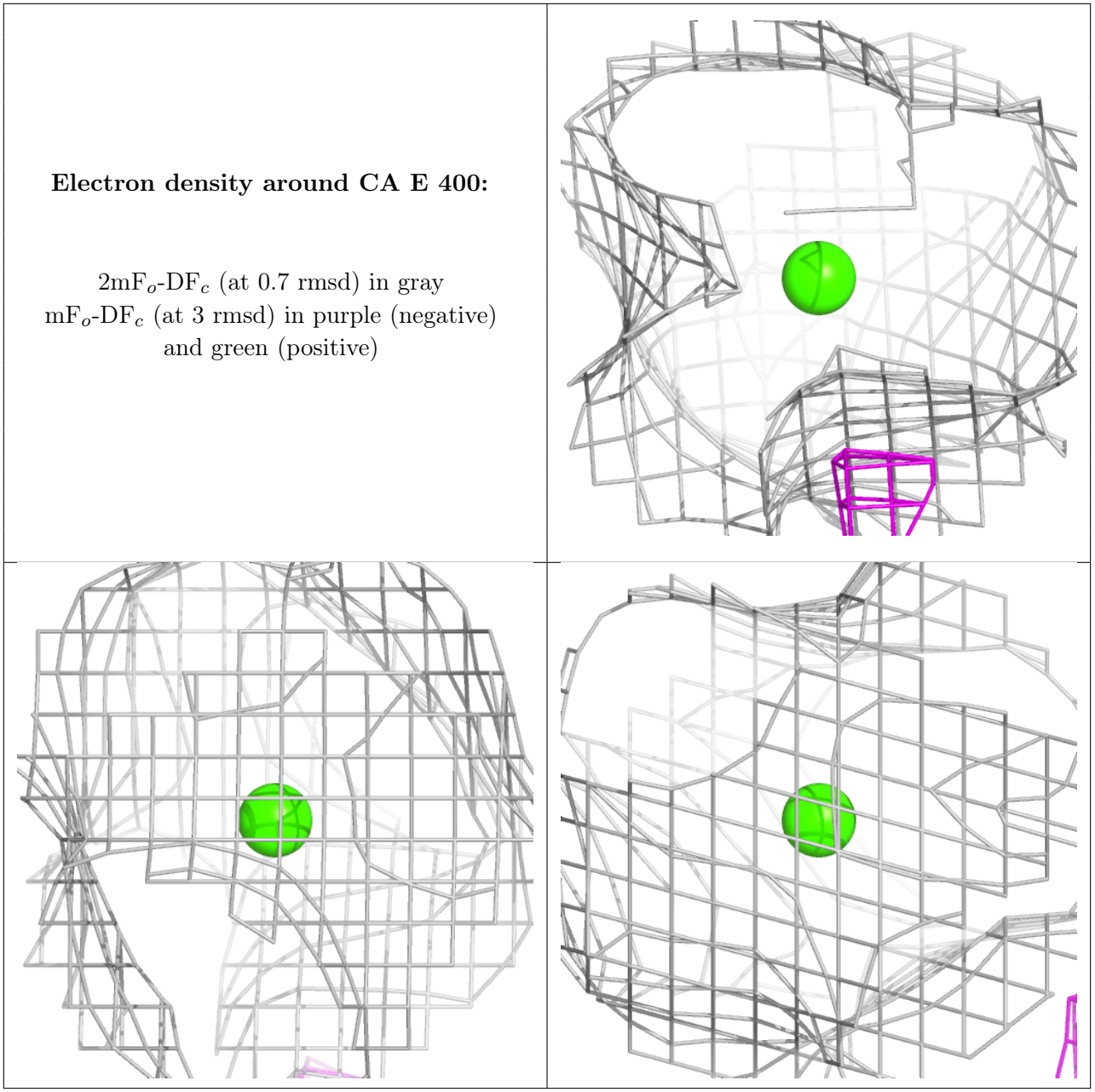
Electron density around CA B 400:

