



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:45 AM UTC

PDB ID : 7XES / pdb\_00007xes  
Title : NifS with L-penicillamine  
Authors : Nakamura, R.; Fujishiro, T.  
Deposited on : 2022-03-31  
Resolution : 3.00 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  
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

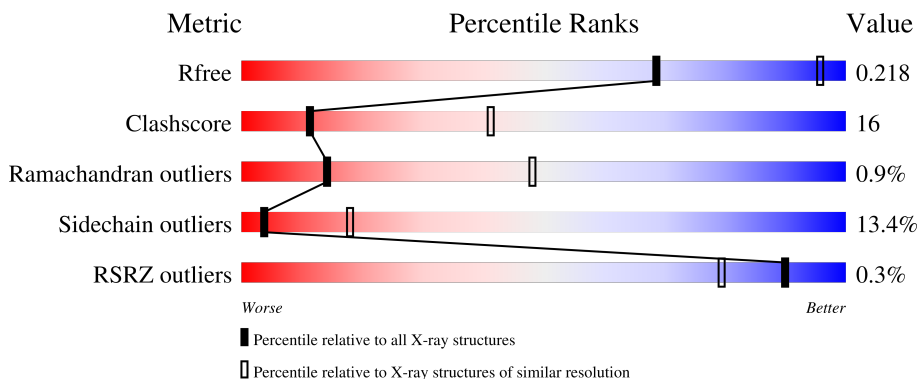
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	401	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2850 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 Cysteine desulfurase IscS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2755	1741	482	521	11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP O25008
A	138	ARG	LYS	engineered mutation	UNP O25008
A	388	VAL	-	expression tag	UNP O25008
A	389	ASP	-	expression tag	UNP O25008
A	390	LEU	-	expression tag	UNP O25008
A	391	VAL	-	expression tag	UNP O25008
A	392	PRO	-	expression tag	UNP O25008
A	393	ARG	-	expression tag	UNP O25008
A	394	GLY	-	expression tag	UNP O25008
A	395	SER	-	expression tag	UNP O25008
A	396	HIS	-	expression tag	UNP O25008
A	397	HIS	-	expression tag	UNP O25008
A	398	HIS	-	expression tag	UNP O25008
A	399	HIS	-	expression tag	UNP O25008
A	400	HIS	-	expression tag	UNP O25008
A	401	HIS	-	expression tag	UNP O25008

- Molecule 2 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).

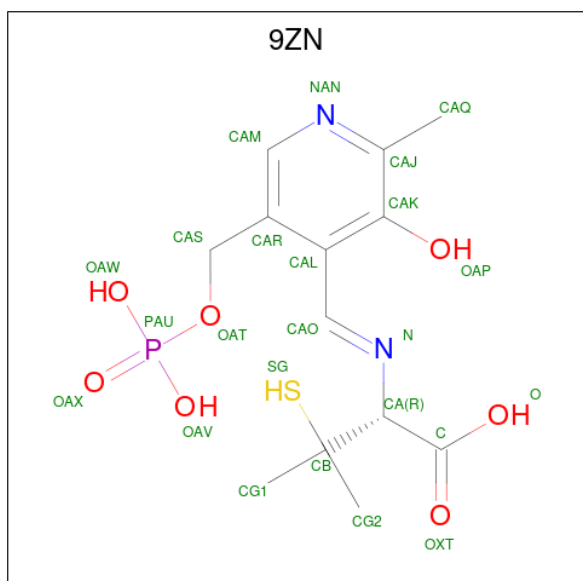


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 3 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is (2 {R})-3-methyl-2-[( {E})-[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylideneamino]-3-sulfanyl-butanoic acid (CCD ID: 9ZN) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>2</sub>O<sub>7</sub>PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	24	13	2	7	1	1	0	0

- Molecule 5 is water.

