



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:57 AM UTC

PDB ID : 9PI4 / pdb_00009pi4
Title : Poly dT bound form of Single stranded DNA-binding protein(ICP8) from Herpes simplex virus-1. Mutations: C254S, C455S
Authors : Erlandsen, H.; Krucinska, J.; Wright, D.
Deposited on : 2025-07-10
Resolution : 3.10 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

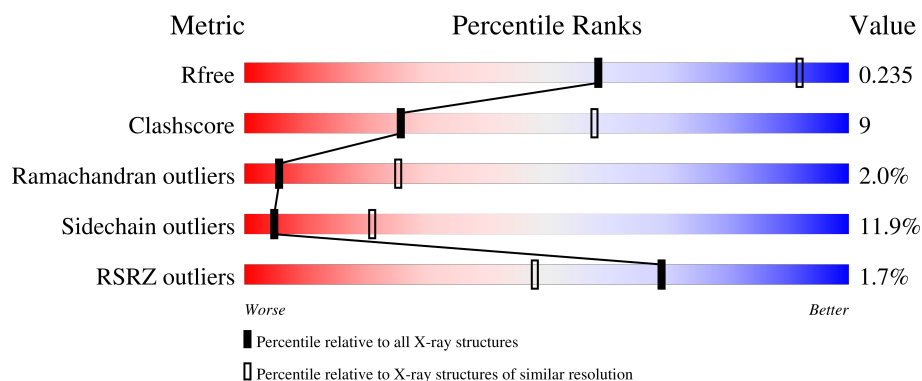
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1128	<div> <div>2%</div> <div>67%</div> <div>23%</div> <div>...</div> </div>
2	G	8	<div> <div>62%</div> <div>38%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8367 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 Major DNA-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1078	Total	C	N	O	S	0	0	0
			8202	5181	1453	1521	47			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	SER	variant	UNP P04296
A	224	ASN	LYS	variant	UNP P04296
A	254	SER	CYS	engineered mutation	UNP P04296
A	306	PRO	ALA	variant	UNP P04296
A	348	CYS	PHE	conflict	UNP P04296
A	455	SER	CYS	engineered mutation	UNP P04296
A	475	GLY	ALA	variant	UNP P04296
A	1039	ASN	SER	conflict	UNP P04296

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			160	80	16	56	8			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

