



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:52 AM UTC

PDB ID : 2FR0 / pdb_00002fr0
Title : The first ketoreductase of the erythromycin synthase (crystal form 1)
Authors : Keatinge-Clay, A.T.; Stroud, R.M.
Deposited on : 2006-01-18
Resolution : 1.81 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

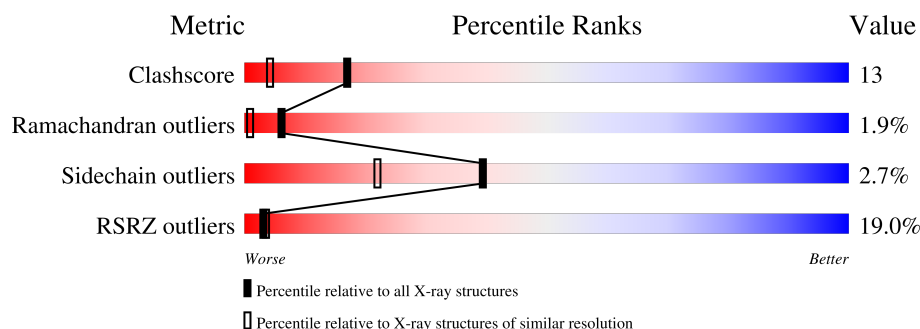
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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))
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	486	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDP	A	201	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3696 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.

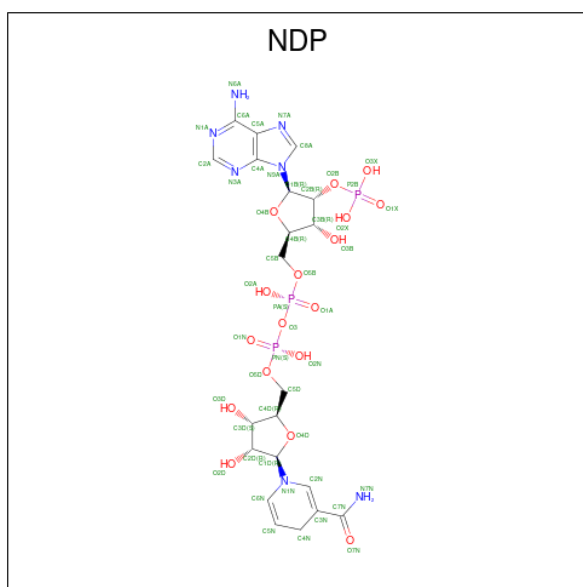
- Molecule 1 is a protein called Erythromycin synthase, EryAI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3468	2155	638	667	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1440	GLY	-	cloning artifact	UNP Q03131
A	1441	SER	-	cloning artifact	UNP Q03131
A	1442	HIS	-	cloning artifact	UNP Q03131
A	1443	MET	-	cloning artifact	UNP Q03131

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



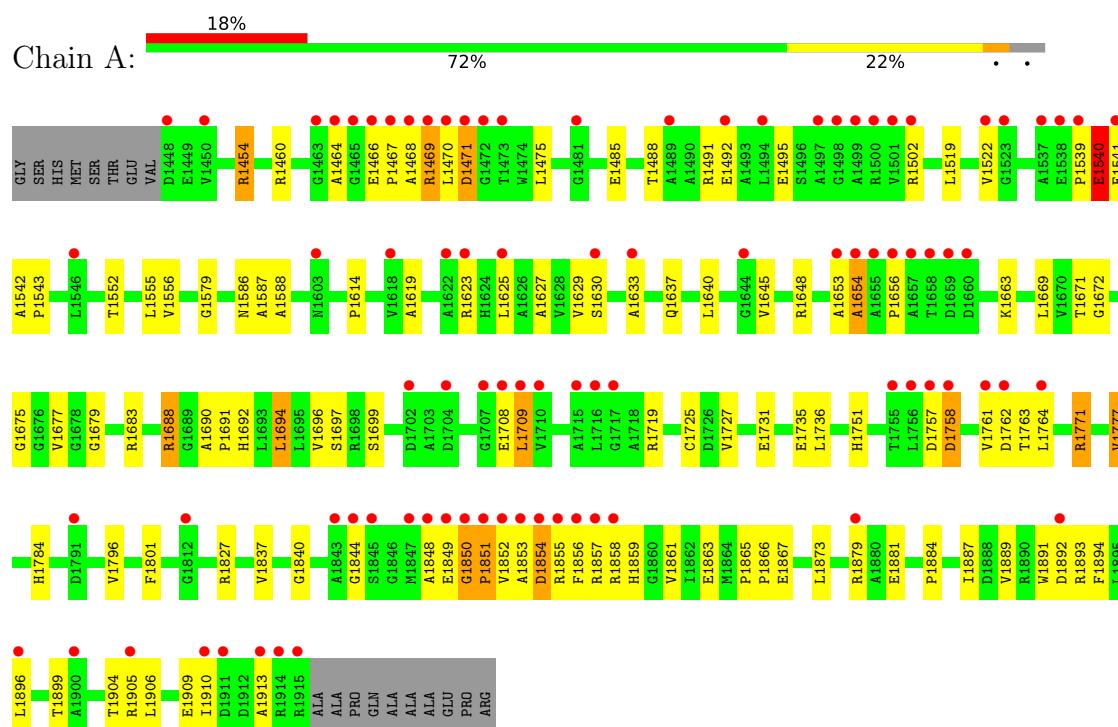
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total 180	O 180	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: Erythromycin synthase, EryAI



