



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:00 AM UTC

PDB ID : 9PI3 / pdb\_00009pi3  
Title : Single stranded DNA-binding protein (ICP8) from Herpes simplex virus-1, apo form. Mutations: C254S, C455S, K769A, E770A  
Authors : Erlandsen, H.; Wright, D.  
Deposited on : 2025-07-10  
Resolution : 2.75 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](mailto: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>.

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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

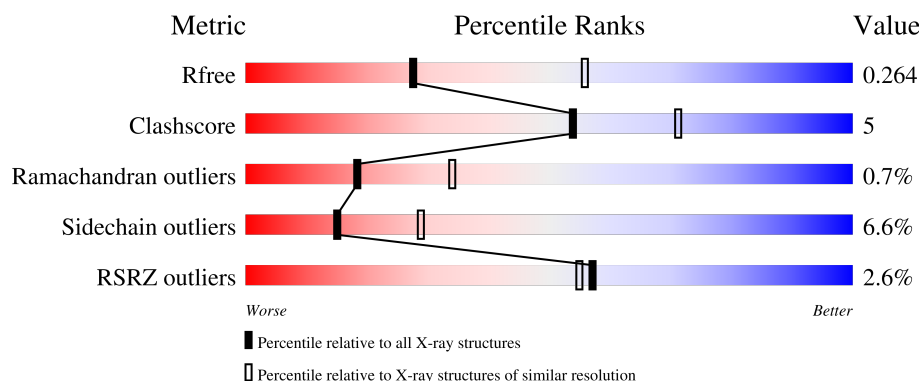
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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  $\geq 3$ , 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	1136	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	1136	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16258 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	1050	Total	C	N	O	S	0	0	0
			8025	5076	1419	1484	46			
1	B	1060	Total	C	N	O	S	0	0	0
			8067	5097	1428	1495	47			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	SER	CYS	engineered mutation	UNP P17470
A	455	SER	CYS	engineered mutation	UNP P17470
A	769	ALA	LYS	engineered mutation	UNP P17470
A	770	ALA	GLU	engineered mutation	UNP P17470
B	254	SER	CYS	engineered mutation	UNP P17470
B	455	SER	CYS	engineered mutation	UNP P17470
B	769	ALA	LYS	engineered mutation	UNP P17470
B	770	ALA	GLU	engineered mutation	UNP P17470

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.99Å 140.20Å 98.80Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	92.20 – 2.75 92.20 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.20-2.75) 100.0 (92.20-2.75)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.184 , 0.263 0.189 , 0.264	Depositor DCC
$R_{free}$ test set	2968 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16258	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.58	0/8197	1.16	27/11135 (0.2%)
1	B	0.60	0/8237	1.17	31/11190 (0.3%)
All	All	0.59	0/16434	1.17	58/22325 (0.3%)

