



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:38 AM UTC

PDB ID : 6ILW / pdb_00006ilw
Title : Crystal structure of PETase from Ideonella sakaiensis
Authors : Liu, C.C.; Shi, C.
Deposited on : 2018-10-19
Resolution : 1.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

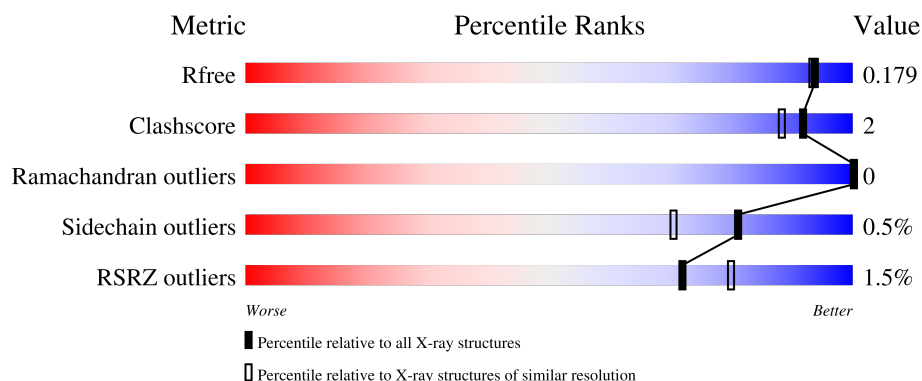
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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

Mol	Chain	Length	Quality of chain
1	A	270	37% 60% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2259 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 Poly(ethylene terephthalate) hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	1	0
			1961	1210	354	386	11			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP A0A0K8P6T7
A	291	HIS	-	expression tag	UNP A0A0K8P6T7
A	292	HIS	-	expression tag	UNP A0A0K8P6T7
A	293	HIS	-	expression tag	UNP A0A0K8P6T7
A	294	HIS	-	expression tag	UNP A0A0K8P6T7
A	295	HIS	-	expression tag	UNP A0A0K8P6T7
A	296	HIS	-	expression tag	UNP A0A0K8P6T7

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

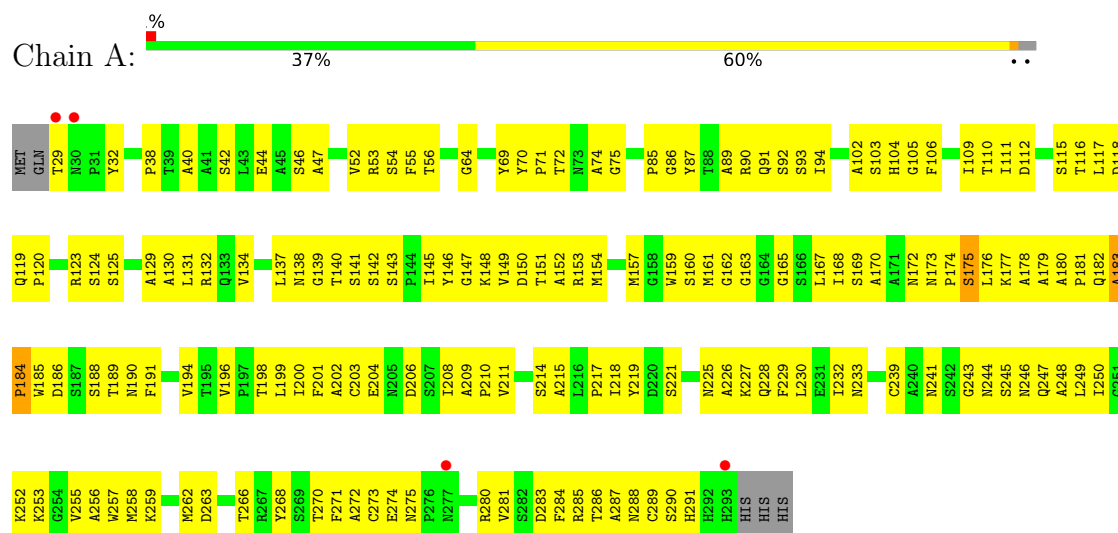
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	296	Total 296	O 296	0	0