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.21Å 46.33Å 61.51Å 94.73° 90.17° 98.89°	Depositor
Resolution (Å)	45.60 – 1.81 45.60 – 1.81	Depositor EDS
% Data completeness (in resolution range)	93.7 (45.60-1.81) 87.8 (45.60-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.263 0.249 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3696	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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: NDP

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	0.43	0/3531	0.89	9/4813 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1840	GLY	N-CA-C	-6.72	100.73	112.55
1	A	1454	ARG	N-CA-C	6.00	118.49	108.96
1	A	1796	VAL	N-CA-C	5.98	116.72	107.99
1	A	1672	GLY	N-CA-C	-5.82	105.94	114.90
1	A	1891	TRP	N-CA-C	5.56	118.06	111.33
1	A	1777	VAL	N-CA-C	5.52	115.72	110.53
1	A	1579	GLY	CA-C-N	5.47	126.67	119.84
1	A	1579	GLY	C-N-CA	5.47	126.67	119.84
1	A	1865	PRO	N-CA-C	-5.25	104.29	110.70

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	3468	0	3418	86	0
2	A	48	0	25	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	180	0	0	5	0
All	All	3696	0	3443	88	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 13.

All (88) 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:1771:ARG:HH11	1:A:1771:ARG:HB3	1.28	0.97
1:A:1849:GLU:HG3	1:A:1853:ALA:HB3	1.48	0.95
1:A:1784:HIS:HD2	1:A:1827:ARG:HH11	1.10	0.93
1:A:1675:GLY:HA3	2:A:201:NDP:H52A	1.59	0.83
1:A:1761:VAL:HA	1:A:1764:LEU:HD12	1.61	0.82
1:A:1699:SER:HB2	2:A:201:NDP:O2X	1.81	0.81
1:A:1677:VAL:HB	2:A:201:NDP:H51N	1.64	0.78
1:A:1784:HIS:CD2	1:A:1827:ARG:HH11	2.02	0.73
1:A:1801:PHE:CE2	2:A:201:NDP:H5N	2.25	0.71
1:A:1762:ASP:OD1	1:A:1763:THR:HG23	1.91	0.69
1:A:1467:PRO:HB3	1:A:1627:ALA:HA	1.75	0.69
1:A:1851:PRO:HB2	1:A:1855:ARG:NH2	2.09	0.68
1:A:1849:GLU:CG	1:A:1853:ALA:HB3	2.22	0.68
1:A:1784:HIS:HD2	1:A:1827:ARG:NH1	1.88	0.67
1:A:1468:ALA:O	1:A:1469:ARG:HG2	1.95	0.67
1:A:1619:ALA:O	1:A:1623:ARG:HD3	1.95	0.66
2:A:201:NDP:P2B	3:A:53:HOH:O	2.52	0.66
1:A:1696:VAL:CG1	1:A:1725:CYS:HB3	2.27	0.64
1:A:1910:ILE:HG22	1:A:1913:ALA:H	1.65	0.61
1:A:1867:GLU:H	1:A:1867:GLU:CD	2.10	0.60
1:A:1542:ALA:HB1	3:A:60:HOH:O	2.02	0.59
1:A:1696:VAL:HG13	1:A:1725:CYS:HB3	1.85	0.59
1:A:1697:SER:HB2	2:A:201:NDP:O2B	2.03	0.58
1:A:1892:ASP:O	1:A:1896:LEU:HD13	2.04	0.58
1:A:1677:VAL:CB	2:A:201:NDP:H51N	2.34	0.58
1:A:1837:VAL:HG21	1:A:1873:LEU:HD13	1.86	0.58
1:A:1771:ARG:HB3	1:A:1771:ARG:NH1	2.09	0.57
1:A:1851:PRO:HD2	1:A:1852:VAL:HG23	1.86	0.57
1:A:1863:GLU:H	1:A:1863:GLU:CD	2.11	0.56
1:A:1623:ARG:HG2	3:A:47:HOH:O	2.05	0.55
1:A:1857:ARG:HG3	3:A:11:HOH:O	2.06	0.55
1:A:1851:PRO:HD2	1:A:1852:VAL:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:PRO:HA	1:A:1630:SER:O	2.07	0.55