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	13
1	B	0	10
All	All	0	23

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	N-CA-CB	-10.18	95.03	110.20
1	B	1132	VAL	N-CA-CB	-7.66	102.41	112.36
1	B	185	THR	CA-CB-OG1	-7.48	98.38	109.60
1	B	353	THR	CA-CB-OG1	-7.09	98.96	109.60
1	A	390	ASP	CA-CB-CG	6.96	119.56	112.60
1	B	821	GLN	N-CA-CB	6.82	120.25	110.16
1	B	705	ASN	CB-CA-C	-6.81	99.10	110.68
1	A	389	ASP	CA-CB-CG	6.77	119.37	112.60
1	B	423	ARG	N-CA-CB	-6.57	99.76	110.14
1	B	379	THR	CA-CB-OG1	-6.49	99.86	109.60
1	B	500	ASN	CB-CA-C	-6.48	97.28	109.72
1	B	134	ASP	CA-CB-CG	6.44	119.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1084	GLN	CB-CA-C	6.39	122.25	110.24
1	A	908	THR	CA-CB-OG1	-6.29	100.17	109.60
1	A	950	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	335	PHE	N-CA-CB	-6.24	101.69	111.05
1	B	142	GLU	N-CA-CB	6.05	119.12	110.16
1	A	514	THR	CA-CB-OG1	-6.05	100.53	109.60
1	B	62	GLU	CB-CA-C	5.98	119.87	110.19
1	A	95	TYR	CB-CA-C	5.96	120.06	110.16
1	B	127	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	538	THR	CA-CB-OG1	-5.89	100.76	109.60
1	B	281	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	1110	GLU	CB-CA-C	-5.79	101.00	110.85
1	B	154	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	B	332	MET	CG-SD-CE	-5.72	88.32	100.90
1	A	598	THR	CA-CB-OG1	-5.71	101.04	109.60
1	A	688	GLN	CB-CA-C	-5.65	100.61	110.17
1	B	335	PHE	CB-CA-C	5.64	120.84	110.24
1	A	643	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	756	PHE	CA-CB-CG	5.63	119.43	113.80
1	A	620	VAL	N-CA-CB	5.59	116.71	110.51
1	B	18	LEU	N-CA-CB	-5.58	101.30	110.40
1	B	287	PHE	CA-C-O	-5.51	111.43	120.80
1	A	960	THR	CA-CB-OG1	-5.47	101.39	109.60
1	B	114	ARG	N-CA-CB	5.44	117.90	110.01
1	B	114	ARG	CB-CA-C	-5.42	102.36	110.88
1	A	707	PHE	CA-CB-CG	-5.39	108.41	113.80
1	B	226	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	217	ASN	CB-CA-C	-5.36	101.15	110.09
1	A	205	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	1081	GLN	N-CA-CB	-5.31	102.09	110.06
1	A	593	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	244	VAL	N-CA-CB	-5.30	107.29	111.64
1	A	1118	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	1021	THR	CA-CB-OG1	-5.27	101.69	109.60
1	B	451	LEU	N-CA-CB	5.23	117.80	110.12
1	A	539	MET	CB-CA-C	5.20	120.37	111.68
1	A	538	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	58	GLU	CB-CG-CD	5.15	121.35	112.60
1	B	995	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	1019	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	74	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	364	TYR	N-CA-C	-5.13	105.58	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	837	GLN	CB-CA-C	5.08	115.64	109.85
1	A	765	LEU	N-CA-CB	-5.06	103.15	110.84
1	A	493	ASN	CB-CA-C	5.04	117.76	109.90
1	A	72	ARG	CB-CA-C	-5.01	99.50	110.67

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	A	234	ARG	Sidechain
1	A	367	ARG	Sidechain
1	A	480	ARG	Sidechain
1	A	517	ARG	Sidechain
1	A	568	ARG	Sidechain
1	A	626	ARG	Sidechain
1	A	639	ARG	Sidechain
1	A	644	ARG	Sidechain
1	A	675	ARG	Sidechain
1	A	714	ARG	Sidechain
1	A	970	ARG	Sidechain
1	A	976	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	147	ARG	Sidechain
1	B	154	ARG	Sidechain
1	B	238	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	471	ARG	Sidechain
1	B	675	ARG	Sidechain
1	B	713	ARG	Sidechain
1	B	714	ARG	Sidechain
1	B	855	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	8025	0	7917	85	0
1	B	8067	0	7964	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	56	0	0	0	0
3	B	108	0	0	0	0
All	All	16258	0	15881	155	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 5.