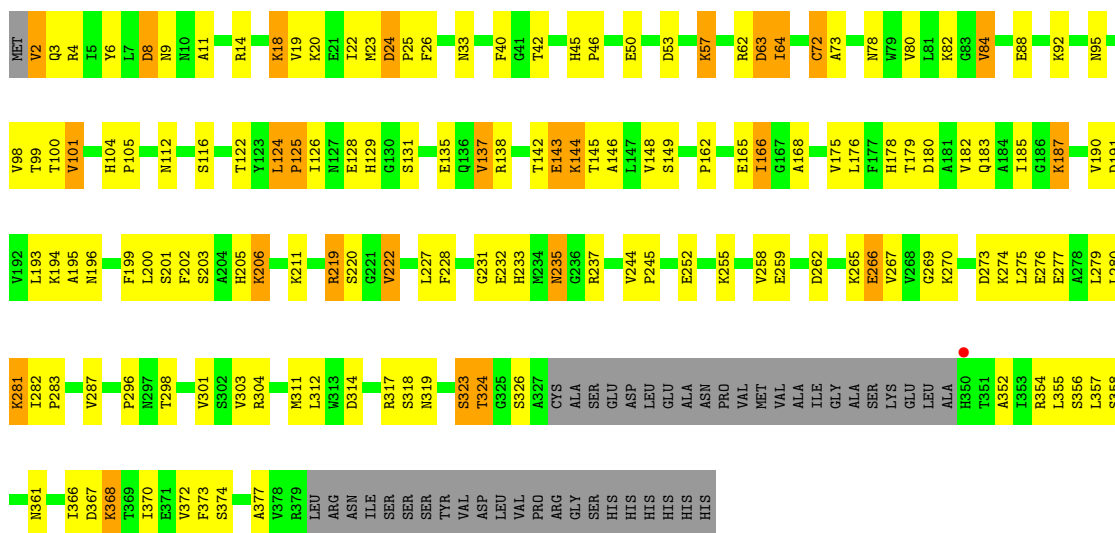
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		

### 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: Cysteine desulfurase IscS

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.94Å 102.94Å 132.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 3.00 48.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-3.00) 99.9 (48.91-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.171 , 0.215 0.173 , 0.218	Depositor DCC
$R_{free}$ test set	740 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.0	Xtrriage
Anisotropy	0.024	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 98.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2850	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, CL, 9ZN

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	0.79	1/2806 (0.0%)	1.60	22/3801 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	VAL	N-CA	5.28	1.56	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	PHE	CA-CB-CG	8.55	122.36	113.80
1	A	125	PRO	CB-CA-C	-7.95	100.57	110.98
1	A	235	ASN	CB-CA-C	-7.70	100.41	111.95
1	A	266	GLU	CB-CA-C	-7.20	98.61	110.85
1	A	24	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	144	LYS	CB-CA-C	7.01	121.92	111.06
1	A	8	ASP	CA-CB-CG	-6.42	106.18	112.60
1	A	227	LEU	N-CA-C	-6.22	105.84	113.50
1	A	298	THR	CA-CB-OG1	-6.14	100.39	109.60
1	A	143	GLU	CB-CA-C	6.11	122.12	110.27
1	A	235	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	99	THR	CA-CB-OG1	-5.59	101.21	109.60
1	A	273	ASP	CB-CA-C	5.48	120.17	110.85
1	A	40	PHE	O-C-N	5.45	128.97	122.27
1	A	42	THR	CB-CA-C	5.40	121.04	110.67
1	A	219	ARG	CG-CD-NE	-5.39	100.14	112.00
1	A	112	ASN	CA-CB-CG	-5.28	107.32	112.60
1	A	283	PRO	N-CA-C	5.25	119.81	111.26
1	A	361	ASN	CA-CB-CG	5.16	117.76	112.60
1	A	18	LYS	N-CA-CB	5.09	118.17	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	26	PHE	CA-CB-CG	-5.05	108.75	113.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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	2755	0	2764	88	0
2	A	4	0	8	0	0
3	A	1	0	0	0	0
4	A	24	0	0	6	0
5	A	66	0	0	2	0
All	All	2850	0	2772	90	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 16.