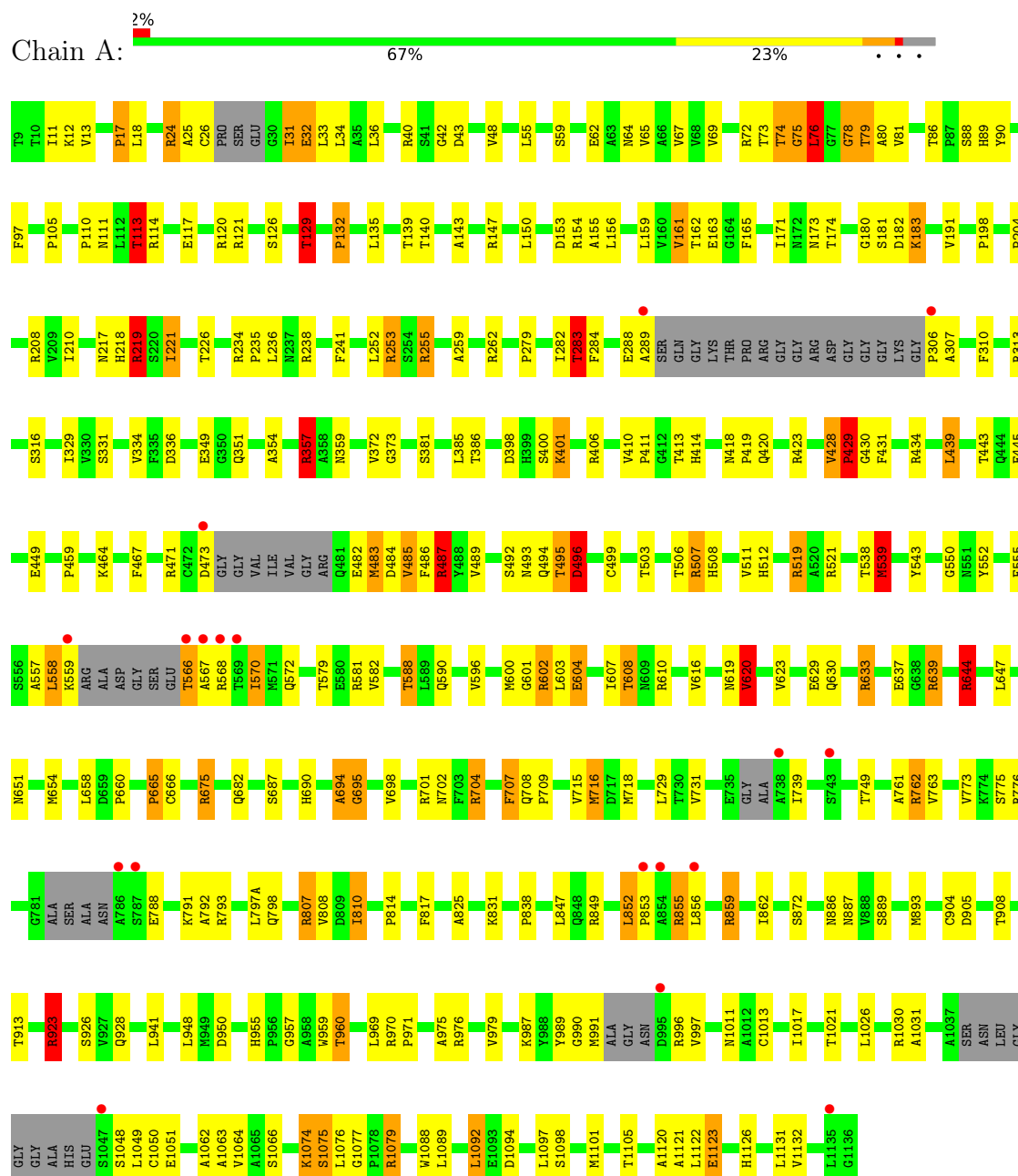
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	G	1	Total 1	O 1	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: Major DNA-binding protein



- Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain G:  62% 38%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.74Å 151.74Å 154.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.51 – 3.10 60.51 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.51-3.10) 99.9 (60.51-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.193 , 0.233 0.203 , 0.235	Depositor DCC
R_{free} test set	1885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8367	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: ZN

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	0.56	0/8375	1.13	29/11369 (0.3%)
2	G	0.45	0/175	1.09	0/268
All	All	0.56	0/8550	1.13	29/11637 (0.2%)

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	A	0	27

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	960	THR	CA-CB-OG1	-8.47	96.89	109.60
1	A	17	PRO	N-CA-CB	-7.65	95.22	103.25
1	A	644	ARG	NE-CZ-NH1	-7.36	114.14	121.50
1	A	588	THR	CA-CB-OG1	-7.31	98.64	109.60
