Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 11:13 PM JST

PDB ID	:	9XGQ / pdb_00009xgq
Title	:	IgM-degrading enzyme
Authors	:	Chen, C.; Gu, Y.; Zhang, K.Y.
Deposited on	:	2025-10-30
Resolution	:	2.21 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 (1)) were used in the production of this report:

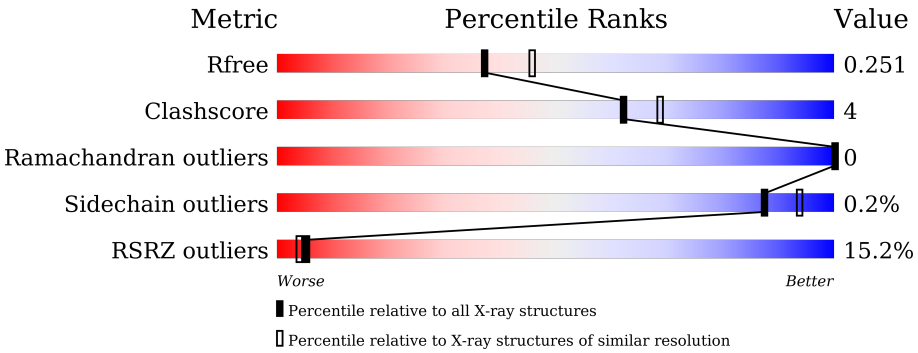
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	325	14% 85% 11% .
1	B	325	16% 90% 6% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5238 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 IdeS/Mac family cysteine endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2513	1588	418	499	8			
1	B	313	Total	C	N	O	S	0	0	0
			2513	1588	418	499	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0ABT2TEQ6
A	-2	PRO	-	expression tag	UNP A0ABT2TEQ6
A	-1	LEU	-	expression tag	UNP A0ABT2TEQ6
A	0	GLY	-	expression tag	UNP A0ABT2TEQ6
A	1	SER	-	expression tag	UNP A0ABT2TEQ6
B	-3	GLY	-	expression tag	UNP A0ABT2TEQ6
B	-2	PRO	-	expression tag	UNP A0ABT2TEQ6
B	-1	LEU	-	expression tag	UNP A0ABT2TEQ6
B	0	GLY	-	expression tag	UNP A0ABT2TEQ6
B	1	SER	-	expression tag	UNP A0ABT2TEQ6

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

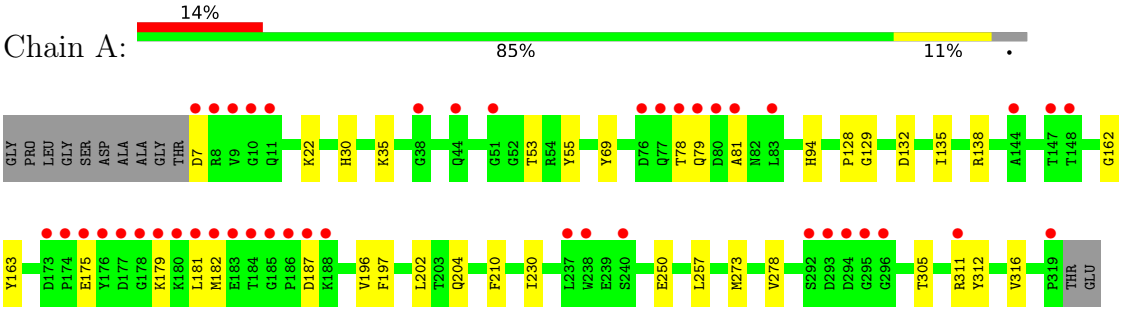
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	108	Total O 108 108	0	0