All (90) 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:312:LEU:HD11	1:A:324:THR:HG22	1.50	0.93
1:A:312:LEU:CD1	1:A:324:THR:HG22	2.06	0.85
1:A:244:VAL:HB	1:A:245:PRO:HD3	1.58	0.83
1:A:219:ARG:HB3	1:A:222:VAL:CG1	2.10	0.81
1:A:219:ARG:HB3	1:A:222:VAL:HG11	1.64	0.78
1:A:275:LEU:HD21	1:A:355:LEU:HD13	1.69	0.75
1:A:101:VAL:HG22	1:A:124:LEU:O	1.89	0.71
1:A:311:MET:HE2	1:A:373:PHE:CD1	2.25	0.71
1:A:219:ARG:O	1:A:222:VAL:HG13	1.89	0.70
1:A:98:VAL:HG13	1:A:148:VAL:HG13	1.72	0.70
1:A:50:GLU:HB3	5:A:625:HOH:O	1.92	0.69
1:A:206:LYS:NZ	4:A:503:9ZN:CAO	2.57	0.67
1:A:62:ARG:HD3	1:A:193:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:HIS:HB2	1:A:46:PRO:HD3	1.78	0.66
1:A:280:LEU:HD13	1:A:287:VAL:HG23	1.78	0.64
1:A:206:LYS:HZ1	4:A:503:9ZN:CAO	2.12	0.63
1:A:64:ILE:HD12	1:A:220:SER:CB	2.29	0.62
1:A:162:PRO:O	1:A:166:ILE:HG13	2.00	0.61
1:A:78:ASN:OD1	1:A:82:LYS:HE3	2.00	0.60
1:A:19:VAL:O	1:A:23:MET:HG3	2.03	0.59
1:A:205:HIS:CE1	1:A:206:LYS:HE3	2.38	0.58
1:A:145:THR:HG22	1:A:175:VAL:HG21	1.88	0.56
1:A:149:SER:HA	1:A:178:HIS:O	2.08	0.54
1:A:219:ARG:O	1:A:222:VAL:CG1	2.55	0.53
1:A:255:LYS:O	1:A:258:VAL:HG22	2.09	0.53
1:A:24:ASP:N	1:A:25:PRO:CD	2.72	0.52
1:A:2:VAL:HG11	1:A:319:ASN:ND2	2.24	0.52
1:A:191:ASP:OD1	1:A:193:LEU:HB2	2.11	0.51
1:A:45:HIS:CB	1:A:46:PRO:HD3	2.41	0.51
1:A:46:PRO:O	1:A:50:GLU:HG3	2.11	0.50
1:A:280:LEU:CD1	1:A:287:VAL:HG23	2.40	0.50
1:A:312:LEU:HD12	1:A:324:THR:HG22	1.91	0.50
1:A:262:ASP:O	1:A:266:GLU:HG2	2.11	0.50
1:A:367:ASP:HA	1:A:370:ILE:HD12	1.92	0.50
1:A:80:VAL:O	1:A:84:VAL:HG13	2.12	0.50
1:A:374:SER:O	1:A:377:ALA:HB3	2.12	0.50
4:A:503:9ZN:CAO	4:A:503:9ZN:SG	3.00	0.50
1:A:185:ILE:HD13	1:A:190:VAL:HG21	1.94	0.49
1:A:180:ASP:HA	1:A:201:SER:HB2	1.94	0.49
1:A:64:ILE:HD12	1:A:220:SER:HB2	1.93	0.49
1:A:24:ASP:N	1:A:25:PRO:HD3	2.27	0.49
1:A:8:ASP:OD1	1:A:323:SER:OG	2.25	0.49
1:A:244:VAL:HB	1:A:245:PRO:CD	2.37	0.48
1:A:182:VAL:HG22	1:A:202:PHE:HA	1.94	0.48
1:A:19:VAL:O	1:A:22:ILE:HG22	2.14	0.48
1:A:135:GLU:O	1:A:138:ARG:HB3	2.14	0.48
