



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:57 AM UTC

PDB ID : 6WV2 / pdb_00006wv2
Title : Crystal Structure of Streptococcal Bacteriophage Hyaluronidase: Presence of a Prokaryotic Collagen and Elucidation of Catalytic Mechanism
Authors : Deivanayagam, C.; Schormann, N.
Deposited on : 2020-05-05
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 ⓘ 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

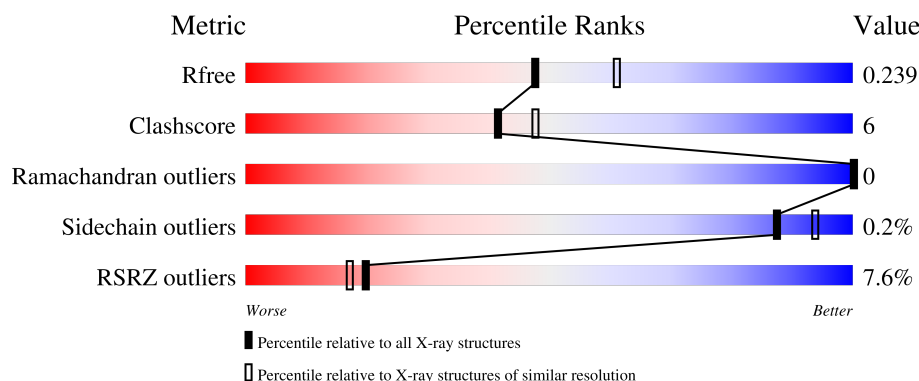
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	293	8% 83% 11% 7%
1	B	293	7% 83% 9% 8%
1	C	293	6% 79% 14% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6383 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 Hyaluronan Lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2044	1266	360	411	7			
1	B	271	Total	C	N	O	S	0	0	0
			2028	1257	358	406	7			
1	C	271	Total	C	N	O	S	0	0	0
			2028	1257	358	406	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	LEU	-	expression tag	UNP P15316
A	373	GLU	-	expression tag	UNP P15316
A	374	HIS	-	expression tag	UNP P15316
A	375	HIS	-	expression tag	UNP P15316
A	376	HIS	-	expression tag	UNP P15316
A	377	HIS	-	expression tag	UNP P15316
A	378	HIS	-	expression tag	UNP P15316
A	379	HIS	-	expression tag	UNP P15316
B	372	LEU	-	expression tag	UNP P15316
B	373	GLU	-	expression tag	UNP P15316
B	374	HIS	-	expression tag	UNP P15316
B	375	HIS	-	expression tag	UNP P15316
B	376	HIS	-	expression tag	UNP P15316
B	377	HIS	-	expression tag	UNP P15316
B	378	HIS	-	expression tag	UNP P15316
B	379	HIS	-	expression tag	UNP P15316
C	372	LEU	-	expression tag	UNP P15316
C	373	GLU	-	expression tag	UNP P15316
C	374	HIS	-	expression tag	UNP P15316
C	375	HIS	-	expression tag	UNP P15316
C	376	HIS	-	expression tag	UNP P15316
C	377	HIS	-	expression tag	UNP P15316
C	378	HIS	-	expression tag	UNP P15316

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Chain	Residue	Modelled	Actual	Comment	Reference
C	379	HIS	-	expression tag	UNP P15316

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

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

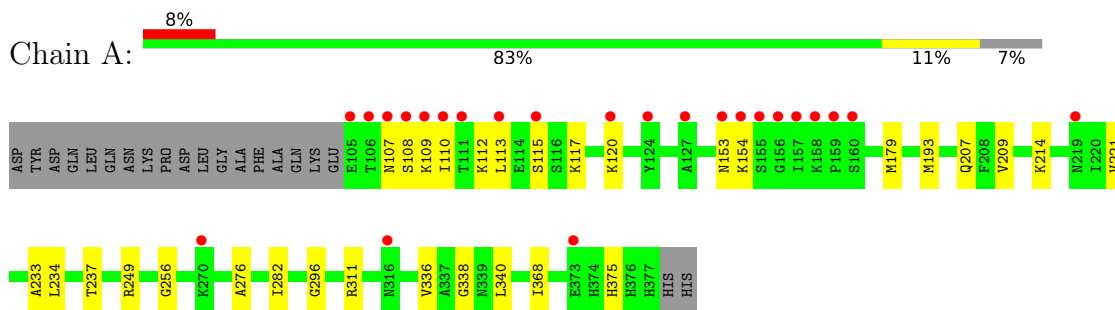
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	89	Total O 89 89	0	0
3	C	94	Total O 94 94	0	0