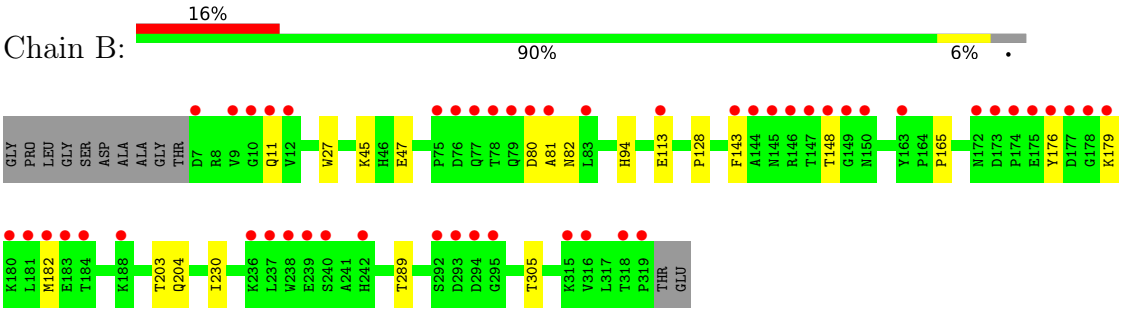
3 Residue-property plots (i)

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: IdeS/Mac family cysteine endopeptidase



• Molecule 1: IdeS/Mac family cysteine endopeptidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.26Å 77.17Å 136.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.09 – 2.21 41.09 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.09-2.21) 92.5 (41.09-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.228 , 0.253 0.228 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5238	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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: NA

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	0.30	0/2586	0.47	0/3516
1	B	0.40	0/2586	0.59	3/3516 (0.1%)
All	All	0.36	0/5172	0.53	3/7032 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	179	LYS	N-CA-C	-5.94	104.88	111.36
1	B	289	THR	N-CA-C	-5.40	106.07	113.30
1	B	176	TYR	CB-CA-C	-5.33	110.41	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2513	0	2320	28	0
1	B	2513	0	2320	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	102	0	0	4	0
3	B	108	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5238	0	4640	40	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 4.

All (40) 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:A:181:LEU:HG	3:A:563:HOH:O	1.48	1.10
1:A:204:GLN:HB2	1:A:305:THR:OG1	1.78	0.83
1:A:311:ARG:HH12	1:B:81:ALA:HB2	1.45	0.80
1:A:311:ARG:HH12	1:B:81:ALA:CB	1.96	0.79
1:B:204:GLN:HB2	1:B:305:THR:OG1	1.83	0.78
1:A:175:GLU:HA	1:A:179:LYS:HB2	1.68	0.76
1:A:53:THR:HG23	1:A:55:TYR:CE2	2.27	0.69
1:A:311:ARG:NH1	1:B:81:ALA:HB2	2.12	0.65
1:A:129:GLY:H	1:A:132:ASP:HB2	1.63	0.62
1:B:45:LYS:NZ	1:B:47:GLU:OE1	2.24	0.62
1:B:113:GLU:O	1:B:113:GLU:HG2	2.01	0.61
1:A:81:ALA:N	3:A:506:HOH:O	2.36	0.57
1:A:138:ARG:NH1	3:A:505:HOH:O	2.36	0.56
1:A:196:VAL:HA	1:A:316:VAL:HG11	1.87	0.55
1:B:143:PHE:HZ	1:B:165:PRO:HG2	1.73	0.53
1:B:94:HIS:CE1	1:B:128:PRO:HG3	2.44	0.52
1:A:204:GLN:CB	1:A:305:THR:OG1	2.53	0.52
1:A:94:HIS:CE1	1:A:135:ILE:HD12	2.46	0.50
1:B:80:ASP:O	1:B:82:ASN:N	2.39	0.50
1:A:204:GLN:NE2	3:A:509:HOH:O	2.45	0.49
1:A:162:GLY:O	1:A:187:ASP:HB2	2.13	0.49
1:B:11:GLN:HB3	1:B:27:TRP:HB2	1.93	0.49
1:B:204:GLN:CB	1:B:305:THR:OG1	2.59	0.48
1:A:7:ASP:HA	1:A:30:HIS:HA	1.98	0.46
1:B:143:PHE:CE1	1:B:148:THR:HG22	2.51	0.46
1:A:78:THR:HG23	1:A:79:GLN:HG3	1.97	0.46
1:A:312:TYR:O	1:A:316:VAL:HG22	2.16	0.46
1:A:197:PHE:CE1	1:A:202:LEU:HD11	2.51	0.45
1:A:273:MET:HE2	1:A:273:MET:HB2	1.92	0.44
1:A:210:PHE:CZ	1:B:47:GLU:HB3	2.53	0.43
1:A:250:GLU:O	1:A:257:LEU:HD12	2.19	0.43
1:A:35:LYS:HA	1:A:35:LYS:HD3	1.78	0.43
1:A:22:LYS:HE2	1:A:22:LYS:HB3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HD23	1:A:278:VAL:HG11	2.02	0.42
1:B:203:THR:HA	1:B:305:THR:O	2.20	0.42
1:A:163:TYR:CE1	1:A:182:MET:HG2	2.54	0.41
1:B:230:ILE:HD12	1:B:230:ILE:HA	1.89	0.41
1:B:113:GLU:O	1:B:113:GLU:CG	2.67	0.41
1:A:69:TYR:CE1	1:A:128:PRO:HD2	2.57	0.40
1:A:230:ILE:HD12	1:A:230:ILE:HA	1.96	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	311/325 (96%)	291 (94%)	20 (6%)	0	100	100
1	B	311/325 (96%)	300 (96%)	11 (4%)	0	100	100
All	All	622/650 (96%)	591 (95%)	31 (5%)	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	262/269 (97%)	262 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	262/269 (97%)	261 (100%)	1 (0%)	84 91
All	All	524/538 (97%)	523 (100%)	1 (0%)	87 94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	182	MET