1	A	413	THR	CA-CB-OG1	-7.07	99.00	109.60
1	A	608	THR	CA-CB-OG1	-6.88	99.28	109.60
1	A	596	VAL	N-CA-CB	6.42	120.19	111.21
1	A	620	VAL	N-CA-CB	6.36	117.99	110.55
1	A	129	THR	CA-CB-OG1	-6.32	100.13	109.60
1	A	1021	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	923	ARG	CB-CA-C	6.14	119.53	109.46
1	A	539	MET	CG-SD-CE	-6.07	87.54	100.90
1	A	665	PRO	N-CA-CB	-6.04	97.75	102.28
1	A	707	PHE	CA-CB-CG	-6.01	107.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	CA-CB-OG1	-5.92	100.71	109.60
1	A	1105	THR	CA-CB-OG1	-5.89	100.76	109.60
1	A	113	THR	CA-CB-OG1	-5.74	100.99	109.60
1	A	443	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	923	ARG	CD-NE-CZ	5.60	132.24	124.40
1	A	644	ARG	NH1-CZ-NH2	5.57	126.54	119.30
1	A	1123	GLU	N-CA-CB	5.55	118.26	109.82
1	A	110	PRO	N-CA-CB	-5.54	97.43	103.25
1	A	219	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	A	283	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	716	MET	CG-SD-CE	-5.46	88.88	100.90
1	A	132	PRO	N-CA-C	-5.30	107.23	113.86
1	A	449	GLU	CB-CG-CD	5.30	121.62	112.60
1	A	651	ASN	CB-CA-C	-5.18	99.09	109.35
1	A	174	THR	CA-CB-OG1	-5.08	101.98	109.60