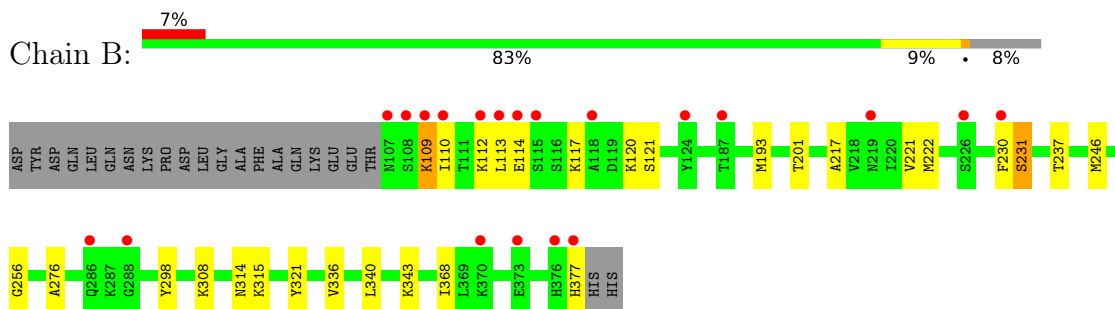
3 Residue-property plots [i](#)

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.

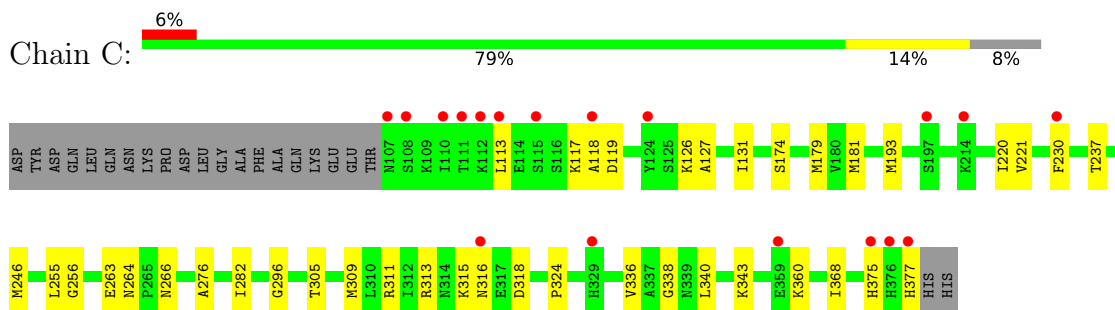
• Molecule 1: Hyaluronan Lyase



• Molecule 1: Hyaluronan Lyase



• Molecule 1: Hyaluronan Lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.45Å 86.79Å 168.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.61 – 2.21 38.61 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.61-2.21) 99.6 (38.61-2.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.79 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.213 , 0.237 0.214 , 0.239	Depositor DCC
R_{free} test set	2396 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6383	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

5.1 Standard geometry

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

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	0/2071	0.56	2/2781 (0.1%)
1	B	0.33	1/2055 (0.0%)	0.49	1/2759 (0.0%)
1	C	0.47	1/2055 (0.0%)	0.53	1/2759 (0.0%)
All	All	0.38	2/6181 (0.0%)	0.52	4/8299 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	SER	C-O	-5.05	1.17	1.23
1	C	174	SER	C-O	-5.03	1.17	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	SER	N-CA-C	-11.03	99.56	113.23
1	B	109	LYS	N-CA-C	-8.69	101.89	111.36
1	C	230	PHE	N-CA-C	5.82	120.24	113.20
1	A	154	LYS	N-CA-C	-5.74	101.61	109.71