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

Mol	Chain	Res	Type
1	A	204	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	313/325 (96%)	0.74	44 (14%)	6	5	23, 39, 98, 141	0
1	B	313/325 (96%)	0.83	51 (16%)	4	3	26, 42, 108, 161	0
All	All	626/650 (96%)	0.78	95 (15%)	5	4	23, 41, 100, 161	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	TRP	8.4
1	A	181	LEU	8.1
1	B	173	ASP	7.6
1	B	181	LEU	7.4
1	B	176	TYR	6.8
1	A	176	TYR	6.5
1	A	182	MET	6.3
1	A	238	TRP	5.9
1	B	174	PRO	5.7
1	B	113	GLU	5.6
1	A	186	PRO	5.5
1	A	178	GLY	5.2
1	B	178	GLY	5.2
1	B	78	THR	5.1
1	A	185	GLY	5.1
1	B	175	GLU	4.8
1	B	177	ASP	4.7
1	A	9	VAL	4.6
1	B	293	ASP	4.6
1	A	7	ASP	4.5
1	A	174	PRO	4.5
1	A	79	GLN	4.3
1	B	237	LEU	4.3
1	B	75	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	143	PHE	4.2
1	B	179	LYS	4.2
1	B	145	ASN	4.1
1	B	319	PRO	4.1
1	A	319	PRO	4.1
1	A	147	THR	4.1
1	A	10	GLY	4.1
1	A	237	LEU	4.0
1	A	184	THR	3.9
1	A	183	GLU	3.9
1	B	182	MET	3.8
1	B	292	SER	3.8
1	B	180	LYS	3.7
1	A	148	THR	3.7
1	A	173	ASP	3.6
1	A	293	ASP	3.6
1	A	80	ASP	3.6
1	B	76	ASP	3.6
1	A	177	ASP	3.5
1	B	10	GLY	3.5
1	A	175	GLU	3.5
1	A	179	LYS	3.4
1	A	144	ALA	3.4
1	A	294	ASP	3.4
1	A	292	SER	3.3
1	A	187	ASP	3.3
1	B	294	ASP	3.3
1	B	295	GLY	3.2
1	A	76	ASP	3.2
1	B	183	GLU	3.1
1	B	7	ASP	3.1
1	A	78	THR	3.0
1	B	316	VAL	3.0
1	B	242	HIS	3.0
1	A	180	LYS	2.8
1	A	51	GLY	2.8
1	A	311	ARG	2.8
1	B	149	GLY	2.8
1	B	77	GLN	2.7
1	B	147	THR	2.6
1	B	79	GLN	2.6
1	A	81	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	318	THR	2.5
1	B	240	SER	2.5
1	B	80	ASP	2.5
1	B	188	LYS	2.4
1	B	81	ALA	2.4
1	B	148	THR	2.4
1	B	172	ASN	2.4
1	A	38	GLY	2.4
1	B	239	GLU	2.4
1	B	150	ASN	2.3
1	A	8	ARG	2.3
1	A	83	LEU	2.3
1	B	236	LYS	2.3
1	A	295	GLY	2.2
1	A	11	GLN	2.2
1	B	144	ALA	2.2
1	B	83	LEU	2.2
1	B	315	LYS	2.2
1	A	77	GLN	2.2
1	A	188	LYS	2.1
1	A	44	GLN	2.1
1	A	296	GLY	2.1
1	A	240	SER	2.1
1	B	12	VAL	2.1
1	B	163	TYR	2.1
1	B	146	ARG	2.1
1	B	184	THR	2.1
1	B	11	GLN	2.1
1	B	9	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 oligosaccharides in this entry.