1:A:281:LYS:HB2	1:A:281:LYS:HE2	1.73	0.48
1:A:73:ALA:CB	1:A:182:VAL:HG21	2.43	0.47
1:A:274:LYS:NZ	1:A:367:ASP:OD1	2.48	0.47
1:A:368:LYS:HD2	1:A:372:VAL:HG23	1.95	0.47
1:A:122:THR:HG22	1:A:124:LEU:HD23	1.95	0.47
1:A:276:GLU:O	1:A:280:LEU:HB2	2.15	0.47
1:A:33:ASN:OD1	1:A:33:ASN:C	2.57	0.46
1:A:137:VAL:HG11	1:A:166:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:CYS:HB2	4:A:503:9ZN:OAW	2.15	0.46
4:A:503:9ZN:OAP	4:A:503:9ZN:N	2.48	0.46
1:A:266:GLU:HB2	1:A:267:VAL:HG23	1.97	0.46
1:A:11:ALA:HB2	1:A:354:ARG:NH1	2.32	0.45
1:A:183:GLN:O	1:A:187:LYS:HD3	2.16	0.45
1:A:9:ASN:CG	1:A:358:SER:HB3	2.42	0.45
1:A:179:THR:HG23	1:A:200:LEU:HD12	1.99	0.45
1:A:195:ALA:O	1:A:196:ASN:C	2.60	0.45
1:A:64:ILE:HD12	1:A:220:SER:HB3	1.96	0.44
1:A:275:LEU:O	1:A:279:LEU:HG	2.18	0.44
1:A:368:LYS:HA	1:A:368:LYS:HD3	1.83	0.44
1:A:2:VAL:CG1	1:A:319:ASN:ND2	2.81	0.44
1:A:311:MET:HE2	1:A:373:PHE:CE1	2.52	0.44
1:A:255:LYS:HE2	1:A:259:GLU:OE1	2.18	0.43
1:A:232:GLU:HB2	1:A:233:HIS:ND1	2.34	0.43
1:A:88:GLU:HA	1:A:92:LYS:HB2	2.01	0.42
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.85	0.42
1:A:124:LEU:HA	1:A:125:PRO:HD2	1.82	0.42
1:A:194:LYS:HE2	1:A:194:LYS:HB3	1.67	0.42
1:A:357:LEU:HD21	1:A:366:ILE:HD11	2.02	0.42
1:A:137:VAL:O	1:A:138:ARG:C	2.63	0.42
1:A:206:LYS:HZ2	4:A:503:9ZN:CAO	2.33	0.42
1:A:205:HIS:CG	1:A:211:LYS:HG2	2.55	0.41
1:A:252:GLU:OE1	1:A:252:GLU:HA	2.20	0.41
1:A:314:ASP:O	1:A:317:ARG:HB2	2.20	0.41
1:A:178:HIS:HB2	1:A:199:PHE:HB2	2.03	0.41
1:A:6:TYR:OH	1:A:8:ASP:HB3	2.20	0.41
1:A:88:GLU:OE1	1:A:92:LYS:HD2	2.21	0.41
1:A:53:ASP:O	1:A:57:LYS:HB2	2.21	0.41
1:A:165:GLU:O	1:A:168:ALA:HB3	2.21	0.41
1:A:269:GLY:HA2	1:A:296:PRO:O	2.20	0.41
1:A:63:ASP:OD1	1:A:63:ASP:N	2.54	0.40
1:A:235:ASN:O	1:A:237:ARG:HG3	2.20	0.40
1:A:301:VAL:O	1:A:352:ALA:HB1	2.21	0.40
1:A:3:GLN:HB2	5:A:658:HOH:O	2.20	0.40
1:A:146:ALA:O	1:A:176:LEU:HB2	2.21	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	352/401 (88%)	328 (93%)	21 (6%)	3 (1%)	14 48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	CYS
1	A	63	ASP
1	A	231	GLY