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	2044	0	2071	34	0
1	B	2028	0	2058	34	0
1	C	2028	0	2058	54	0
2	A	1	0	0	0	0
3	A	99	0	0	1	0
3	B	89	0	0	0	0
3	C	94	0	0	0	0
All	All	6383	0	6187	78	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 (78) 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:B:377:HIS:CE1	1:C:377:HIS:CD2	2.21	1.28
1:A:375:HIS:CE1	1:C:375:HIS:CE1	2.33	1.17
1:C:375:HIS:CE1	1:C:377:HIS:CE1	2.49	0.99
1:B:377:HIS:HE1	1:C:377:HIS:CD2	1.71	0.99
1:C:311:ARG:CZ	1:C:313:ARG:NH2	2.32	0.92
1:B:377:HIS:CE1	1:C:377:HIS:HD2	1.84	0.86
1:A:117:LYS:HD3	1:B:117:LYS:HB3	1.57	0.84
1:A:375:HIS:HE1	1:C:375:HIS:CE1	1.95	0.81
1:B:377:HIS:CE1	1:C:377:HIS:NE2	2.48	0.81
1:A:375:HIS:CE1	1:C:375:HIS:HE1	1.96	0.79
1:A:375:HIS:NE2	1:C:375:HIS:CE1	2.51	0.78
1:A:120:LYS:HE2	1:C:118:ALA:HA	1.66	0.76
1:A:375:HIS:NE2	1:C:375:HIS:HE1	1.85	0.73
1:C:311:ARG:NH1	1:C:313:ARG:NH2	2.35	0.73
1:C:313:ARG:NE	1:C:318:ASP:OD1	2.23	0.71
1:C:305:THR:HG23	1:C:309:MET:HE1	1.73	0.70
1:A:368:ILE:HG21	1:C:368:ILE:HD13	1.73	0.70
1:A:113:LEU:HD11	1:B:110:ILE:HG23	1.75	0.69
1:A:234:LEU:HD23	1:C:246:MET:HE3	1.74	0.68
1:C:375:HIS:HE1	1:C:377:HIS:CE1	2.13	0.67
1:C:311:ARG:CZ	1:C:313:ARG:HH21	2.10	0.64
1:B:121:SER:O	1:C:126:LYS:NZ	2.20	0.64
1:B:377:HIS:NE2	1:C:377:HIS:NE2	2.47	0.62
1:A:120:LYS:HE2	1:C:119:ASP:H	1.63	0.62
1:C:309:MET:HE3	1:C:324:PRO:HA	1.81	0.61
1:A:117:LYS:HE3	1:B:114:GLU:HA	1.81	0.61
1:A:209:VAL:HG22	1:C:220:ILE:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ILE:HD13	1:C:368:ILE:HG21	1.84	0.60
1:B:109:LYS:O	1:B:112:LYS:N	2.36	0.58
1:A:214:LYS:HE2	1:B:201:THR:HA	1.85	0.58
1:C:113:LEU:O	1:C:117:LYS:HB2	2.03	0.58
1:B:343:LYS:HE2	1:C:338:GLY:HA2	1.84	0.58
1:A:115:SER:O	1:B:120:LYS:HE2	2.05	0.57
1:A:336:VAL:HG23	1:C:340:LEU:HD11	1.86	0.57
1:C:313:ARG:HG2	1:C:318:ASP:OD1	2.06	0.54
1:A:340:LEU:HD11	1:B:336:VAL:HG23	1.89	0.54
1:C:305:THR:CG2	1:C:309:MET:HE1	2.38	0.53
1:C:375:HIS:CE1	1:C:377:HIS:NE2	2.76	0.53
1:A:110:ILE:HA	1:A:113:LEU:HD12	1.92	0.52
1:C:375:HIS:NE2	1:C:377:HIS:CE1	2.77	0.52
1:B:193:MET:HE1	1:C:193:MET:HE1	1.93	0.51
1:A:338:GLY:HA2	1:C:343:LYS:HE3	1.92	0.51
1:C:264:ASN:ND2	1:C:266:ASN:O	2.44	0.51
1:B:222:MET:HE1	1:B:231:SER:O	2.12	0.49
1:A:179:MET:HE1	1:C:179:MET:HE1	1.95	0.48
1:B:113:LEU:O	1:B:117:LYS:HB2	2.14	0.48
1:B:237:THR:HG23	1:B:237:THR:O	2.13	0.48
1:C:179:MET:SD	1:C:181:MET:HE2	2.53	0.48
1:B:377:HIS:NE2	1:C:377:HIS:CD2	2.78	0.47
1:B:314:ASN:O	1:B:315:LYS:HB2	2.15	0.47
1:A:311:ARG:HD3	1:B:298:TYR:CD1	2.50	0.47
1:A:109:LYS:NZ	1:A:112:LYS:HD2	2.30	0.46
1:A:237:THR:HG22	1:B:221:VAL:HG22	1.98	0.46
1:C:315:LYS:O	1:C:316:ASN:HB2	2.16	0.46
1:C:127:ALA:O	1:C:131:ILE:HG12	2.16	0.45
1:B:308:LYS:HD3	1:B:321:TYR:CG	2.52	0.45
1:B:246:MET:HE1	1:C:246:MET:HE1	1.98	0.45
1:A:117:LYS:HD3	1:B:117:LYS:CB	2.37	0.45
1:B:340:LEU:HD11	1:C:336:VAL:HG23	1.98	0.45
1:A:221:VAL:HG22	1:C:237:THR:HG22	1.99	0.44
1:B:276:ALA:O	1:C:256:GLY:HA2	2.19	0.43
1:A:207:GLN:HE21	1:A:209:VAL:CG1	2.31	0.43
3:A:573:HOH:O	1:C:360:LYS:HD2	2.18	0.43
1:A:276:ALA:O	1:B:256:GLY:HA2	2.18	0.42
1:C:375:HIS:CE1	1:C:377:HIS:HE1	2.23	0.42
1:C:311:ARG:HD3	1:C:313:ARG:NE	2.34	0.42
1:A:233:ALA:O	1:B:217:ALA:HB3	2.20	0.42
1:A:249:ARG:NH1	1:C:263:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:THR:CG2	1:C:221:VAL:HG22	2.49	0.42
1:B:222:MET:HE1	1:B:231:SER:C	2.45	0.42
1:B:230:PHE:CE1	1:C:255:LEU:HD11	2.56	0.41
1:A:282:ILE:HD11	1:A:296:GLY:HA2	2.01	0.41
1:C:313:ARG:HG2	1:C:318:ASP:HA	2.02	0.41
1:A:193:MET:HE1	1:B:193:MET:HE1	2.02	0.41
1:C:282:ILE:HD11	1:C:296:GLY:HA2	2.02	0.41
1:A:256:GLY:HA2	1:C:276:ALA:O	2.21	0.41
1:A:120:LYS:HG2	1:C:118:ALA:HA	2.03	0.40
1:A:107:ASN:OD1	1:A:107:ASN:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	271/293 (92%)	267 (98%)	4 (2%)	0	100	100
1	B	269/293 (92%)	263 (98%)	6 (2%)	0	100	100
1	C	269/293 (92%)	265 (98%)	4 (2%)	0	100	100
All	All	809/879 (92%)	795 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	223/240 (93%)	222 (100%)	1 (0%)	84	91
1	B	221/240 (92%)	221 (100%)	0	100	100
1	C	221/240 (92%)	221 (100%)	0	100	100
All	All	665/720 (92%)	664 (100%)	1 (0%)	87	94