6.4 Ligands (i)

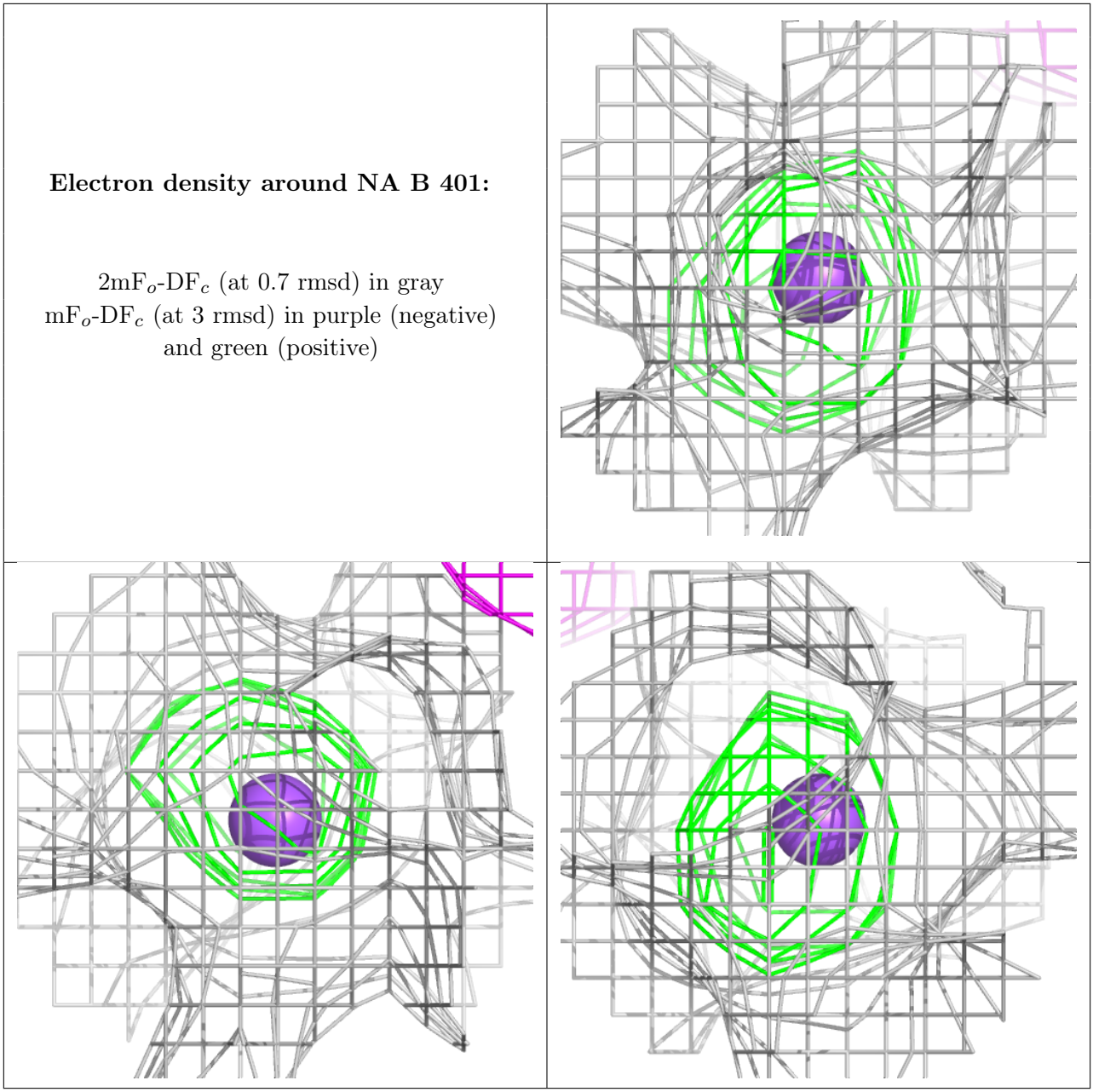
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NA	B	401	1/1	0.96	0.19	27,27,27,27	0
2	NA	A	401	1/1	0.97	0.06	22,22,22,22	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.