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



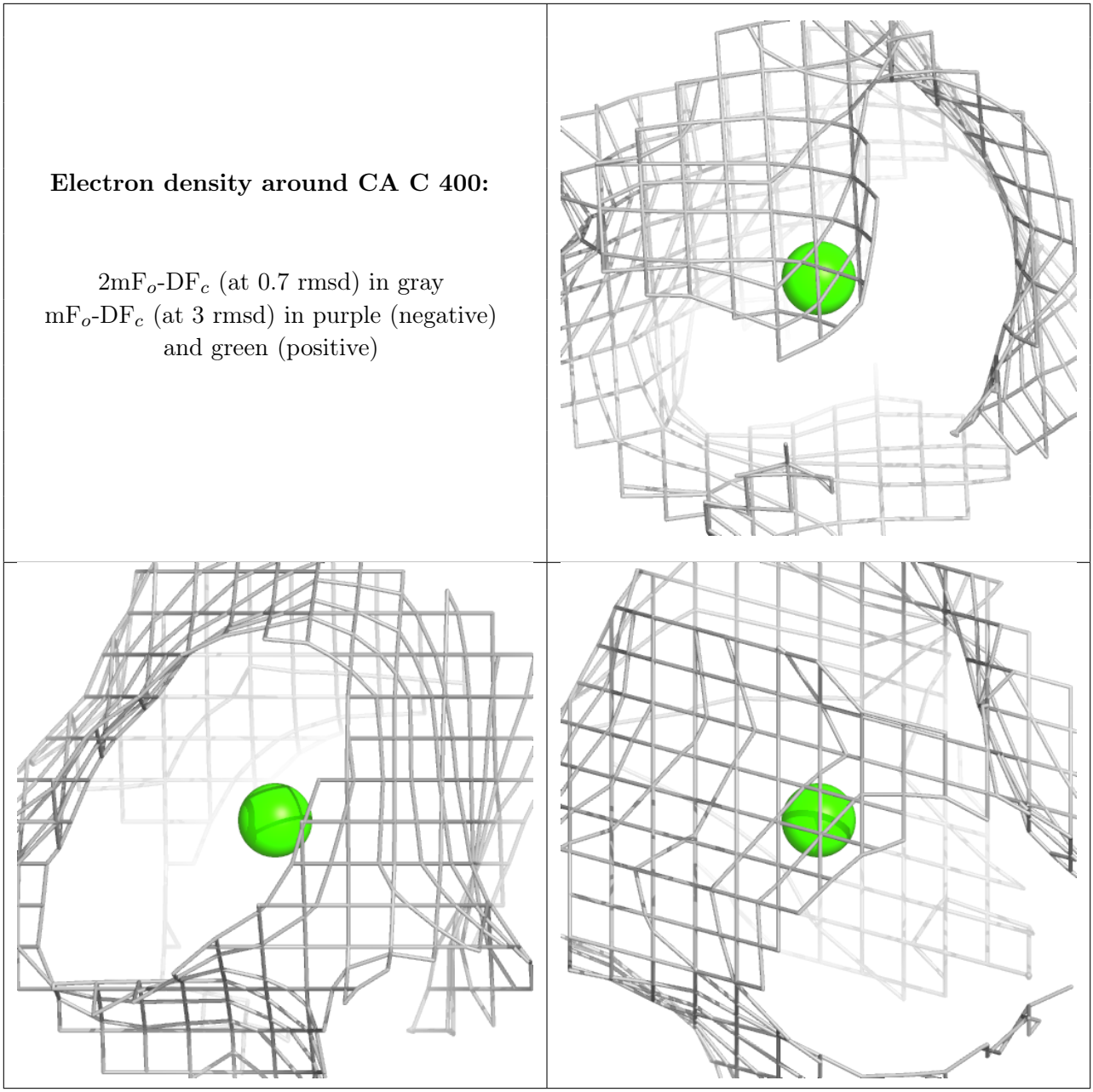
Electron density around CA E 400:

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



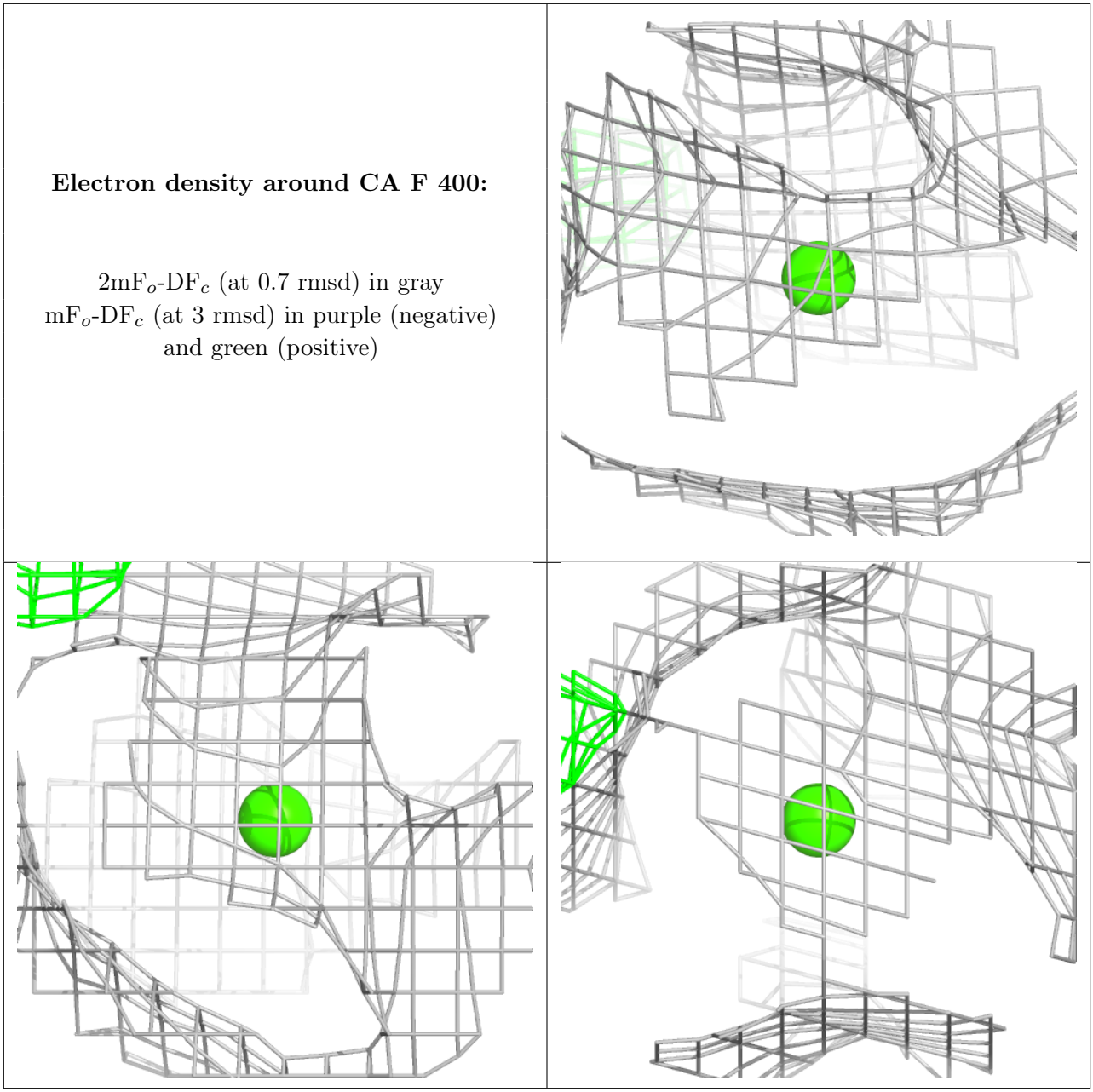
Electron density around CA C 400:

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



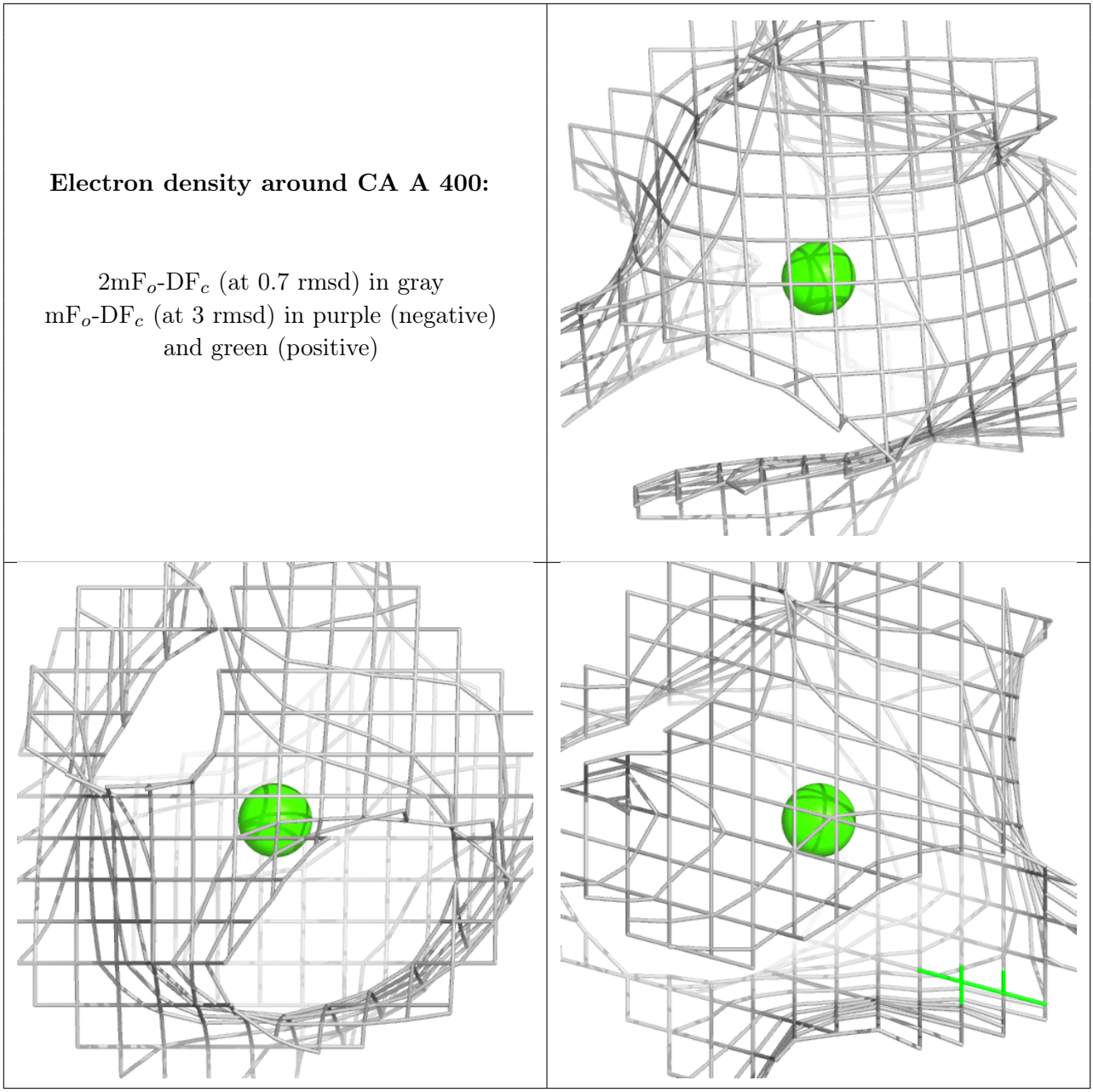
Electron density around CA F 400:

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



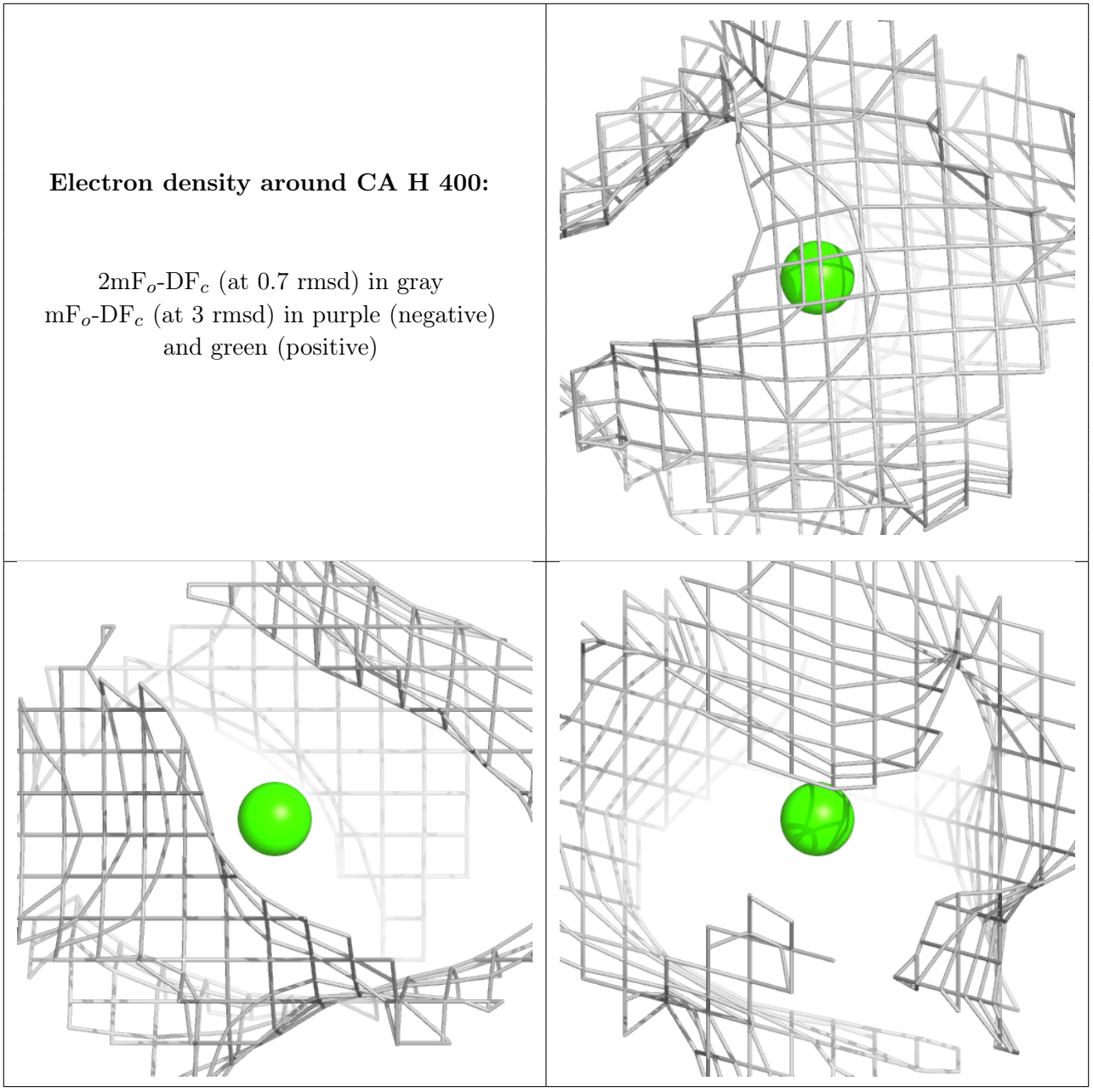
Electron density around CA A 400:

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



Electron density around CA H 400:

$2mF_o$-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.