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

Mol	Chain	Res	Type
1	A	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	207	GLN
1	A	247	GLN
1	B	207	GLN
1	B	247	GLN
1	B	300	ASN
1	B	374	HIS
1	C	149	GLN
1	C	207	GLN
1	C	375	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

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, 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	273/293 (93%)	0.44	24 (8%) 15 13	22, 36, 84, 136	0
1	B	271/293 (92%)	0.39	20 (7%) 20 18	22, 35, 86, 115	0
1	C	271/293 (92%)	0.40	18 (6%) 24 21	22, 36, 85, 111	0
All	All	815/879 (92%)	0.41	62 (7%) 20 17	22, 36, 85, 136	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	ILE	6.9
1	A	106	THR	5.9
1	C	376	HIS	5.3
1	C	359	GLU	5.1
1	B	107	ASN	4.9
1	B	230	PHE	4.4
1	C	375	HIS	4.4
1	A	120	LYS	4.2
1	A	111	THR	4.2
1	C	377	HIS	4.1
1	C	107	ASN	4.1
1	A	154	LYS	3.9
1	A	270	LYS	3.6
1	B	377	HIS	3.6
1	C	316	ASN	3.5
1	B	286	GLN	3.5
1	A	153	ASN	3.4
1	A	157	ILE	3.4
1	C	230	PHE	3.4
1	B	110	ILE	3.3
1	C	108	SER	3.3
1	B	113	LEU	3.2
1	B	108	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	124	TYR	3.1
1	C	110	ILE	3.1
1	A	107	ASN	3.0
1	A	105	GLU	2.9
1	C	124	TYR	2.8
1	A	373	GLU	2.8
1	B	376	HIS	2.8
1	B	109	LYS	2.8
1	C	112	LYS	2.7
1	B	114	GLU	2.7
1	A	156	GLY	2.6
1	A	219	ASN	2.6
1	A	124	TYR	2.5
1	B	112	LYS	2.5
1	B	373	GLU	2.4
1	C	115	SER	2.4
1	A	108	SER	2.4
1	A	158	LYS	2.4
1	A	316	ASN	2.4
1	B	187	THR	2.4
1	A	109	LYS	2.4
1	B	115	SER	2.4
1	B	118	ALA	2.3
1	A	159	PRO	2.3
1	C	111	THR	2.3
1	A	160	SER	2.2
1	C	197	SER	2.2
1	B	226	SER	2.2
1	B	219	ASN	2.1
1	A	155	SER	2.1
1	C	113	LEU	2.1
1	B	288	GLY	2.1
1	A	127	ALA	2.1
1	C	118	ALA	2.1
1	A	115	SER	2.1
1	B	370	LYS	2.1
1	C	214	LYS	2.0
1	C	329	HIS	2.0
1	A	113	LEU	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](#)