All (155) 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:1017:ILE:HD11	1:B:1054:ARG:HH12	1.35	0.87
1:A:970:ARG:HG3	1:A:970:ARG:HH11	1.43	0.83
1:B:11:ILE:HD11	1:B:731:VAL:HG22	1.62	0.79
1:B:545:ASP:OD1	1:B:576:ARG:NH2	2.18	0.77
1:A:11:ILE:HD12	1:A:334:VAL:HG11	1.71	0.71
1:B:353:THR:HG22	1:B:356:ALA:H	1.59	0.68
1:B:36:LEU:O	1:B:464:LYS:NZ	2.28	0.66
1:A:572:GLN:O	1:A:581:ARG:NH2	2.31	0.63
1:B:847:LEU:C	1:B:847:LEU:HD23	2.24	0.63
1:B:90:TYR:HA	1:B:162:THR:HA	1.82	0.62
1:A:829:ASN:O	1:A:831:LYS:N	2.32	0.62
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.65	0.61
1:B:234:ARG:HB3	1:B:235:PRO:HD3	1.83	0.60
1:A:476:VAL:HG21	1:B:1079:ARG:HE	1.67	0.60
1:A:1017:ILE:HD11	1:B:1054:ARG:NH1	2.14	0.59
1:B:675:ARG:HG2	1:B:675:ARG:HH11	1.68	0.59
1:A:268:ALA:HA	1:A:332:MET:HE3	1.85	0.59
1:B:485:VAL:HG22	1:B:928:GLN:HE21	1.68	0.58
1:B:471:ARG:NH1	1:B:957:GLY:O	2.37	0.58
1:A:519:ARG:HD3	1:B:588:THR:O	2.03	0.58
1:A:11:ILE:CD1	1:A:334:VAL:HG11	2.33	0.57
1:B:713:ARG:HH11	1:B:716:MET:HB2	1.69	0.57
1:A:647:LEU:HD21	1:A:901:LEU:HD23	1.86	0.57
1:B:1111:ARG:HH11	1:B:1111:ARG:HG3	1.70	0.57
1:A:53:VAL:O	1:A:342:ILE:HG22	2.05	0.56
1:B:1015:LEU:O	1:B:1017:ILE:HD12	2.06	0.56
1:A:89:HIS:CE1	1:A:660:PRO:HG3	2.41	0.55
1:B:610:ARG:NH2	1:B:860:GLU:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:NH2	1:B:682:GLN:OE1	2.37	0.55
1:B:554:ALA:HA	1:B:574:THR:HG22	1.87	0.55
1:A:728:THR:HA	1:A:765:LEU:O	2.06	0.55
1:A:62:GLU:HA	1:A:62:GLU:OE1	2.05	0.55
1:A:310:PHE:C	1:A:310:PHE:CD1	2.85	0.54
1:B:991:MET:O	1:B:992:ALA:C	2.50	0.54
1:A:590:GLN:HB3	1:A:602:ARG:HG3	1.88	0.54
1:A:591:TYR:O	1:A:603:LEU:HD11	2.06	0.53
1:B:614:HIS:HE1	1:B:864:THR:OG1	1.91	0.53
1:A:167:GLU:HG3	1:A:264:ALA:HB3	1.90	0.52
1:A:1031:ALA:HA	1:A:1035:CYS:O	2.10	0.52
1:B:1133:SER:O	1:B:1134:GLN:C	2.53	0.52
1:A:652:HIS:O	1:A:774:LYS:HA	2.10	0.51
1:A:45:ASP:CG	1:A:45:ASP:O	2.53	0.51
1:A:860:GLU:O	1:A:863:GLU:HB2	2.10	0.51
1:A:1070:VAL:HG22	1:A:1122:LEU:HD23	1.91	0.51
1:A:600:MET:O	1:A:601:GLY:C	2.52	0.51
1:B:359:ASN:OD1	1:B:956:PRO:HA	2.10	0.51
1:A:633:ARG:C	1:A:635:LEU:H	2.19	0.51
1:B:567:ALA:HB1	1:B:1070:VAL:HG21	1.93	0.50
1:A:934:SER:OG	1:A:936:GLN:O	2.28	0.50
1:A:613:LEU:HD13	1:A:826:ILE:HD11	1.92	0.50
1:A:357:ARG:O	1:A:361:VAL:HG23	2.12	0.50
1:A:478:VAL:HB	1:A:480:ARG:HD2	1.92	0.50
1:A:1088:TRP:CE3	1:A:1101:MET:HG3	2.46	0.50
1:B:144:LEU:HA	1:B:147:ARG:HG2	1.94	0.50
1:A:13:VAL:HG12	1:A:66:ALA:HB2	1.93	0.50
1:A:516:MET:HG2	1:A:519:ARG:NH2	2.27	0.49
1:A:970:ARG:HB3	1:A:971:PRO:HD3	1.93	0.49
1:B:89:HIS:CE1	1:B:660:PRO:HG2	2.47	0.49
1:B:173:ASN:HD21	1:B:210:ILE:H	1.61	0.49
1:B:498:PRO:O	1:B:499:CYS:HB2	2.11	0.49
1:B:778:LEU:HD22	1:B:911:ILE:HG22	1.94	0.49
1:B:610:ARG:NH1	1:B:864:THR:OG1	2.45	0.49
1:B:67:VAL:O	1:B:85:LEU:HA	2.13	0.49
1:A:138:GLU:OE1	1:A:234:ARG:NH1	2.46	0.48
1:B:651:ASN:N	1:B:651:ASN:OD1	2.45	0.48
1:A:616:VAL:O	1:A:620:VAL:HG23	2.14	0.48
1:B:347:LEU:HG	1:B:1033:PHE:O	2.12	0.48
1:A:410:VAL:HG21	1:A:439:LEU:HD21	1.96	0.48
1:B:724:LEU:HD11	1:B:768:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PRO:HB3	1:B:748:GLN:HB3	1.96	0.47
1:A:46:VAL:HG22	1:A:97:PHE:HA	1.94	0.47
1:B:232:PHE:CD1	1:B:232:PHE:C	2.92	0.47
1:B:1062:ALA:HB1	1:B:1132:VAL:CG1	2.45	0.47
1:B:1062:ALA:HB1	1:B:1132:VAL:HG12	1.97	0.47
1:A:186:ILE:HD12	1:A:191:VAL:HG21	1.95	0.47
1:A:554:ALA:O	1:A:556:SER:N	2.47	0.47
1:B:703:PHE:CE1	1:B:707:PHE:CD2	3.02	0.47
1:A:46:VAL:CG1	1:A:239:LEU:HD13	2.45	0.47
1:A:636:VAL:HG23	1:A:637:GLU:HG3	1.96	0.47
1:B:464:LYS:HE2	1:B:666:CYS:SG	2.55	0.47
1:B:465:MET:HE3	1:B:668:LEU:HD11	1.96	0.46
1:A:86:THR:OG1	1:A:762:ARG:NH1	2.48	0.46
1:A:615:THR:HG22	1:A:619:ASN:ND2	2.30	0.46