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1030	ARG	Sidechain
1	A	1079	ARG	Sidechain
1	A	147	ARG	Sidechain
1	A	154	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	357	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	434	ARG	Sidechain
1	A	487	ARG	Sidechain
1	A	507	ARG	Sidechain
1	A	519	ARG	Sidechain
1	A	568	ARG	Sidechain
1	A	602	ARG	Sidechain
1	A	633	ARG	Sidechain
1	A	639	ARG	Sidechain
1	A	644	ARG	Sidechain
1	A	701	ARG	Sidechain
1	A	762	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	793	ARG	Sidechain
1	A	807	ARG	Sidechain
1	A	849	ARG	Sidechain
1	A	855	ARG	Sidechain
1	A	859	ARG	Sidechain

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	8202	0	8103	156	2
2	G	160	0	97	4	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
4	G	1	0	0	0	0
All	All	8367	0	8200	157	2

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 9.

All (157) 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:329:ILE:HD11	1:A:716:MET:HE1	1.63	0.80
1:A:508:HIS:HB3	1:A:941:LEU:HD11	1.71	0.73
1:A:11:ILE:HG13	1:A:729:LEU:HD13	1.74	0.69
1:A:159:LEU:HD22	1:A:236:LEU:HD21	1.77	0.66
1:A:675:ARG:HH11	1:A:675:ARG:CG	2.10	0.63
1:A:307:ALA:HB3	1:A:310:PHE:HB2	1.82	0.62
1:A:117:GLU:OE1	1:A:121:ARG:NH1	2.32	0.61
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.66	0.61
1:A:675:ARG:CG	1:A:675:ARG:NH1	2.64	0.60
1:A:788:GLU:HB2	2:G:1:DT:H5''	1.82	0.59
1:A:74:THR:O	1:A:75:GLY:C	2.45	0.59
1:A:495:THR:O	1:A:496:ASP:C	2.47	0.58
1:A:704:ARG:HG2	1:A:704:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:CE1	1:A:660:PRO:HG3	2.38	0.58
1:A:893:MET:HA	1:A:893:MET:HE2	1.86	0.57
1:A:283:THR:OG1	1:A:420:GLN:HB3	2.04	0.57
1:A:1088:TRP:CE3	1:A:1101:MET:HG3	2.38	0.57
1:A:471:ARG:NH1	1:A:957:GLY:O	2.36	0.57
1:A:18:LEU:HD13	1:A:198:PRO:HD3	1.86	0.57
1:A:78:GLY:O	1:A:79:THR:C	2.48	0.56
1:A:429:PRO:O	1:A:431:PHE:N	2.34	0.56
1:A:329:ILE:CD1	1:A:716:MET:HE1	2.35	0.55
1:A:132:PRO:HA	1:A:135:LEU:CD1	2.37	0.55
1:A:1075:SER:O	1:A:1076:LEU:C	2.50	0.54
1:A:381:SER:O	1:A:385:LEU:HD13	2.07	0.54
1:A:36:LEU:O	1:A:464:LYS:NZ	2.37	0.54
1:A:173:ASN:ND2	1:A:210:ILE:H	2.05	0.54
1:A:64:ASN:OD1	1:A:334:VAL:HA	2.08	0.53
1:A:557:ALA:C	1:A:559:LYS:H	2.15	0.53
1:A:608:THR:HA	1:A:825:ALA:HB1	1.90	0.53
1:A:428:VAL:HB	1:A:429:PRO:HD2	1.90	0.53
1:A:75:GLY:O	1:A:76:LEU:C	2.52	0.53
1:A:791:LYS:O	1:A:792:ALA:C	2.52	0.53
1:A:923:ARG:HG2	1:A:923:ARG:HH11	1.75	0.52
1:A:1063:ALA:O	1:A:1064:VAL:C	2.53	0.52
1:A:489:VAL:HG21	1:A:941:LEU:HD13	1.91	0.52
1:A:159:LEU:HG	1:A:161:VAL:HG22	1.91	0.52
1:A:853:PRO:C	1:A:855:ARG:N	2.67	0.52