### 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	299/337 (89%)	259 (87%)	40 (13%)	4 18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	14	ARG
1	A	18	LYS
1	A	20	LYS
1	A	57	LYS
1	A	64	ILE
1	A	84	VAL
1	A	95	ASN

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Mol	Chain	Res	Type
1	A	100	THR
1	A	101	VAL
1	A	104	HIS
1	A	105	PRO
1	A	116	SER
1	A	124	LEU
1	A	126	ILE
1	A	128	GLU
1	A	129	HIS
1	A	131	SER
1	A	137	VAL
1	A	142	THR
1	A	143	GLU
1	A	144	LYS
1	A	166	ILE
1	A	187	LYS
1	A	203	SER
1	A	206	LYS
1	A	222	VAL
1	A	265	LYS
1	A	270	LYS
1	A	277	GLU
1	A	281	LYS
1	A	282	ILE
1	A	303	VAL
1	A	304	ARG
1	A	318	SER
1	A	323	SER
1	A	324	THR
1	A	326	SER
1	A	356	SER
1	A	368	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	229	HIS
1	A	260	HIS
1	A	319	ASN

### 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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	IPA	A	501	-	3,3,3	0.59	0	3,3,3	0.73	0
4	9ZN	A	503	-	21,24,24	2.96	10 (47%)	27,36,36	2.05	9 (33%)

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
4	9ZN	A	503	-	-	6/20/21/21	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	9ZN	CAQ-CAJ	-7.32	1.38	1.50
4	A	503	9ZN	CAS-CAR	-5.47	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	9ZN	CAL-CAO	-4.46	1.37	1.46
4	A	503	9ZN	PAU-OAX	4.24	1.63	1.50
4	A	503	9ZN	CAO-N	3.58	1.33	1.27
4	A	503	9ZN	CA-N	-3.25	1.43	1.46
4	A	503	9ZN	CAM-NAN	2.73	1.40	1.34
4	A	503	9ZN	PAU-OAV	2.72	1.64	1.54
4	A	503	9ZN	CAK-CAJ	-2.60	1.38	1.41
4	A	503	9ZN	CAL-CAR	-2.54	1.38	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	9ZN	CAL-CAO-N	-4.86	113.18	122.73
4	A	503	9ZN	CAL-CAK-CAJ	3.86	122.32	120.14
4	A	503	9ZN	OAW-PAU-OAT	3.17	114.93	106.67
4	A	503	9ZN	OAW-PAU-OAV	3.13	119.55	107.80
4	A	503	9ZN	OAV-PAU-OAX	-2.93	99.41	110.83
4	A	503	9ZN	CAR-CAM-NAN	-2.84	119.21	123.83
4	A	503	9ZN	CAQ-CAJ-CAK	2.51	123.74	120.80
4	A	503	9ZN	CAK-CAJ-NAN	-2.42	117.91	120.96
4	A	503	9ZN	CA-N-CAO	2.38	120.44	116.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	9ZN	OXT-C-CA-CB
4	A	503	9ZN	CAL-CAR-CAS-OAT
4	A	503	9ZN	CB-CA-N-CAO
4	A	503	9ZN	O-C-CA-CB
4	A	503	9ZN	CAM-CAR-CAS-OAT
4	A	503	9ZN	CAK-CAL-CAO-N