1:A:1727:VAL:HG22	2:A:201:NDP:N1A	2.24	0.52
1:A:1848:ALA:O	1:A:1849:GLU:HB3	2.08	0.52
1:A:1663:LYS:HG3	1:A:1688:ARG:NH2	2.26	0.51
1:A:1488:THR:O	1:A:1492:GLU:HG2	2.10	0.50
1:A:1454:ARG:HH22	1:A:1881:GLU:CD	2.20	0.50
1:A:1691:PRO:HB2	1:A:1692:HIS:ND1	2.26	0.50
1:A:1460:ARG:NH1	1:A:1909:GLU:HG2	2.27	0.50
1:A:1801:PHE:HE2	2:A:201:NDP:H5N	1.74	0.49
1:A:1654:ALA:HB3	1:A:1879:ARG:NH1	2.27	0.49
1:A:1669:LEU:HD13	1:A:1694:LEU:HD13	1.95	0.49
1:A:1586:ASN:ND2	1:A:1588:ALA:H	2.11	0.49
1:A:1697:SER:HB2	2:A:201:NDP:P2B	2.53	0.48
1:A:1696:VAL:HG11	1:A:1725:CYS:HB3	1.96	0.48
1:A:1552:THR:O	1:A:1556:VAL:HG23	2.14	0.48
1:A:1771:ARG:HH11	1:A:1771:ARG:CB	2.14	0.47
1:A:1519:LEU:O	1:A:1522:VAL:HG12	2.14	0.47
1:A:1475:LEU:HA	1:A:1502:ARG:O	2.14	0.47
1:A:1757:ASP:O	1:A:1758:ASP:HB2	2.15	0.47
1:A:1464:ALA:O	1:A:1633:ALA:HB2	2.15	0.47
1:A:1851:PRO:O	1:A:1854:ASP:OD1	2.33	0.46
1:A:1696:VAL:HG21	1:A:1736:LEU:HD21	1.98	0.46
1:A:1731:GLU:O	1:A:1735:GLU:HG3	2.15	0.46
1:A:1633:ALA:HB1	1:A:1905:ARG:NH1	2.30	0.46
1:A:1640:LEU:HD23	1:A:1645:VAL:HG13	1.98	0.46
1:A:1692:HIS:HD2	1:A:1719:ARG:CZ	2.28	0.46
1:A:1540:GLU:HB3	1:A:1541:GLU:H	1.58	0.45
1:A:1454:ARG:HB3	1:A:1653:ALA:HB3	1.98	0.45
1:A:1899:THR:HG22	1:A:1904:THR:HG22	1.98	0.45
1:A:1586:ASN:C	1:A:1586:ASN:HD22	2.23	0.45
1:A:1637:GLN:OE1	1:A:1648:ARG:HD3	2.16	0.45
1:A:1679:GLY:O	1:A:1683:ARG:HG3	2.17	0.45
1:A:1859:HIS:O	1:A:1894:PHE:HA	2.16	0.45
1:A:1697:SER:OG	2:A:201:NDP:O2X	2.27	0.45
1:A:1614:PRO:HD3	1:A:1640:LEU:O	2.17	0.44
1:A:1625:LEU:O	1:A:1629:VAL:HG22	2.18	0.44
1:A:1654:ALA:HB3	1:A:1879:ARG:HH12	1.81	0.44
1:A:1470:LEU:O	1:A:1471:ASP:HB2	2.17	0.44
1:A:1856:PHE:HB3	1:A:1861:VAL:HG23	1.99	0.44
1:A:1858:ARG:HA	1:A:1893:ARG:HH11	1.83	0.44
2:A:201:NDP:O2B	3:A:53:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1586:ASN:HD22	1:A:1587:ALA:N	2.15	0.44
1:A:1699:SER:HB2	2:A:201:NDP:P2B	2.58	0.43
1:A:1671:THR:OG1	1:A:1751:HIS:HA	2.18	0.43
1:A:1543:PRO:HG2	1:A:1777:VAL:CG1	2.49	0.42
1:A:1656:PRO:HA	1:A:1879:ARG:CG	2.49	0.42
1:A:1708:GLU:HG3	1:A:1709:LEU:N	2.33	0.42
1:A:1540:GLU:O	1:A:1541:GLU:HB2	2.18	0.42
1:A:1690:ALA:HA	1:A:1691:PRO:HD3	1.86	0.41
1:A:1887:ILE:HG12	1:A:1889:VAL:HG23	2.00	0.41
1:A:1543:PRO:HG2	1:A:1777:VAL:HG11	2.01	0.41
1:A:1844:GLY:HA3	1:A:1866:PRO:HG2	2.03	0.41
1:A:1586:ASN:ND2	1:A:1586:ASN:C	2.79	0.41
1:A:1837:VAL:HG22	1:A:1884:PRO:HG2	2.03	0.41
1:A:1491:ARG:O	1:A:1495:GLU:HG3	2.20	0.40
1:A:1849:GLU:HG2	1:A:1850:GLY:N	2.36	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	466/486 (96%)	446 (96%)	11 (2%)	9 (2%)	6 1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1850	GLY
1	A	1469	ARG
1	A	1471	ASP
1	A	1540	GLU
1	A	1654	ALA
1	A	1758	ASP