1:B:403:SER:HB3	1:B:406:ARG:HB2	1.97	0.46
1:B:81:VAL:HG11	1:B:744:LEU:CD1	2.46	0.46
1:A:108:GLN:O	1:A:109:ALA:C	2.57	0.46
1:A:185:THR:HA	1:A:189:ALA:O	2.16	0.46
1:A:73:THR:HA	1:A:80:ALA:O	2.15	0.46
1:B:970:ARG:HB3	1:B:971:PRO:HD3	1.97	0.46
1:B:17:PRO:HG3	1:B:20:TYR:CZ	2.51	0.46
1:B:1111:ARG:HH11	1:B:1111:ARG:CG	2.29	0.46
1:A:89:HIS:HD2	1:A:333:ALA:O	1.99	0.45
1:A:329:ILE:CD1	1:A:716:MET:HE1	2.47	0.45
1:A:494:GLN:C	1:A:496:ASP:H	2.24	0.45
1:A:874:ASP:O	1:A:878:ILE:HG12	2.16	0.45
1:A:842:TRP:HB2	1:B:1132:VAL:HG13	1.98	0.45
1:A:494:GLN:O	1:A:496:ASP:N	2.48	0.45
1:A:806:LYS:HA	1:A:806:LYS:HE2	1.98	0.45
1:A:979:VAL:HA	1:A:1026:LEU:O	2.16	0.45
1:A:715:VAL:HA	1:A:718:MET:HE2	1.99	0.45
1:B:583:MET:SD	1:B:893:MET:HE3	2.56	0.45
1:A:13:VAL:CG1	1:A:66:ALA:HB2	2.47	0.45
1:B:701:ARG:HG2	1:B:701:ARG:HH11	1.82	0.45
1:A:330:VAL:HG22	1:A:768:PRO:HG2	1.97	0.45
1:A:170:CYS:SG	1:A:241:PHE:CD1	3.10	0.45
1:A:183:LYS:HE3	1:A:183:LYS:HB2	1.46	0.45
1:A:483:MET:HE3	1:A:483:MET:HB2	1.79	0.44
1:B:647:LEU:HD21	1:B:901:LEU:HD23	1.99	0.44
1:A:849:ARG:O	1:A:850:ASN:C	2.60	0.44
1:A:1072:THR:HG21	1:A:1088:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:511:VAL:HG11	1.99	0.44
1:A:46:VAL:HG13	1:A:239:LEU:HD13	2.00	0.44
1:A:639:ARG:O	1:A:640:ASN:C	2.61	0.44
1:B:823:HIS:HB2	1:B:840:PRO:HB3	1.99	0.43
1:B:398:ASP:C	1:B:400:SER:H	2.27	0.43
1:A:1019:ASP:OD1	1:A:1021:THR:HG22	2.19	0.43
1:B:583:MET:HB3	1:B:594:GLN:HG2	1.99	0.43
1:B:1107:ARG:O	1:B:1110:GLU:N	2.52	0.43
1:B:720:ASN:ND2	1:B:726:ALA:H	2.16	0.43
1:A:197:TYR:CZ	1:A:742:PRO:HD3	2.54	0.43
1:B:631:LEU:HG	1:B:632:MET:HE2	2.01	0.42
1:A:917:ILE:HD12	1:A:1015:LEU:HB3	2.01	0.42
1:B:613:LEU:HD22	1:B:826:ILE:HD13	2.01	0.42
1:A:476:VAL:HG12	1:A:477:ILE:HD12	2.01	0.42
1:B:906:HIS:NE2	1:B:909:TYR:O	2.37	0.42
1:A:67:VAL:HG22	1:A:69:VAL:HG23	2.01	0.42
1:A:810:ILE:HG21	1:A:844:TRP:CE3	2.54	0.42
1:A:1088:TRP:CE2	1:A:1101:MET:HB3	2.55	0.42
1:B:610:ARG:HH21	1:B:860:GLU:HB3	1.83	0.42
1:A:366:ALA:HB2	1:A:959:TRP:HB2	2.02	0.42
1:A:924:PRO:O	1:A:949:MET:HE1	2.19	0.42
1:A:970:ARG:HG3	1:A:970:ARG:NH1	2.19	0.42
1:B:818:LEU:HD23	1:B:818:LEU:HA	1.95	0.42
1:B:713:ARG:HA	1:B:713:ARG:HD2	1.31	0.41
1:A:433:GLY:O	1:A:434:ARG:O	2.39	0.41
1:B:200:GLN:OE1	1:B:200:GLN:N	2.51	0.41
1:B:268:ALA:HA	1:B:332:MET:HE3	2.02	0.41
1:B:98:HIS:HB3	1:B:157:LEU:HB2	2.02	0.41
1:A:632:MET:HA	1:A:632:MET:HE2	2.03	0.41
1:A:1131:LEU:H	1:A:1131:LEU:HG	1.48	0.41
1:B:353:THR:HG22	1:B:355:ALA:N	2.36	0.41
1:B:852:LEU:HG	1:B:853:PRO:HD2	2.03	0.41
1:A:735:GLU:OE2	1:A:735:GLU:HA	2.20	0.41
1:B:395:ASP:C	1:B:397:LYS:H	2.29	0.41
1:A:642:LYS:HD2	1:A:642:LYS:HA	1.87	0.41
1:B:464:LYS:CE	1:B:666:CYS:SG	3.09	0.41
1:A:359:ASN:OD1	1:A:956:PRO:HA	2.21	0.41
1:A:814:PRO:HG3	1:A:875:TYR:CD1	2.56	0.41
1:A:846:ALA:HB3	1:A:852:LEU:HD13	2.03	0.41
1:B:801:TYR:CE1	1:B:1021:THR:HG22	2.56	0.41
1:B:968:LEU:HA	1:B:968:LEU:HD12	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:ALA:O	1:B:1101:MET:HE1	2.21	0.40
1:A:384:HIS:O	1:A:411:PRO:HA	2.21	0.40
1:B:202:PHE:CE2	1:B:744:LEU:HA	2.57	0.40
1:B:444:GLN:HE22	1:B:525:PHE:H	1.69	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	1030/1136 (91%)	983 (95%)	37 (4%)	10 (1%)	12	24
1	B	1040/1136 (92%)	984 (95%)	52 (5%)	4 (0%)	30	50
All	All	2070/2272 (91%)	1967 (95%)	89 (4%)	14 (1%)	18	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	PHE
1	A	830	GLY
1	A	434	ARG
1	A	601	GLY
1	A	444	GLN
1	B	499	CYS
1	A	634	ASN
1	A	850	ASN
1	A	908	THR
1	B	992	ALA
1	B	993	GLY
1	B	1131	LEU
1	A	29	GLU
1	A	638	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	839/885 (95%)	784 (93%)	55 (7%)	15	29
1	B	840/885 (95%)	784 (93%)	56 (7%)	15	28
All	All	1679/1770 (95%)	1568 (93%)	111 (7%)	15	29