3 Residue-property plots

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

- Molecule 1: Poly(ethylene terephthalate) hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.96Å 51.41Å 85.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.08 – 1.57 44.08 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.08-1.57) 99.5 (44.08-1.57)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.18 (at 1.58Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.160 , 0.176 0.165 , 0.179	Depositor DCC
R_{free} test set	1607 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2259	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2.33	153/2009 (7.6%)	1.20	11/2737 (0.4%)

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	ALA	C-O	-19.87	1.14	1.23
1	A	160	SER	C-O	-9.98	1.15	1.24
1	A	194	VAL	C-O	-9.71	1.14	1.24
1	A	70	TYR	C-O	-8.67	1.14	1.24
1	A	71	PRO	C-O	-8.66	1.14	1.23
1	A	284	PHE	C-O	-8.60	1.14	1.24
1	A	125	SER	C-O	-8.58	1.14	1.24
1	A	198	THR	C-O	-8.56	1.14	1.24
1	A	270	THR	C-O	-8.43	1.14	1.24
1	A	203	CYS	C-O	-8.39	1.14	1.24
1	A	229	PHE	C-O	-8.39	1.14	1.24
1	A	258	MET	C-O	-8.36	1.14	1.24
1	A	182	GLN	C-O	-8.26	1.14	1.24
1	A	169	SER	C-O	-8.24	1.14	1.24
1	A	176	LEU	C-O	-8.20	1.14	1.23
1	A	219	TYR	C-O	-8.18	1.14	1.24
1	A	106	PHE	C-O	-8.16	1.13	1.23
1	A	230	LEU	C-O	-8.08	1.14	1.24
1	A	173	ASN	C-O	-8.08	1.14	1.24
1	A	140	THR	C-O	-8.07	1.14	1.24
1	A	181	PRO	C-O	-8.06	1.14	1.23
1	A	52	VAL	C-O	-8.06	1.15	1.24
1	A	249	LEU	C-O	-8.03	1.14	1.24
1	A	153	ARG	C-O	-8.02	1.14	1.23
1	A	109	ILE	C-O	-8.00	1.15	1.24
1	A	272	ALA	C-O	-7.97	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	TRP	C-O	-7.94	1.15	1.24
1	A	159	TRP	C-O	-7.92	1.14	1.24
1	A	131	LEU	C-O	-7.81	1.15	1.24
1	A	154	MET	C-O	-7.78	1.14	1.23
1	A	248	ALA	C-O	-7.78	1.15	1.24
1	A	110	THR	C-O	-7.77	1.14	1.24
1	A	149	VAL	C-O	-7.68	1.15	1.24
1	A	157	MET	C-O	-7.66	1.14	1.23
1	A	150	ASP	C-O	-7.62	1.14	1.23
1	A	253	LYS	C-O	-7.55	1.15	1.24
1	A	268	TYR	C-O	-7.53	1.13	1.24
1	A	90	ARG	C-O	-7.52	1.14	1.24
1	A	134	VAL	C-O	-7.51	1.15	1.24
1	A	102	ALA	C-O	-7.50	1.14	1.24
1	A	285	ARG	C-O	-7.48	1.14	1.23