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Mol	Chain	Res	Type
1	A	1851	PRO
1	A	1466	GLU
1	A	1539	PRO

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	339/351 (97%)	330 (97%)	9 (3%)	39	22

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1485	GLU
1	A	1540	GLU
1	A	1555	LEU
1	A	1688	ARG
1	A	1694	LEU
1	A	1709	LEU
1	A	1771	ARG
1	A	1854	ASP
1	A	1906	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1586	ASN
1	A	1680	GLN
1	A	1784	HIS
1	A	1875	ASN
1	A	1901	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](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	NDP	A	201	-	51,52,52	2.08	15 (29%)	71,80,80	3.05	18 (25%)

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
2	NDP	A	201	-	1/1/14/17	9/34/77/77	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	NDP	PA-O3	6.61	1.66	1.59
2	A	201	NDP	C5B-C4B	4.83	1.66	1.51
2	A	201	NDP	C1D-N1N	4.79	1.59	1.46
2	A	201	NDP	O4B-C4B	3.63	1.53	1.45
2	A	201	NDP	C6N-N1N	3.32	1.45	1.37
2	A	201	NDP	P2B-O2B	3.05	1.64	1.59
2	A	201	NDP	C2N-C3N	2.78	1.42	1.35
2	A	201	NDP	C3B-C4B	2.59	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	NDP	C4N-C5N	-2.53	1.42	1.49
2	A	201	NDP	C4N-C3N	-2.34	1.45	1.50
2	A	201	NDP	O5B-C5B	-2.28	1.36	1.44
2	A	201	NDP	C2A-N3A	2.27	1.38	1.33
2	A	201	NDP	C4A-N3A	2.19	1.38	1.34
2	A	201	NDP	C8A-N7A	2.15	1.35	1.31
2	A	201	NDP	C1B-N9A	2.13	1.52	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	NDP	C5B-C4B-C3B	15.73	171.85	115.21
2	A	201	NDP	O4B-C1B-N9A	10.64	128.53	108.09
2	A	201	NDP	O4B-C4B-C5B	-6.36	88.97	109.33
2	A	201	NDP	O5B-PA-O1A	-5.53	87.01	108.94
2	A	201	NDP	C2B-C1B-N9A	-5.09	105.38	113.75
2	A	201	NDP	O4B-C4B-C3B	-4.79	95.64	105.15
2	A	201	NDP	O5B-C5B-C4B	-4.66	93.14	108.99
2	A	201	NDP	O2B-C2B-C1B	4.33	125.28	110.05
2	A	201	NDP	O3B-C3B-C4B	3.99	122.54	111.08
2	A	201	NDP	PA-O5B-C5B	3.39	140.77	121.35
2	A	201	NDP	O4D-C1D-N1N	3.38	114.53	108.08
2	A	201	NDP	O2A-PA-O5B	3.08	121.51	107.57
2	A	201	NDP	O3-PA-O1A	-2.91	101.96	110.70
2	A	201	NDP	C3B-C2B-C1B	-2.80	97.45	102.81
2	A	201	NDP	C2B-C3B-C4B	2.62	107.62	101.99
2	A	201	NDP	C4B-O4B-C1B	2.30	114.56	109.47
2	A	201	NDP	O5D-C5D-C4D	2.24	116.61	108.99
2	A	201	NDP	C2A-N1A-C6A	2.21	122.37	118.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	201	NDP	C4B