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	18	LEU
1	A	46	VAL
1	A	67	VAL
1	A	82	SER
1	A	86	THR
1	A	107	THR
1	A	110	PRO
1	A	117	GLU
1	A	171	ILE
1	A	173	ASN
1	A	183	LYS
1	A	234	ARG
1	A	241	PHE
1	A	439	LEU
1	A	473	ASP
1	A	476	VAL
1	A	477	ILE
1	A	478	VAL
1	A	480	ARG
1	A	482	GLU
1	A	483	MET
1	A	495	THR
1	A	497	VAL
1	A	512	HIS
1	A	517	ARG
1	A	521	ARG

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Mol	Chain	Res	Type
1	A	539	MET
1	A	573	GLU
1	A	596	VAL
1	A	598	THR
1	A	602	ARG
1	A	631	LEU
1	A	633	ARG
1	A	642	LYS
1	A	651	ASN
1	A	655	SER
1	A	675	ARG
1	A	702	ASN
1	A	728	THR
1	A	760	VAL
1	A	763	VAL
1	A	775	SER
1	A	806	LYS
1	A	821	GLN
1	A	851	GLN
1	A	857	LEU
1	A	858	SER
1	A	863	GLU
1	A	970	ARG
1	A	1005	SER
1	A	1021	THR
1	A	1089	LEU
1	A	1113	ASN
1	A	1131	LEU
1	B	9	THR
1	B	18	LEU
1	B	29	GLU
1	B	32	GLU
1	B	81	VAL
1	B	92	SER
1	B	142	GLU
1	B	154	ARG
1	B	156	LEU
1	B	184	VAL
1	B	193	ARG
1	B	204	PRO
1	B	342	ILE
1	B	353	THR