1:A:253:ARG:HH12	1:A:682:GLN:HE22	1.57	0.52
1:A:675:ARG:HH11	1:A:675:ARG:HG3	1.75	0.52
1:A:588:THR:C	1:A:590:GLN:H	2.18	0.51
1:A:675:ARG:NH1	1:A:675:ARG:HG2	2.24	0.51
1:A:464:LYS:HE2	1:A:666:CYS:SG	2.50	0.51
1:A:173:ASN:HD21	1:A:210:ILE:H	1.57	0.51
1:A:923:ARG:HH11	1:A:923:ARG:CG	2.24	0.51
1:A:687:SER:HB3	1:A:987:LYS:HE2	1.93	0.50
1:A:570:ILE:HA	1:A:639:ARG:HH22	1.76	0.50
1:A:1062:ALA:HB1	1:A:1132:VAL:HG11	1.94	0.50
1:A:351:GLN:O	1:A:357:ARG:NH2	2.45	0.50
1:A:600:MET:O	1:A:601:GLY:C	2.55	0.50
1:A:572:GLN:O	1:A:581:ARG:NH2	2.45	0.50
1:A:484:ASP:O	1:A:485:VAL:C	2.53	0.50
1:A:336:ASP:N	1:A:336:ASP:OD1	2.45	0.49
1:A:494:GLN:O	1:A:495:THR:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.28	0.49
1:A:550:GLY:C	1:A:552:TYR:H	2.21	0.49
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.66	0.48
1:A:252:LEU:C	1:A:253:ARG:HG2	2.39	0.48
1:A:566:THR:OG1	1:A:567:ALA:N	2.45	0.48
1:A:97:PHE:CD1	1:A:236:LEU:HD13	2.49	0.48
1:A:776:ARG:NH1	2:G:1:DT:H71	2.29	0.48
1:A:492:SER:O	1:A:493:ASN:C	2.56	0.48
1:A:521:ARG:HA	1:A:1011:ASN:HB3	1.96	0.48
1:A:619:ASN:O	1:A:623:VAL:HG23	2.13	0.48
1:A:120:ARG:HD3	1:A:126:SER:O	2.12	0.48
1:A:180:GLY:O	1:A:182:ASP:N	2.46	0.48
1:A:926:SER:OG	1:A:928:GLN:HB2	2.14	0.48
1:A:507:ARG:O	1:A:508:HIS:C	2.57	0.47
1:A:707:PHE:O	1:A:708:GLN:C	2.57	0.47
1:A:975:ALA:HA	1:A:1031:ALA:HB3	1.97	0.47
1:A:31:ILE:O	1:A:32:GLU:C	2.57	0.47
1:A:970:ARG:HB3	1:A:971:PRO:HD3	1.96	0.47
1:A:132:PRO:HA	1:A:135:LEU:HD12	1.97	0.47
1:A:539:MET:O	1:A:539:MET:HG3	2.15	0.47
1:A:354:ALA:HA	1:A:357:ARG:HD2	1.97	0.46
1:A:1131:LEU:HD23	1:A:1131:LEU:C	2.40	0.46
1:A:217:ASN:O	1:A:218:HIS:C	2.58	0.46
1:A:484:ASP:HB3	1:A:487:ARG:HB2	1.95	0.46
1:A:163:GLU:HB3	1:A:331:SER:HB3	1.98	0.46
1:A:359:ASN:OD1	1:A:923:ARG:NH2	2.49	0.46
1:A:975:ALA:O	1:A:976:ARG:C	2.59	0.46
1:A:1077:GLY:C	1:A:1079:ARG:H	2.23	0.46
1:A:486:PHE:O	1:A:487:ARG:C	2.58	0.46
1:A:288:GLU:O	1:A:289:ALA:HB3	2.16	0.45
1:A:1122:LEU:O	1:A:1126:HIS:CD2	2.69	0.45
1:A:644:ARG:HG2	1:A:904:CYS:HB3	1.99	0.45
1:A:406:ARG:HH11	1:A:690:HIS:CD2	2.35	0.45
1:A:1089:LEU:O	1:A:1092:LEU:O	2.35	0.45
1:A:410:VAL:HB	1:A:411:PRO:CD	2.46	0.45
1:A:853:PRO:C	1:A:855:ARG:H	2.25	0.45
1:A:234:ARG:HB2	1:A:235:PRO:HD3	1.99	0.45
1:A:1120:ALA:O	1:A:1121:ALA:C	2.59	0.45
1:A:253:ARG:HD3	1:A:386:THR:O	2.17	0.45
1:A:113:THR:HA	1:A:459:PRO:HG3	1.99	0.44
1:A:814:PRO:HG3	1:A:872:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:LEU:O	1:A:1050:CYS:C	2.60	0.44
1:A:372:VAL:O	1:A:373:GLY:C	2.60	0.44
1:A:610:ARG:HH11	1:A:610:ARG:HG3	1.82	0.44
1:A:853:PRO:HB2	1:A:855:ARG:HB3	1.99	0.44