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	NDP	O4D-C1D-N1N-C6N
2	A	201	NDP	O4B-C4B-C5B-O5B
2	A	201	NDP	C3B-C4B-C5B-O5B
2	A	201	NDP	O4D-C4D-C5D-O5D

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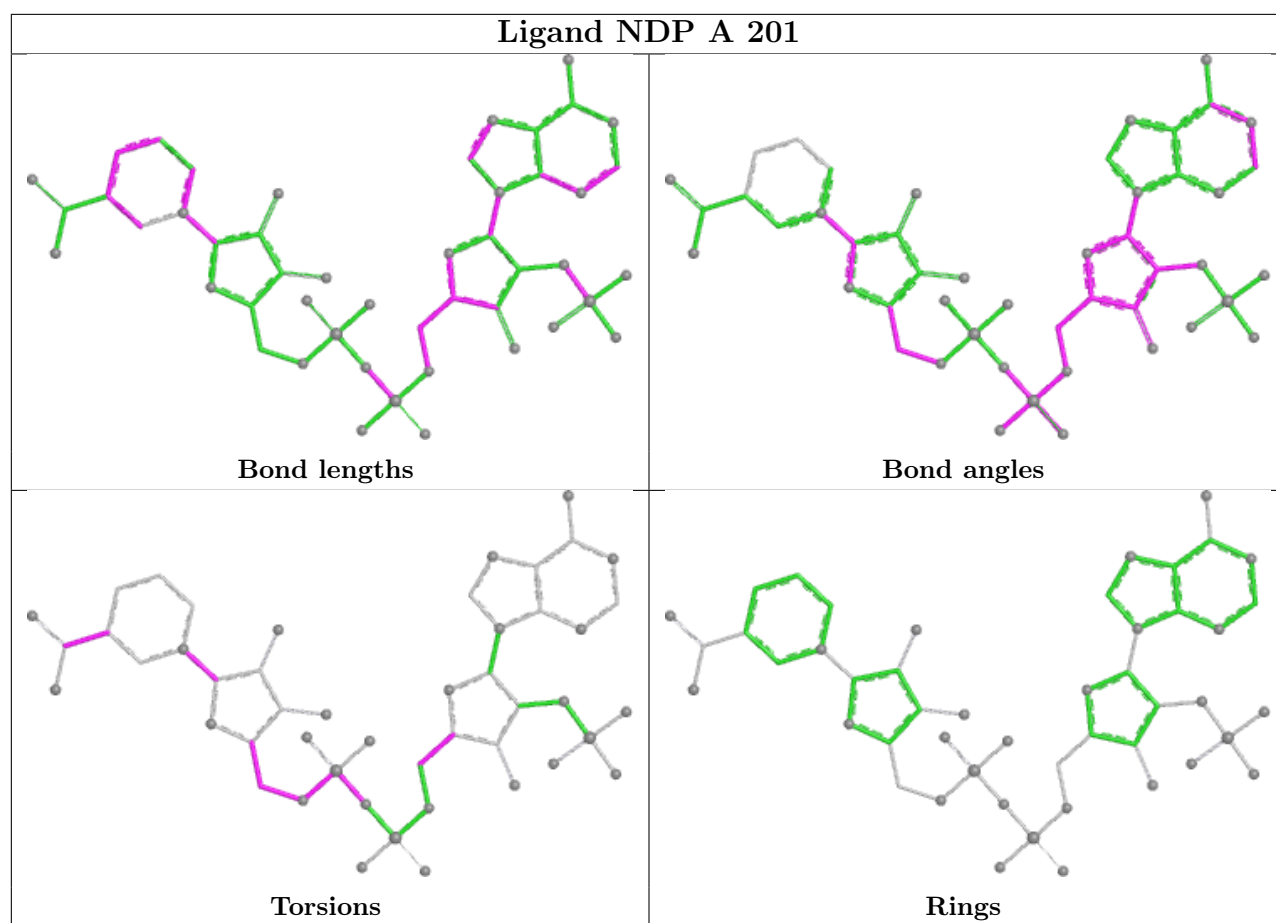
Mol	Chain	Res	Type	Atoms
2	A	201	NDP	PA-O3-PN-O2N
2	A	201	NDP	C5D-O5D-PN-O1N
2	A	201	NDP	C4D-C5D-O5D-PN
2	A	201	NDP	C2N-C3N-C7N-N7N
2	A	201	NDP	PA-O3-PN-O1N