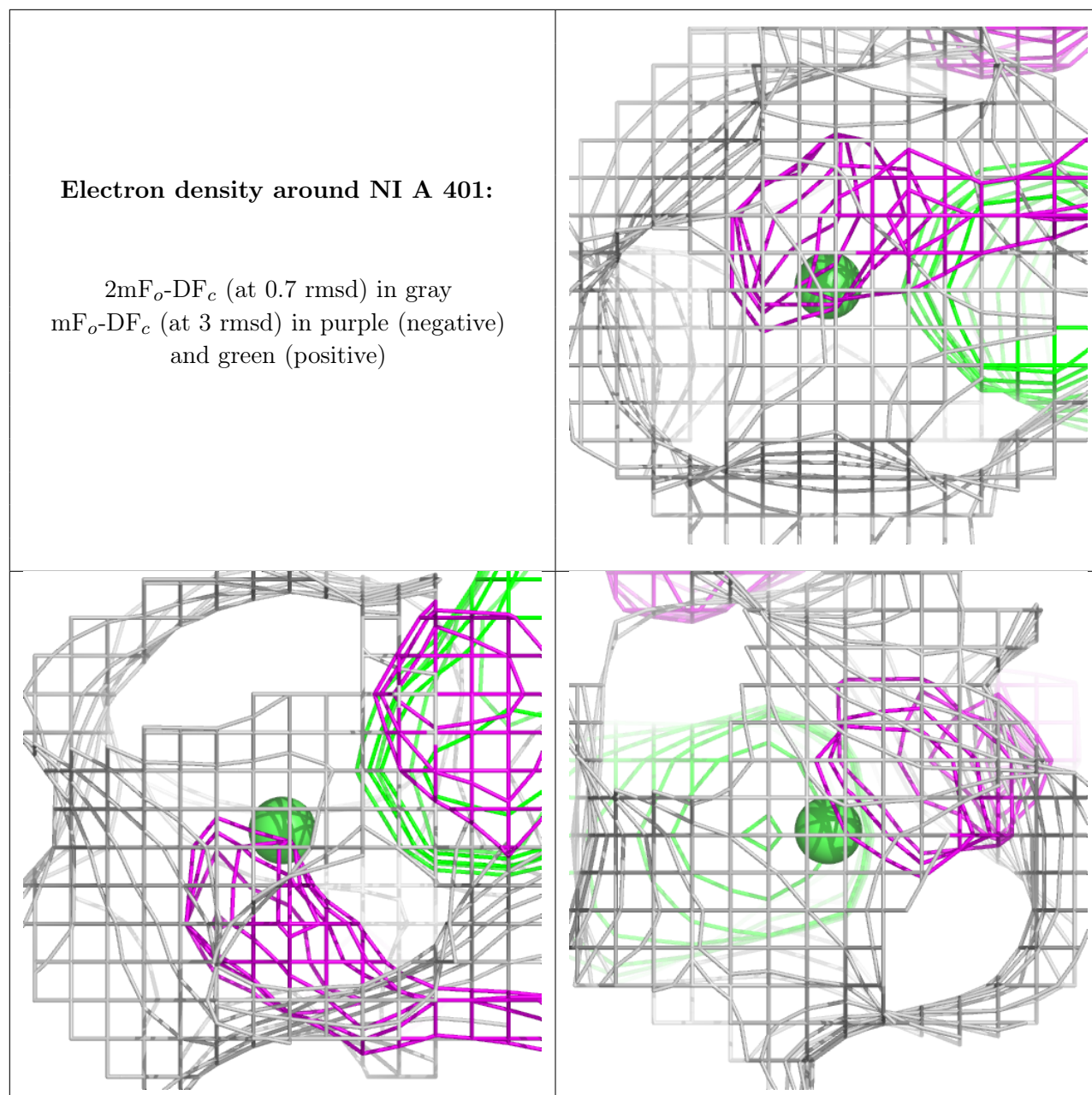
There are no oligosaccharides in this entry.

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, 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($\text{\AA}^2$)	Q<0.9
2	NI	A	401	1/1	0.91	0.09	65,65,65,65	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.