1:A:43:ASP:OD2	1:A:113:THR:OG1	2.36	0.44
1:A:284:PHE:CD1	1:A:313:ARG:HD2	2.53	0.44
1:A:90:TYR:HA	1:A:162:THR:HA	1.99	0.44
1:A:588:THR:C	1:A:590:GLN:N	2.75	0.44
1:A:25:ALA:HA	1:A:155:ALA:HA	1.99	0.43
1:A:464:LYS:O	1:A:467:PHE:HB3	2.19	0.43
1:A:581:ARG:O	1:A:582:VAL:C	2.61	0.43
1:A:904:CYS:O	1:A:905:ASP:C	2.61	0.43
1:A:1094:ASP:O	1:A:1098:SER:OG	2.31	0.43
1:A:183:LYS:HE2	1:A:183:LYS:HB2	1.46	0.43
1:A:979:VAL:HA	1:A:1026:LEU:O	2.18	0.43
1:A:18:LEU:HG	1:A:165:PHE:CB	2.49	0.43
1:A:234:ARG:O	1:A:235:PRO:C	2.60	0.43
1:A:1122:LEU:O	1:A:1126:HIS:HD2	2.01	0.43
1:A:111:ASN:HB3	1:A:114:ARG:HB2	2.00	0.43
1:A:471:ARG:HG2	1:A:959:TRP:O	2.19	0.43
1:A:398:ASP:HB3	1:A:401:LYS:HD2	2.00	0.43
1:A:708:GLN:N	1:A:709:PRO:CD	2.82	0.43
1:A:73:THR:HG23	1:A:204:PRO:HB3	2.01	0.42
1:A:1097:LEU:O	1:A:1101:MET:HG2	2.19	0.42
1:A:1120:ALA:O	1:A:1123:GLU:N	2.53	0.42
1:A:797(A):LEU:O	1:A:798:GLN:C	2.63	0.42
1:A:810:ILE:H	1:A:810:ILE:HG12	1.69	0.42
1:A:831:LYS:HA	1:A:838:PRO:HA	2.00	0.42
1:A:1074:LYS:HD2	1:A:1074:LYS:HA	1.74	0.42
1:A:503:THR:H	1:A:506:THR:HG1	1.65	0.42
1:A:74:THR:H	1:A:80:ALA:HB1	1.84	0.42
1:A:88:SER:OG	1:A:89:HIS:N	2.52	0.42
1:A:129:THR:O	1:A:129:THR:CG2	2.67	0.42
1:A:259:ALA:HB1	1:A:279:PRO:HG3	2.01	0.42
1:A:602:ARG:O	1:A:603:LEU:C	2.62	0.42
1:A:948:LEU:HD12	1:A:955:HIS:CD2	2.55	0.42
1:A:129:THR:O	1:A:129:THR:HG23	2.19	0.42
1:A:969:LEU:O	1:A:970:ARG:C	2.62	0.42
1:A:414:HIS:ND1	1:A:414:HIS:N	2.68	0.42
1:A:439:LEU:HD13	1:A:439:LEU:HA	1.94	0.42
1:A:288:GLU:O	1:A:289:ALA:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:HB3	1:A:419:PRO:HD2	2.02	0.41
1:A:616:VAL:O	1:A:620:VAL:HG13	2.21	0.41
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.87	0.41
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.82	0.41
1:A:555:PHE:HE1	1:A:570:ILE:HD13	1.85	0.41
1:A:852:LEU:O	1:A:853:PRO:C	2.63	0.41
1:A:715:VAL:O	1:A:718:MET:HB2	2.20	0.41
1:A:694:ALA:O	1:A:695:GLY:C	2.64	0.41
1:A:817:PHE:CE2	1:A:887:ASN:HA	2.56	0.41
1:A:406:ARG:HH11	1:A:690:HIS:HD2	1.68	0.41
1:A:543:TYR:CZ	2:G:8:DT:H3'	2.56	0.41
1:A:558:LEU:O	1:A:559:LYS:C	2.63	0.41
1:A:629:GLU:O	1:A:630:GLN:C	2.64	0.41
1:A:259:ALA:CB	1:A:279:PRO:HG3	2.51	0.41
2:G:1:DT:H4'	2:G:2:DT:OP1	2.21	0.41
1:A:42:GLY:HA2	1:A:105:PRO:HB3	2.03	0.40
1:A:852:LEU:HA	1:A:853:PRO:HD2	1.94	0.40
1:A:24:ARG:HB3	1:A:191:VAL:HG22	2.02	0.40
1:A:140:THR:HG23	1:A:143:ALA:HB2	2.04	0.40
1:A:604:GLU:H	1:A:604:GLU:HG2	1.56	0.40
1:A:886:ASN:O	1:A:887:ASN:HB3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:NH1	1:A:644:ARG:NH1[4_545]	2.04	0.16
1:A:219:ARG:NH1	1:A:644:ARG:CZ[4_545]	2.19	0.01