1	A	286	THR	C-O	-7.46	1.14	1.23
1	A	55	PHE	C-O	-7.28	1.14	1.23
1	A	263	ASP	C-O	-7.25	1.14	1.23
1	A	69	TYR	C-O	-7.22	1.15	1.24
1	A	209	ALA	C-O	-7.20	1.15	1.24
1	A	167	LEU	C-O	-7.17	1.15	1.24
1	A	44	GLU	C-O	-7.14	1.14	1.24
1	A	91	GLN	C-O	-7.12	1.15	1.24
1	A	38	PRO	C-O	-7.11	1.15	1.23
1	A	215	ALA	C-O	-7.03	1.15	1.24
1	A	129	ALA	C-O	-7.02	1.16	1.24
1	A	281	VAL	C-O	-6.99	1.16	1.24
1	A	170	ALA	C-O	-6.98	1.16	1.24
1	A	142	SER	C-O	-6.97	1.14	1.24
1	A	233	ASN	C-O	-6.89	1.15	1.23
1	A	287	ALA	C-O	-6.89	1.15	1.23
1	A	289	CYS	C-O	-6.87	1.15	1.23
1	A	226	ALA	C-O	-6.83	1.15	1.23
1	A	117	LEU	C-O	-6.82	1.15	1.24
1	A	53	ARG	C-O	-6.81	1.15	1.23
1	A	283	ASP	C-O	-6.80	1.15	1.24
1	A	256	ALA	C-O	-6.75	1.16	1.24
1	A	124	SER	C-O	-6.73	1.16	1.24
1	A	139	GLY	C-O	-6.72	1.17	1.24
1	A	291	HIS	C-O	-6.71	1.15	1.23
1	A	87	TYR	C-O	-6.71	1.15	1.23
1	A	178	ALA	C-O	-6.69	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	VAL	C-O	-6.67	1.16	1.24
1	A	250	ILE	C-O	-6.64	1.16	1.24
1	A	185	TRP	C-O	-6.62	1.15	1.23
1	A	145	ILE	C-O	-6.62	1.14	1.23
1	A	206	ASP	C-O	-6.61	1.16	1.23
1	A	56	THR	C-O	-6.58	1.16	1.23
1	A	116	THR	C-O	-6.55	1.15	1.24
1	A	227	LYS	C-O	-6.53	1.15	1.23
1	A	163	GLY	C-O	-6.53	1.16	1.23
1	A	146	TYR	C-O	-6.53	1.16	1.24
1	A	210	PRO	C-O	-6.52	1.15	1.23
1	A	252	LYS	C-O	-6.51	1.16	1.24
1	A	143	SER	C-O	-6.46	1.15	1.23
1	A	85	PRO	C-O	-6.44	1.13	1.23
1	A	196	VAL	C-O	-6.43	1.16	1.24
1	A	228	GLN	C-O	-6.37	1.16	1.23
1	A	245	SER	C-O	-6.36	1.15	1.24
1	A	120	PRO	C-O	-6.33	1.16	1.24
1	A	255	VAL	C-O	-6.26	1.16	1.24
1	A	141	SER	C-O	-6.25	1.16	1.24
1	A	130	ALA	C-O	-6.24	1.16	1.24
1	A	190	ASN	C-O	-6.24	1.16	1.23
1	A	119	GLN	C-O	-6.22	1.14	1.23
1	A	179	ALA	C-O	-6.20	1.16	1.23
1	A	271	PHE	C-O	-6.19	1.16	1.24
1	A	184	PRO	C-O	-6.18	1.16	1.23
1	A	214	SER	C-O	-6.18	1.16	1.24
1	A	32	TYR	C-O	-6.14	1.15	1.23
1	A	118	ASP	C-O	-6.11	1.16	1.23
1	A	262	MET	C-O	-6.10	1.16	1.24
1	A	115	SER	C-O	-6.09	1.16	1.23
1	A	241	ASN	C-O	-6.09	1.16	1.23
1	A	175[A]	SER	C-O	-6.06	1.16	1.24
1	A	175[B]	SER	C-O	-6.06	1.16	1.24
1	A	244	ASN	C-O	-6.04	1.16	1.23
1	A	288	ASN	C-O	-6.02	1.15	1.23
1	A	208	ILE	C-O	-5.97	1.17	1.23