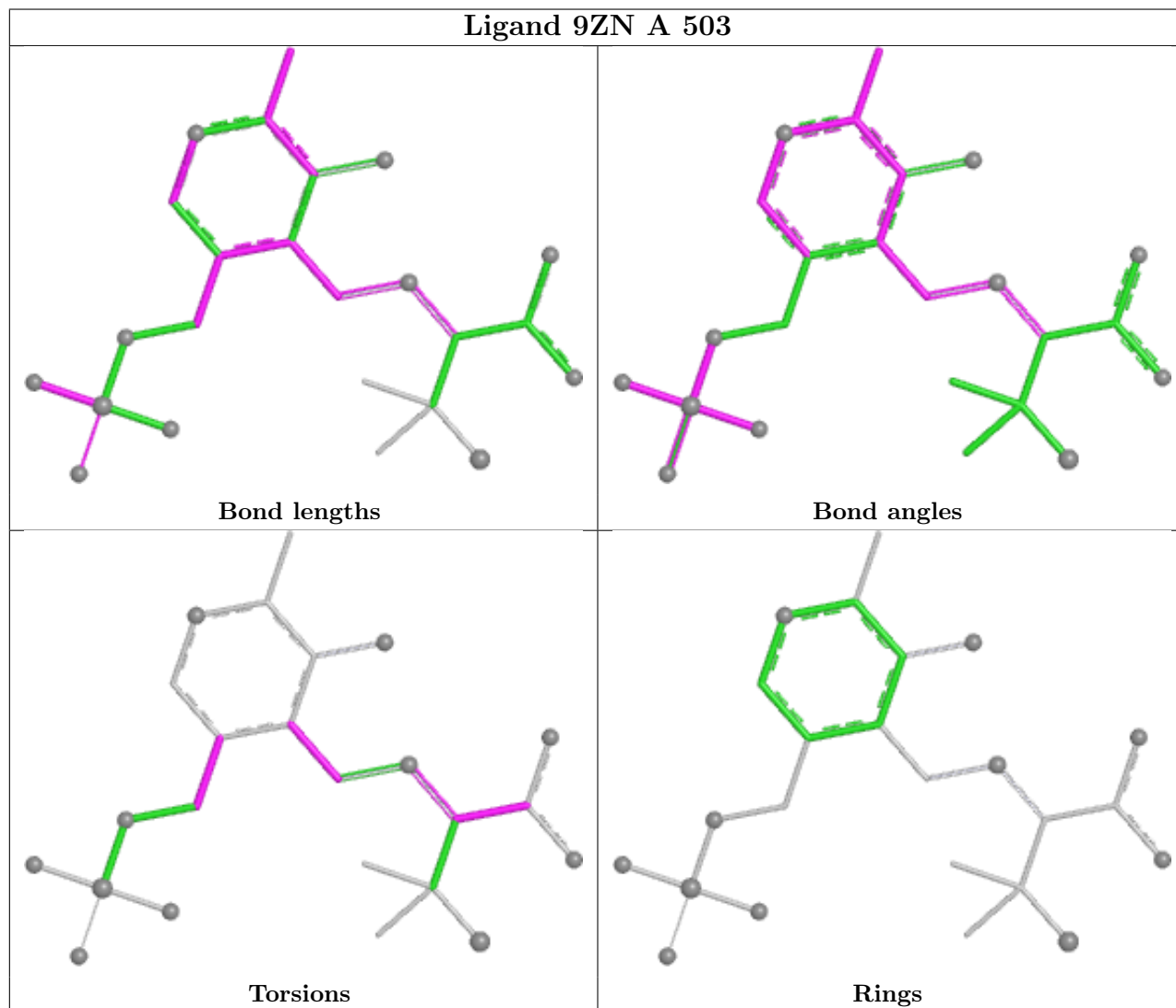
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	9ZN	6	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	356/401 (88%)	-0.67	1 (0%) 90 79	63, 111, 168, 199	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	HIS	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.