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	NDP	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 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	468/486 (96%)	1.10	89 (19%) 3 3	14, 31, 61, 80	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1848	ALA	6.7
1	A	1468	ALA	6.1
1	A	1467	PRO	6.0
1	A	1850	GLY	6.0
1	A	1656	PRO	5.7
1	A	1851	PRO	5.7
1	A	1464	ALA	5.5
1	A	1470	LEU	5.0
1	A	1657	ALA	4.7
1	A	1843	ALA	4.6
1	A	1465	GLY	4.3
1	A	1854	ASP	4.0
1	A	1522	VAL	4.0
1	A	1658	THR	3.8
1	A	1498	GLY	3.7
1	A	1852	VAL	3.7
1	A	1655	ALA	3.7
1	A	1494	LEU	3.6
1	A	1845	SER	3.6
1	A	1757	ASP	3.6
1	A	1758	ASP	3.6
1	A	1466	GLU	3.5
1	A	1660	ASP	3.4
1	A	1847	MET	3.4
1	A	1541	GLU	3.2
1	A	1630	SER	3.2
1	A	1471	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1856	PHE	3.2
1	A	1654	ALA	3.2
1	A	1644	GLY	3.2
1	A	1896	LEU	3.1
1	A	1497	ALA	3.1
1	A	1523	GLY	3.0
1	A	1844	GLY	3.0
1	A	1761	VAL	2.9
1	A	1911	ASP	2.9
1	A	1463	GLY	2.9
1	A	1472	GLY	2.9
1	A	1717	GLY	2.9
1	A	1492	GLU	2.9
1	A	1849	GLU	2.9
1	A	1659	ASP	2.9
1	A	1853	ALA	2.8
1	A	1623	ARG	2.8
1	A	1502	ARG	2.8
1	A	1914	ARG	2.8
1	A	1915	ARG	2.7
1	A	1879	ARG	2.7
1	A	1855	ARG	2.7
1	A	1473	THR	2.7
1	A	1858	ARG	2.6
1	A	1756	LEU	2.6
1	A	1501	VAL	2.6
1	A	1633	ALA	2.6
1	A	1762	ASP	2.5
1	A	1704	ASP	2.5
1	A	1546	LEU	2.5
1	A	1715	ALA	2.5
1	A	1900	ALA	2.5
1	A	1913	ALA	2.5
1	A	1538	GLU	2.5
1	A	1618	VAL	2.5
1	A	1764	LEU	2.4
1	A	1755	THR	2.4
1	A	1892	ASP	2.4
1	A	1539	PRO	2.4
1	A	1500	ARG	2.4
1	A	1709	LEU	2.4
1	A	1708	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1537	ALA	2.3
1	A	1469	ARG	2.3
1	A	1905	ARG	2.3
1	A	1603	ASN	2.3
1	A	1625	LEU	2.2
1	A	1622	ALA	2.2
1	A	1857	ARG	2.2
1	A	1707	GLY	2.2
1	A	1812	GLY	2.2
1	A	1448	ASP	2.2
1	A	1489	ALA	2.2
1	A	1910	ILE	2.1
1	A	1481	GLY	2.1
1	A	1499	ALA	2.1
1	A	1450	VAL	2.1
1	A	1716	LEU	2.1
1	A	1653	ALA	2.1
1	A	1791	ASP	2.1
1	A	1710	VAL	2.0
1	A	1702	ASP	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.