1	A	148	LYS	C-O	-5.96	1.16	1.24
1	A	103	SER	C-O	-5.95	1.16	1.24
1	A	42	SER	C-O	-5.95	1.17	1.24
1	A	217	PRO	C-O	-5.88	1.16	1.24
1	A	105	GLY	C-O	-5.86	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	ILE	C-O	-5.85	1.17	1.24
1	A	93	SER	C-O	-5.81	1.16	1.24
1	A	202	ALA	C-O	-5.80	1.16	1.23
1	A	201	PHE	C-O	-5.79	1.17	1.24
1	A	92	SER	C-O	-5.79	1.16	1.24
1	A	218	ILE	C-O	-5.77	1.17	1.24
1	A	132	ARG	C-O	-5.76	1.17	1.24
1	A	89	ALA	C-O	-5.74	1.16	1.23
1	A	111	ILE	C-O	-5.74	1.16	1.23
1	A	232	ILE	C-O	-5.73	1.17	1.24
1	A	138	ASN	C-O	-5.72	1.17	1.24
1	A	221	SER	C-O	-5.72	1.16	1.24
1	A	86	GLY	C-O	-5.70	1.16	1.23
1	A	273	CYS	C-O	-5.66	1.16	1.24
1	A	46	SER	C-O	-5.64	1.17	1.24
1	A	200	ILE	C-O	-5.63	1.18	1.24
1	A	123	ARG	C-O	-5.63	1.17	1.24
1	A	161	MET	C-O	-5.60	1.17	1.24
1	A	165	GLY	C-O	-5.60	1.16	1.23
1	A	247	GLN	C-O	-5.52	1.17	1.24
1	A	188	SER	C-O	-5.51	1.17	1.24
1	A	152	ALA	C-O	-5.47	1.16	1.24
1	A	47	ALA	C-O	-5.46	1.17	1.23
1	A	112	ASP	C-O	-5.41	1.17	1.23
1	A	40	ALA	C-O	-5.38	1.17	1.24
1	A	137	LEU	C-O	-5.34	1.17	1.24
1	A	75	GLY	C-O	-5.29	1.16	1.24
1	A	162	GLY	C-O	-5.28	1.17	1.23
1	A	54	SER	C-O	-5.28	1.17	1.23
1	A	243	GLY	C-O	-5.28	1.17	1.24
1	A	72	THR	C-O	-5.26	1.17	1.24
1	A	259	LYS	C-O	-5.25	1.18	1.24
1	A	191	PHE	C-O	-5.23	1.16	1.23
1	A	266	THR	C-O	-5.22	1.17	1.24
1	A	186	ASP	C-O	-5.18	1.17	1.23
1	A	151	THR	C-O	-5.17	1.17	1.24
1	A	290	SER	C-O	-5.13	1.17	1.23
1	A	147	GLY	C-O	-5.11	1.17	1.23
1	A	104	HIS	C-O	-5.11	1.17	1.24
1	A	189	THR	C-O	-5.09	1.17	1.24
1	A	172	ASN	C-O	-5.07	1.17	1.24
1	A	225	ASN	C-O	-5.07	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	PRO	C-O	-5.03	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	GLY	N-CA-C	7.37	121.41	112.49
1	A	52	VAL	N-CA-C	6.63	118.15	108.53
1	A	111	ILE	N-CA-C	6.47	119.08	108.99
1	A	141	SER	N-CA-C	5.95	118.56	111.71
1	A	74	ALA	N-CA-C	5.76	118.34	111.71
1	A	239	CYS	N-CA-C	5.74	119.38	112.38
1	A	275	ASN	N-CA-C	-5.59	101.47	109.24
1	A	273	CYS	N-CA-C	5.44	119.98	113.23
1	A	274	GLU	N-CA-C	5.19	117.82	110.50
1	A	204	GLU	N-CA-C	5.07	116.81	111.28
1	A	94	ILE	CB-CA-C	-5.02	105.41	110.93