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Mol	Chain	Res	Type
1	B	379	THR
1	B	397	LYS
1	B	496	ASP
1	B	505	ASP
1	B	566	THR
1	B	568	ARG
1	B	569	THR
1	B	572	GLN
1	B	574	THR
1	B	588	THR
1	B	592	VAL
1	B	600	MET
1	B	605	THR
1	B	621	ARG
1	B	629	GLU
1	B	636	VAL
1	B	637	GLU
1	B	644	ARG
1	B	647	LEU
1	B	651	ASN
1	B	675	ARG
1	B	699	GLU
1	B	701	ARG
1	B	702	ASN
1	B	713	ARG
1	B	714	ARG
1	B	717	ASP
1	B	725	SER
1	B	739	ILE
1	B	754	SER
1	B	763	VAL
1	B	775	SER
1	B	836	ASN
1	B	902	ARG
1	B	936	GLN
1	B	952	VAL
1	B	1048	SER
1	B	1050	CYS
1	B	1058	SER
1	B	1064	VAL
1	B	1070	VAL
1	B	1122	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	177	HIS
1	A	266	HIS
1	A	272	ASN
1	A	614	HIS
1	A	619	ASN
1	A	702	ASN
1	A	708	GLN
1	A	851	GLN
1	A	955	HIS
1	A	1002	ASN
1	A	1052	GLN
1	A	1081	GLN
1	A	1134	GLN
1	B	89	HIS
1	B	98	HIS
1	B	173	ASN
1	B	218	HIS
1	B	399	HIS
1	B	420	GLN
1	B	444	GLN
1	B	572	GLN
1	B	614	HIS
1	B	708	GLN
1	B	720	ASN
1	B	836	ASN
1	B	928	GLN
1	B	936	GLN
1	B	967	ASN
1	B	1002	ASN
1	B	1126	HIS

### 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1050/1136 (92%)	-0.06	28 (2%) 56 54	16, 36, 68, 103	0
1	B	1060/1136 (93%)	-0.19	26 (2%) 58 56	11, 30, 66, 107	0
All	All	2110/2272 (92%)	-0.12	54 (2%) 57 55	11, 33, 68, 107	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	555	PHE	5.2
1	B	992	ALA	5.0
1	B	792	ALA	4.1
1	A	779	PHE	3.6
1	B	566	THR	3.4
1	A	566	THR	3.3
1	A	528	ALA	3.3
1	A	801	TYR	3.3
1	A	80	ALA	3.3
1	B	308	GLY	3.2
1	A	639	ARG	3.1
1	A	833	PRO	3.0
1	A	854	ALA	3.0
1	B	795	ALA	3.0
1	A	497	VAL	2.9
1	B	601	GLY	2.9
1	B	80	ALA	2.8
1	A	737	ALA	2.8
1	B	440	VAL	2.8
1	B	567	ALA	2.8
1	A	29	GLU	2.8
1	A	1131	LEU	2.7
1	B	1108	ALA	2.6
1	B	8	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1048	SER	2.6
1	A	495	THR	2.6
1	A	556	SER	2.6
1	A	642	LYS	2.6
1	B	30	GLY	2.5
1	A	756	PHE	2.5
1	A	81	VAL	2.5
1	B	600	MET	2.5
1	B	28	SER	2.3
1	B	570	ILE	2.3
1	A	1036	ALA	2.3
1	A	1135	LEU	2.3
1	B	903	TYR	2.3
1	A	480	ARG	2.3
1	B	1116	TRP	2.3
1	A	600	MET	2.2
1	A	72	ARG	2.2
1	B	738	ALA	2.2
1	A	443	THR	2.2
1	B	430	GLY	2.2
1	B	759	ASP	2.2
1	B	1122	LEU	2.2
1	A	477	ILE	2.2
1	B	780	ALA	2.2
1	B	762	ARG	2.1
1	B	1109	LEU	2.1
1	A	435	PRO	2.0
1	A	994	ASN	2.0
1	A	434	ARG	2.0
1	A	636	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands