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	1060/1128 (94%)	924 (87%)	115 (11%)	21 (2%)	6	25

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	GLY
1	A	181	SER
1	A	429	PRO
1	A	76	LEU
1	A	496	ASP
1	A	695	GLY
1	A	495	THR
1	A	499	CYS
1	A	908	THR
1	A	1075	SER
1	A	79	THR
1	A	694	ALA
1	A	761	ALA
1	A	483	MET
1	A	558	LEU
1	A	852	LEU
1	A	221	ILE
1	A	430	GLY
1	A	485	VAL
1	A	990	GLY
1	A	78	GLY

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	852/880 (97%)	751 (88%)	101 (12%)	5	21

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	13	VAL
1	A	17	PRO
1	A	26	CYS
1	A	31	ILE
1	A	32	GLU
1	A	33	LEU
1	A	48	VAL
1	A	59	SER
1	A	62	GLU
1	A	65	VAL
1	A	67	VAL
1	A	69	VAL
1	A	72	ARG
1	A	74	THR
1	A	76	LEU
1	A	81	VAL
1	A	86	THR
1	A	113	THR
1	A	129	THR
1	A	150	LEU
1	A	153	ASP
1	A	156	LEU
1	A	161	VAL
1	A	171	ILE
1	A	183	LYS
1	A	208	ARG
1	A	219	ARG
1	A	221	ILE
1	A	226	THR
1	A	241	PHE
1	A	255	ARG
1	A	282	ILE
1	A	283	THR
1	A	306	PRO
1	A	316	SER
1	A	349	GLU
1	A	357	ARG
1	A	400	SER
1	A	401	LYS
1	A	423	ARG
1	A	428	VAL
1	A	429	PRO

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Mol	Chain	Res	Type
1	A	439	LEU
1	A	445	GLU
1	A	473	ASP
1	A	482	GLU
1	A	483	MET
1	A	487	ARG
1	A	496	ASP
1	A	511	VAL
1	A	512	HIS
1	A	519	ARG
1	A	538	THR
1	A	539	MET
1	A	566	THR
1	A	570	ILE
1	A	579	THR
1	A	604	GLU
1	A	607	ILE
1	A	620	VAL
1	A	633	ARG
1	A	637	GLU
1	A	647	LEU
1	A	654	MET
1	A	658	LEU
1	A	665	PRO
1	A	675	ARG
1	A	698	VAL
1	A	702	ASN
1	A	704	ARG
1	A	731	VAL
1	A	739	ILE
1	A	749	THR
1	A	762	ARG
1	A	763	VAL
1	A	773	VAL
1	A	775	SER
1	A	807	ARG
1	A	808	VAL
1	A	810	ILE
1	A	847	LEU
1	A	856	LEU
1	A	859	ARG
1	A	862	ILE

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Mol	Chain	Res	Type
1	A	889	SER
1	A	913	THR
1	A	923	ARG
1	A	950	ASP
1	A	960	THR
1	A	989	TYR
1	A	991	MET
1	A	996	ARG
1	A	997	VAL
1	A	1013	CYS
1	A	1017	ILE
1	A	1048	SER
1	A	1051	GLU
1	A	1066	SER
1	A	1074	LYS
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	111	ASN
1	A	172	ASN
1	A	173	ASN
1	A	682	GLN
1	A	696	GLN
1	A	702	ASN
1	A	748	GLN
1	A	836	ASN
1	A	837	GLN
1	A	879	ASN
1	A	912	ASN
1	A	1082	GLN
1	A	1126	HIS

5.3.3 RNA ⓘ

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 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 [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 [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	1078/1128 (95%)	-0.08	18 (1%) 69 48	36, 72, 124, 166	0
2	G	8/8 (100%)	0.74	0 100 100	143, 161, 176, 192	0
All	All	1086/1136 (95%)	-0.07	18 (1%) 69 48	36, 72, 126, 192	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1047	SER	4.1
1	A	566	THR	4.0
1	A	738	ALA	3.4
1	A	559	LYS	3.4
1	A	854	ALA	3.3
1	A	853	PRO	3.0
1	A	856	LEU	3.0
1	A	786	ALA	3.0
1	A	473	ASP	2.7
1	A	995	ASP	2.6
1	A	743	SER	2.6
1	A	568	ARG	2.5
1	A	787	SER	2.4
1	A	567	ALA	2.4
1	A	569	THR	2.2
1	A	289	ALA	2.1
1	A	306	PRO	2.1
1	A	1135	LEU	2.1

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](#)