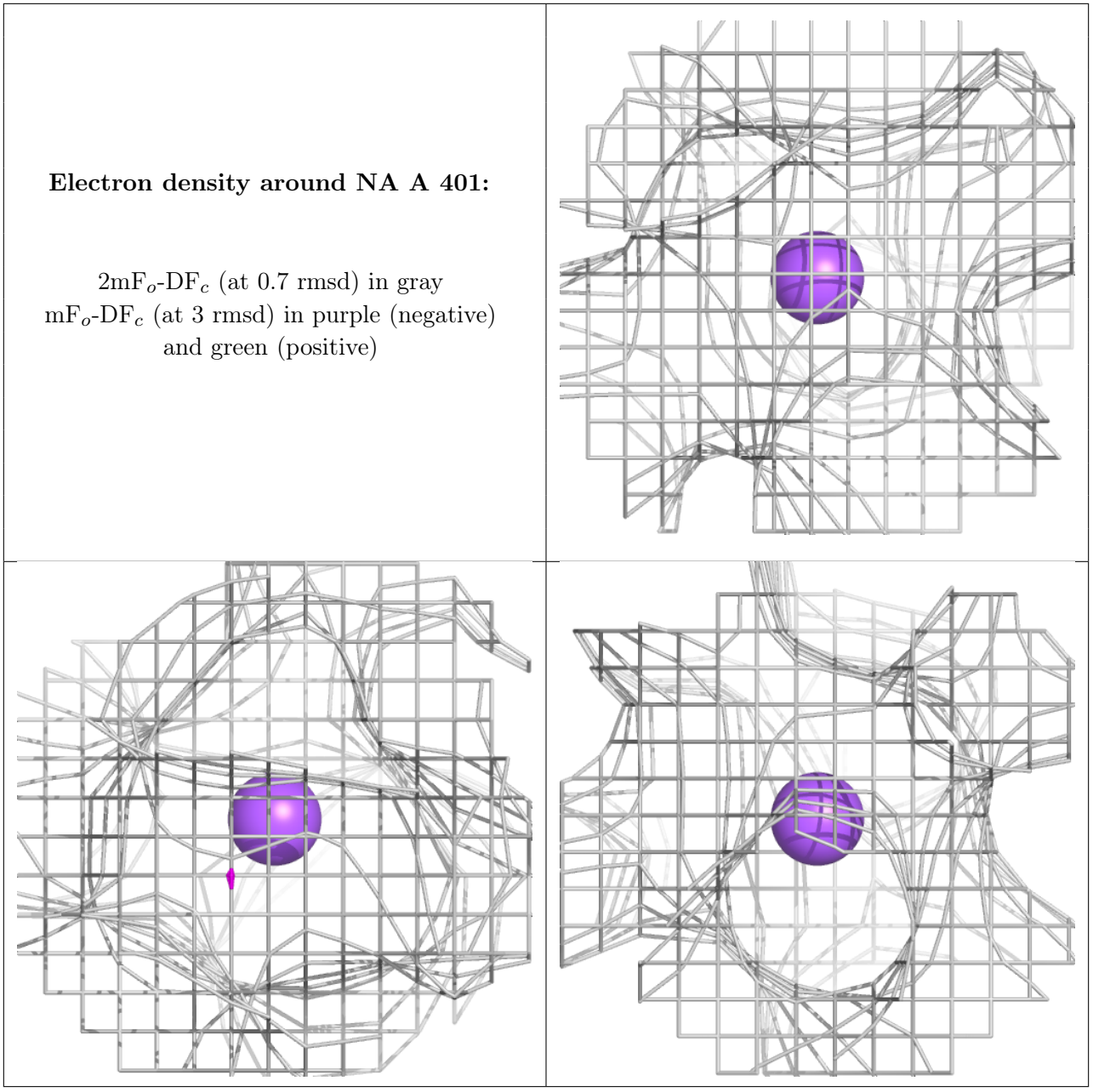
Electron density around NA B 401:

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



Electron density around NA A 401:

$2mF_o$-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.