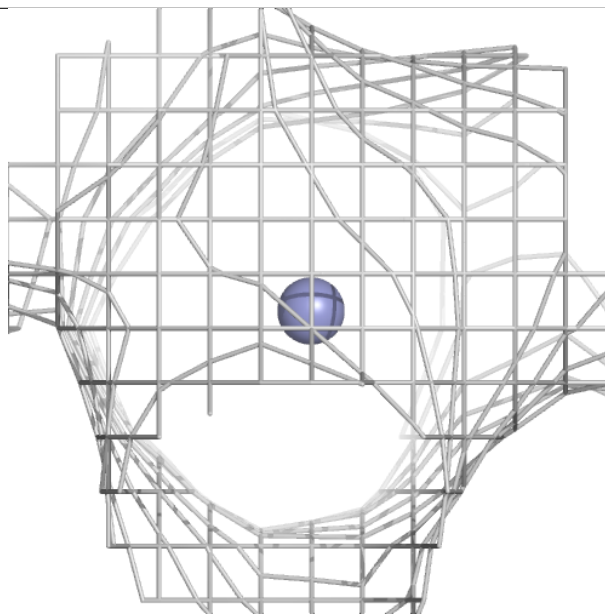
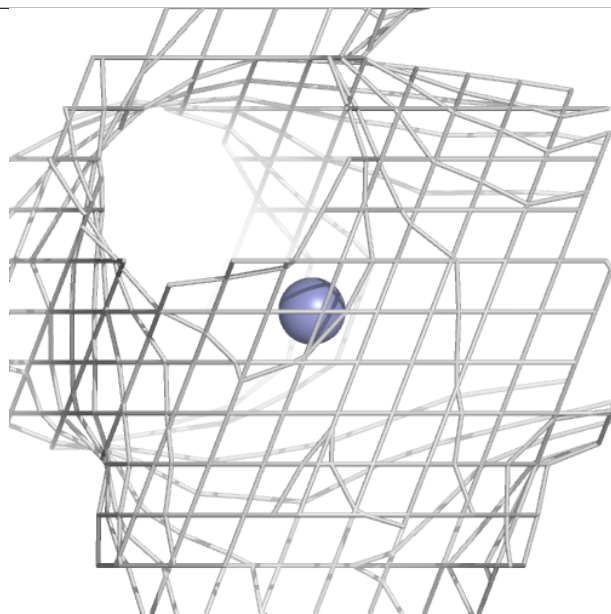
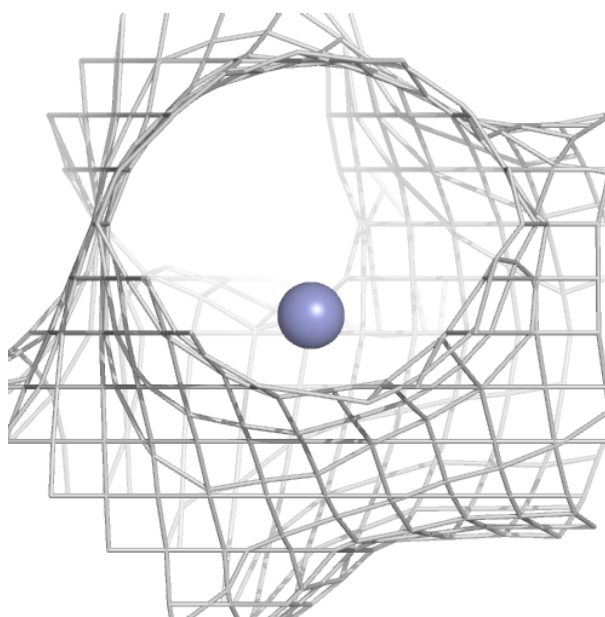
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	ZN	A	1201	1/1	0.99	0.03	40,40,40,40	0
2	ZN	B	1201	1/1	0.99	0.02	27,27,27,27	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 ZN A 1201:**