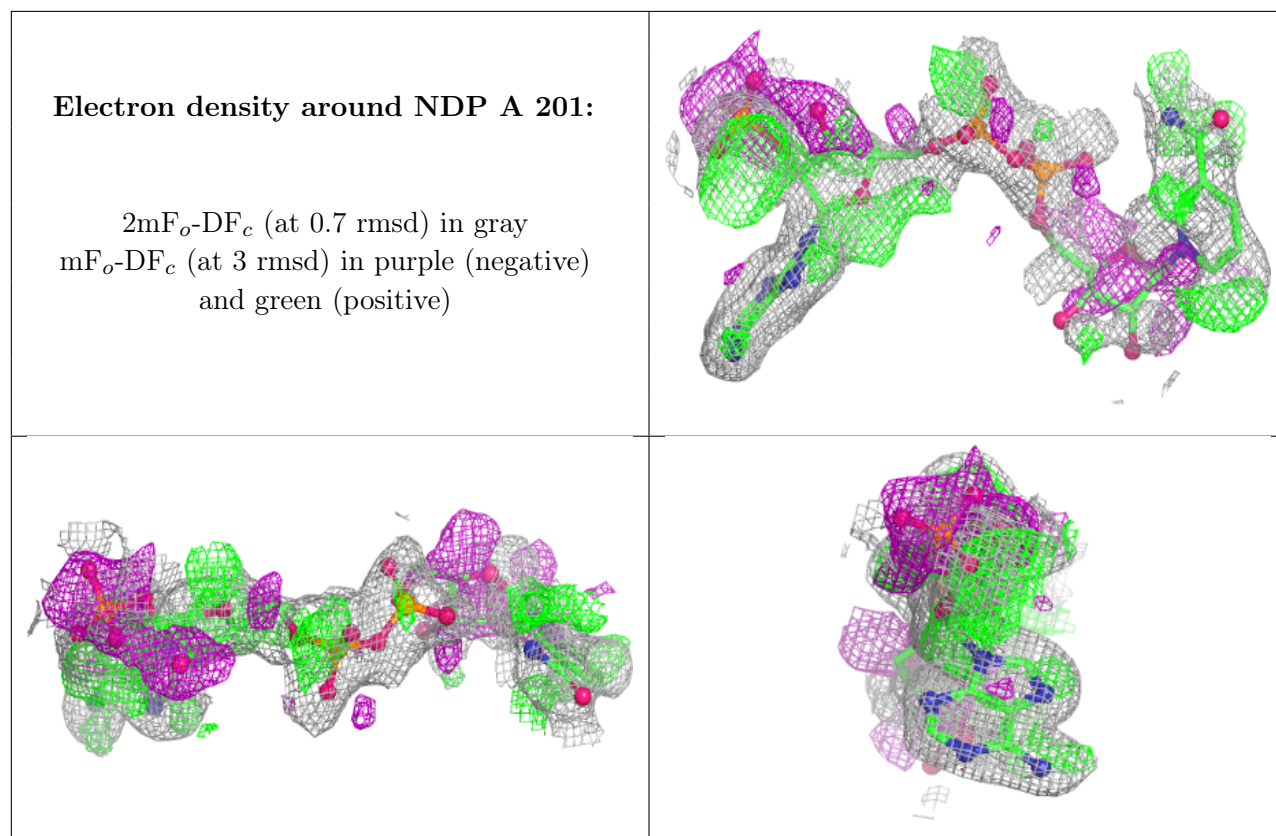
6.4 Ligands [i](#)

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	NDP	A	201	48/48	0.66	0.26	24,58,67,68	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.