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	1961	0	1877	6	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	296	0	0	0	0
All	All	2259	0	1877	6	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 2.

All (6) 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:246:ASN:OD1	1:A:280:ARG:HD3	2.03	0.58
1:A:183:ALA:N	1:A:184:PRO:CD	2.80	0.45
1:A:175[A]:SER:O	1:A:177:LYS:HE3	2.17	0.45
1:A:177:LYS:HA	1:A:177:LYS:HD3	1.84	0.43
1:A:180:ALA:HA	1:A:199:LEU:O	2.18	0.43
1:A:175[B]:SER:O	1:A:177:LYS:HE3	2.21	0.41

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	264/270 (98%)	260 (98%)	4 (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	212/216 (98%)	211 (100%)	1 (0%)	81 70

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

Mol	Chain	Res	Type
1	A	29	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	247	GLN
1	A	288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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 ⓘ

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 [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	265/270 (98%)	-0.16	4 (1%) 72 80	7, 12, 24, 44	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	HIS	5.5
1	A	29	THR	5.0
1	A	277	ASN	4.6
1	A	30	ASN	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

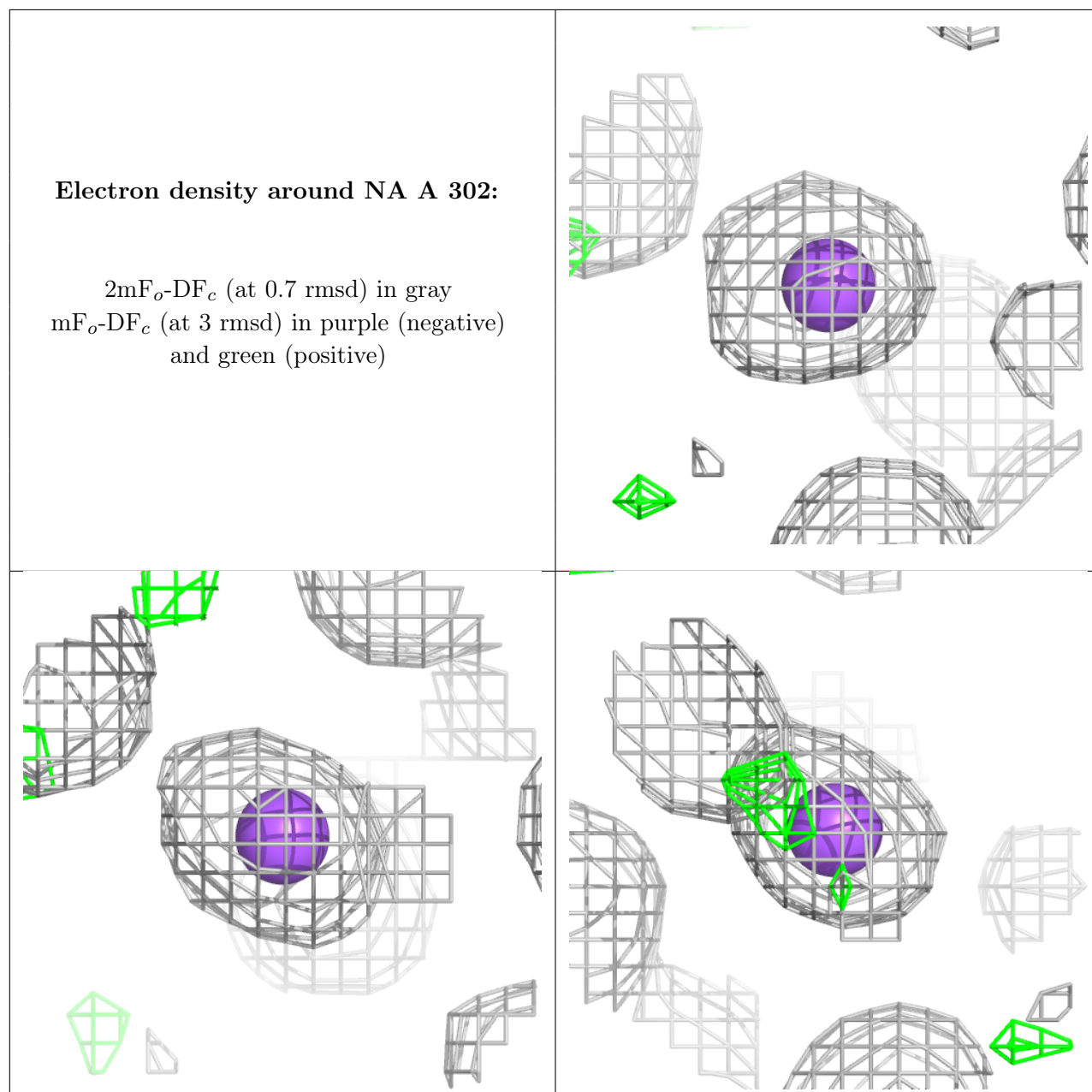
6.4 Ligands [i](#)