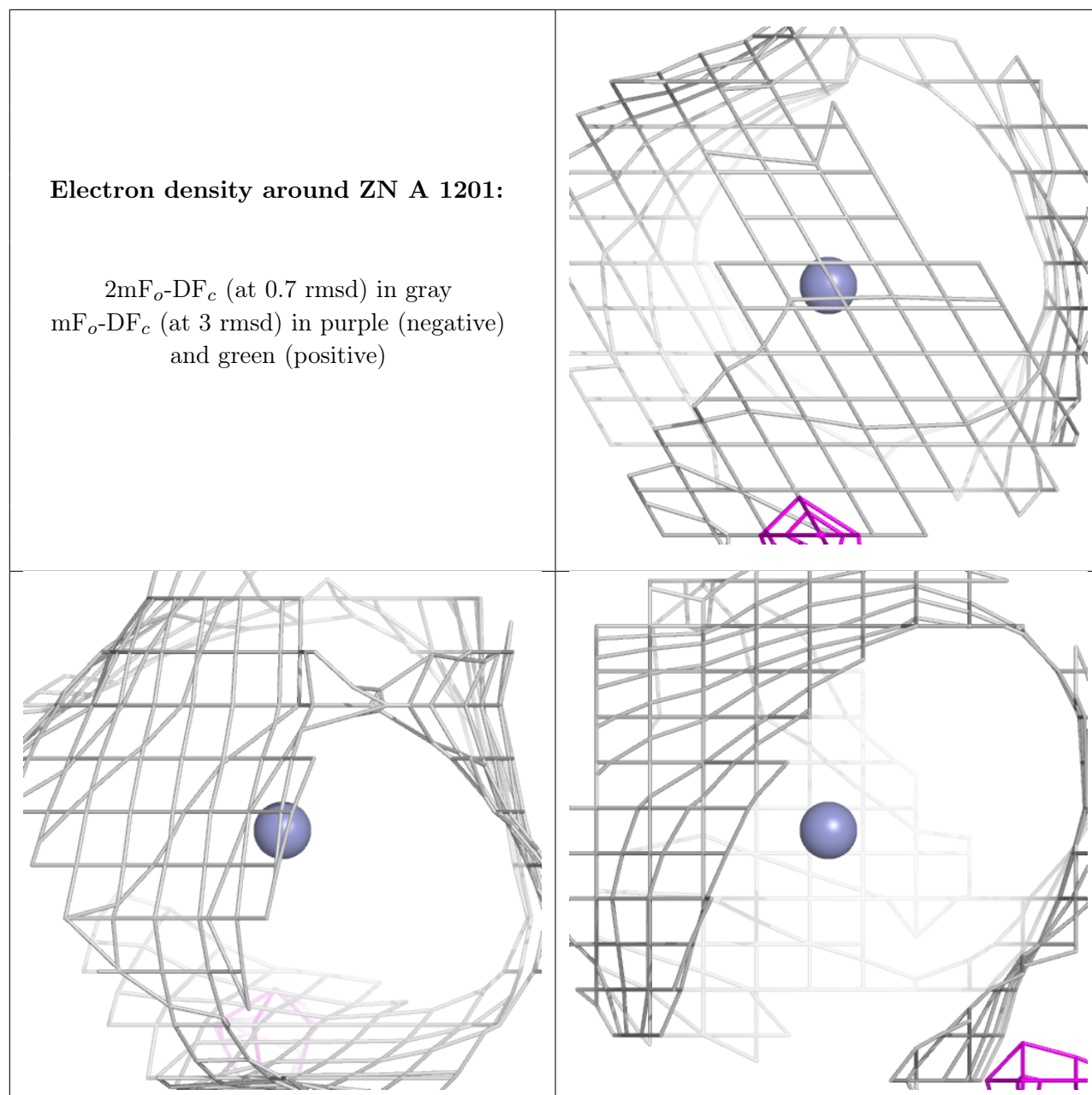
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
3	ZN	A	1201	1/1	1.00	0.02	74,74,74,74	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.