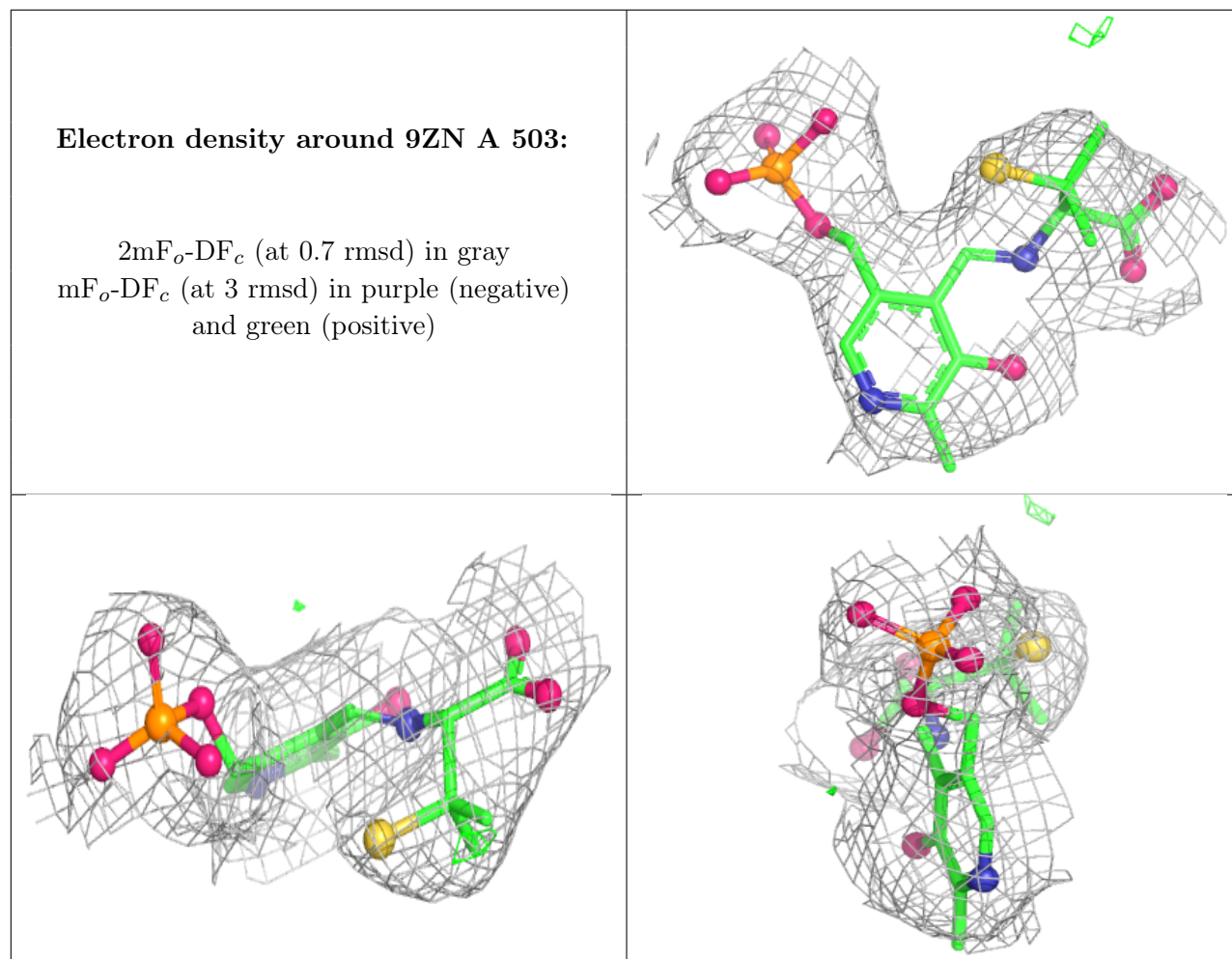
### 6.4 Ligands [i](#)

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, 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(Å <sup>2</sup> )	Q<0.9
2	IPA	A	501	4/4	0.93	0.27	67,68,72,89	0
3	CL	A	502	1/1	0.95	0.15	84,84,84,84	0
4	9ZN	A	503	24/24	0.98	0.06	70,96,112,140	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 [i](#)

There are no such residues in this entry.