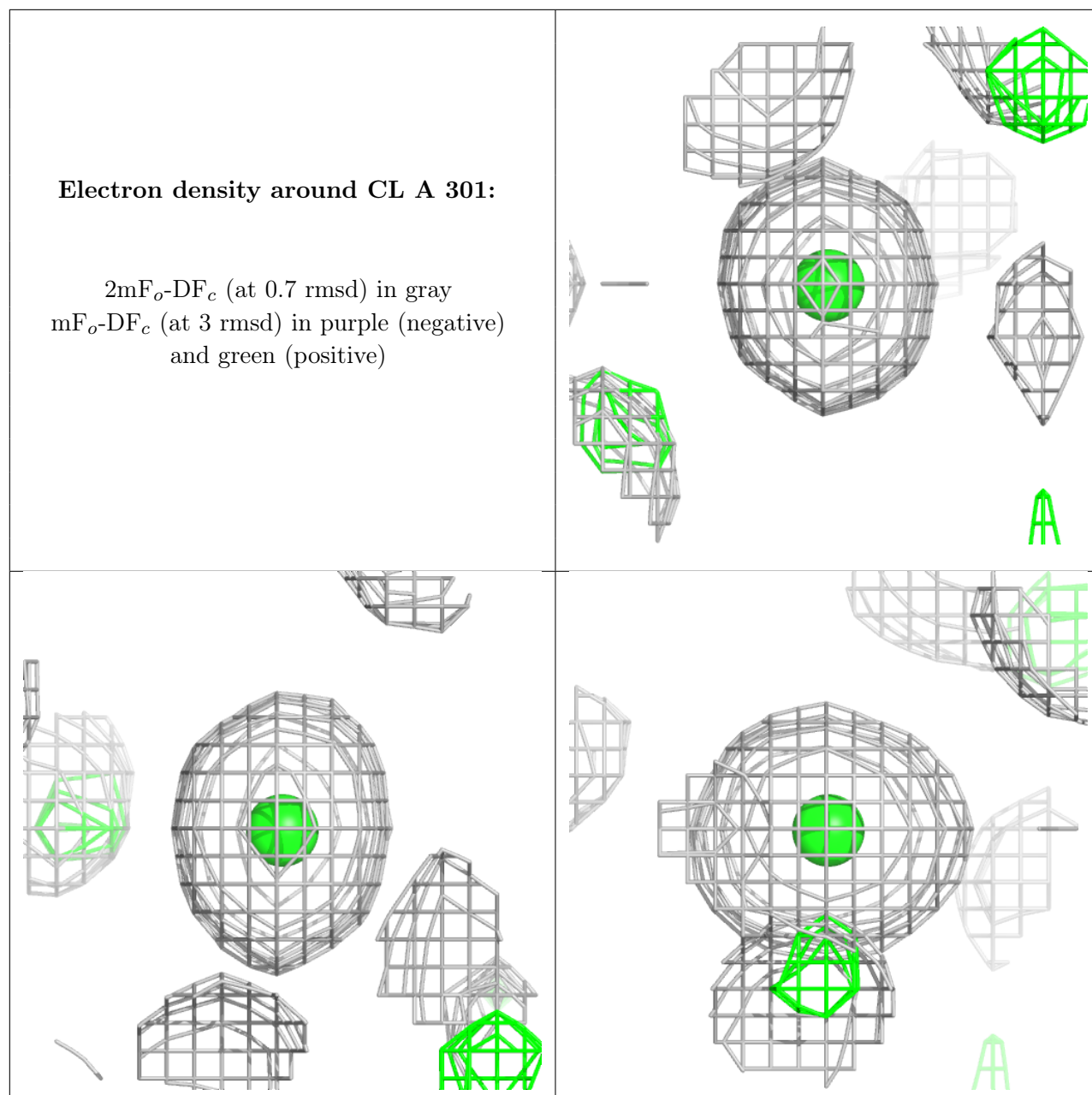
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	A	302	1/1	0.92	0.12	30,30,30,30	0
2	CL	A	301	1/1	0.99	0.05	20,20,20,20	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.