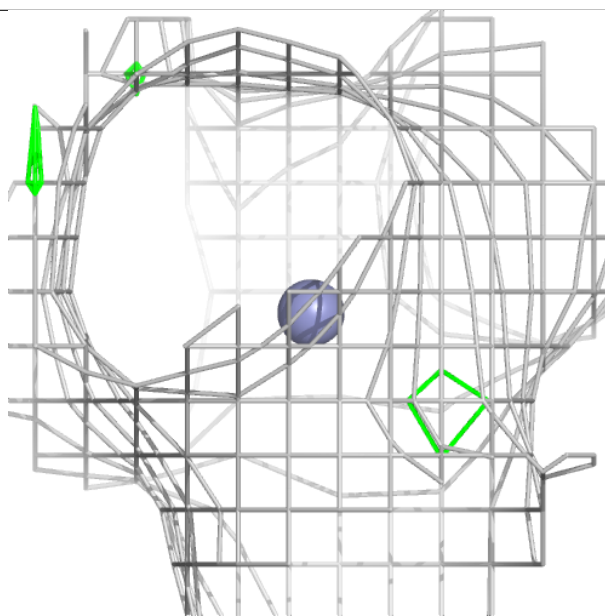
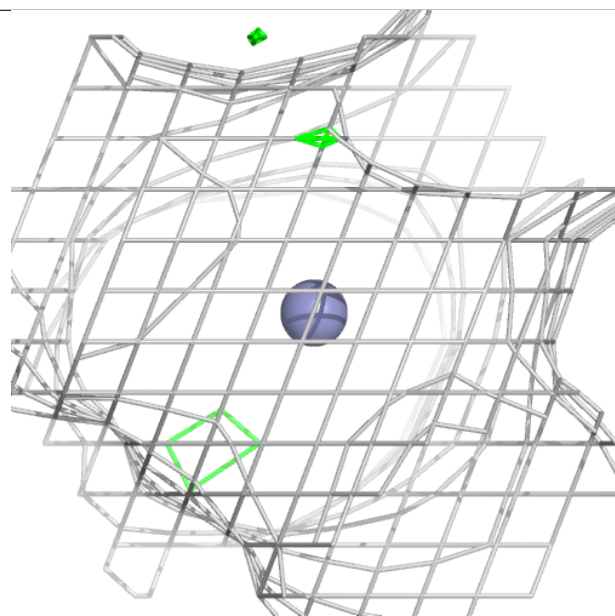
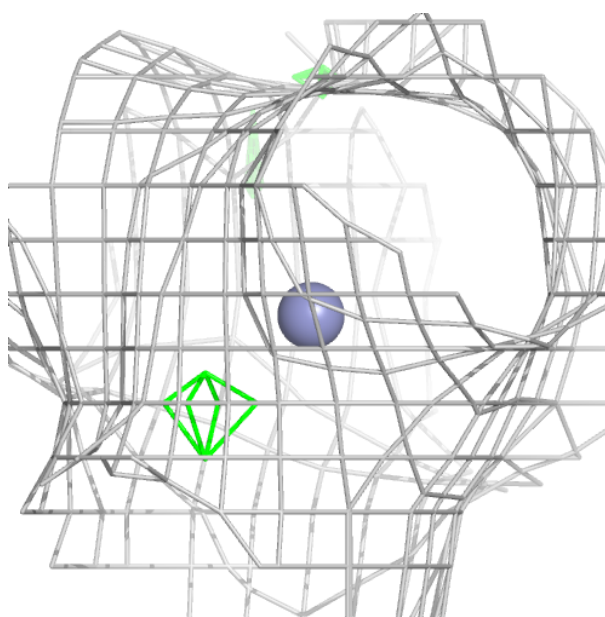
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ZN B 1201:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.