



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 8UL6 / pdb_00008ul6
Title : LSD1-CoREST in complex with T16, long soaking
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2023-10-16
Resolution : 2.74 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

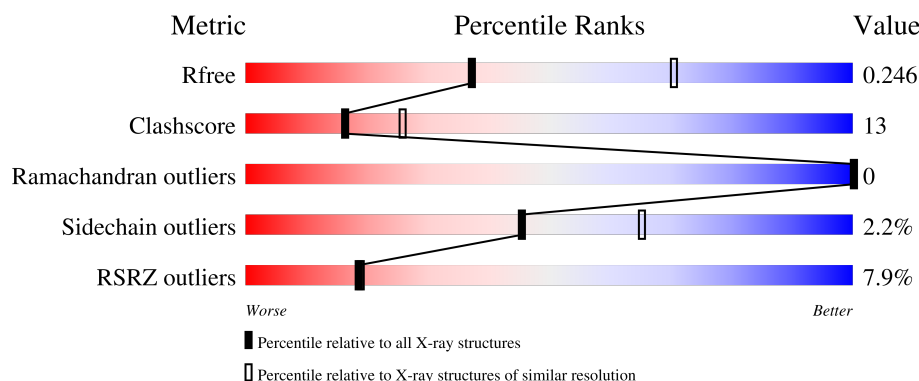
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	871	4% 59% 17% • 24%
2	B	144	17% 61% 28% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6360 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O60341
A	-17	SER	-	expression tag	UNP O60341
A	-16	SER	-	expression tag	UNP O60341
A	-15	HIS	-	expression tag	UNP O60341
A	-14	HIS	-	expression tag	UNP O60341
A	-13	HIS	-	expression tag	UNP O60341
A	-12	HIS	-	expression tag	UNP O60341
A	-11	HIS	-	expression tag	UNP O60341
A	-10	HIS	-	expression tag	UNP O60341
A	-9	SER	-	expression tag	UNP O60341
A	-8	SER	-	expression tag	UNP O60341
A	-7	GLY	-	expression tag	UNP O60341
A	-6	LEU	-	expression tag	UNP O60341
A	-5	VAL	-	expression tag	UNP O60341
A	-4	PRO	-	expression tag	UNP O60341
A	-3	ARG	-	expression tag	UNP O60341
A	-2	GLY	-	expression tag	UNP O60341
A	-1	SER	-	expression tag	UNP O60341
A	0	HIS	-	expression tag	UNP O60341

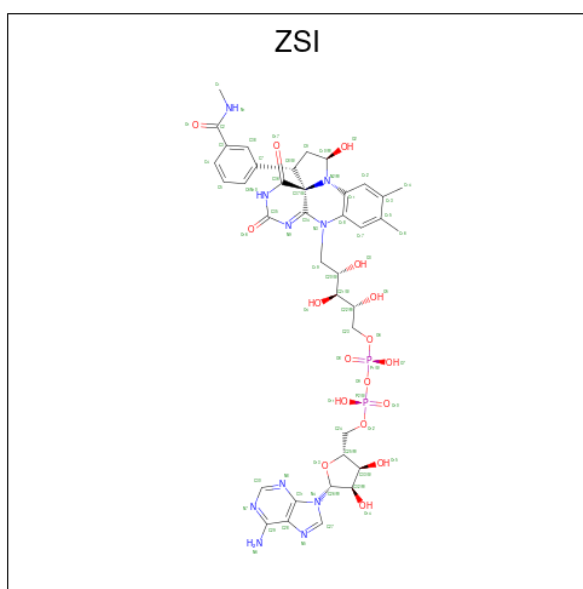
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag	UNP Q9UKL0
B	304	PHE	-	expression tag	UNP Q9UKL0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2R,3S,4S)-2,3,4-trihydroxy-5-[(1R,3S,3aS,13R)-1-hydroxy-10,11-dimethyl-3-[3-(methylcarbamoyl)phenyl]-4,6-dioxo-2,3,5,6-tetrahydro-1H-benzo[g]pyrrolo[2,1-e]pteridin-8(4H)-yl]pentyl dihydrogen diphosphate (non-preferred name) (CCD ID: ZSI) (formula: C₃₈H₄₆N₁₀O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

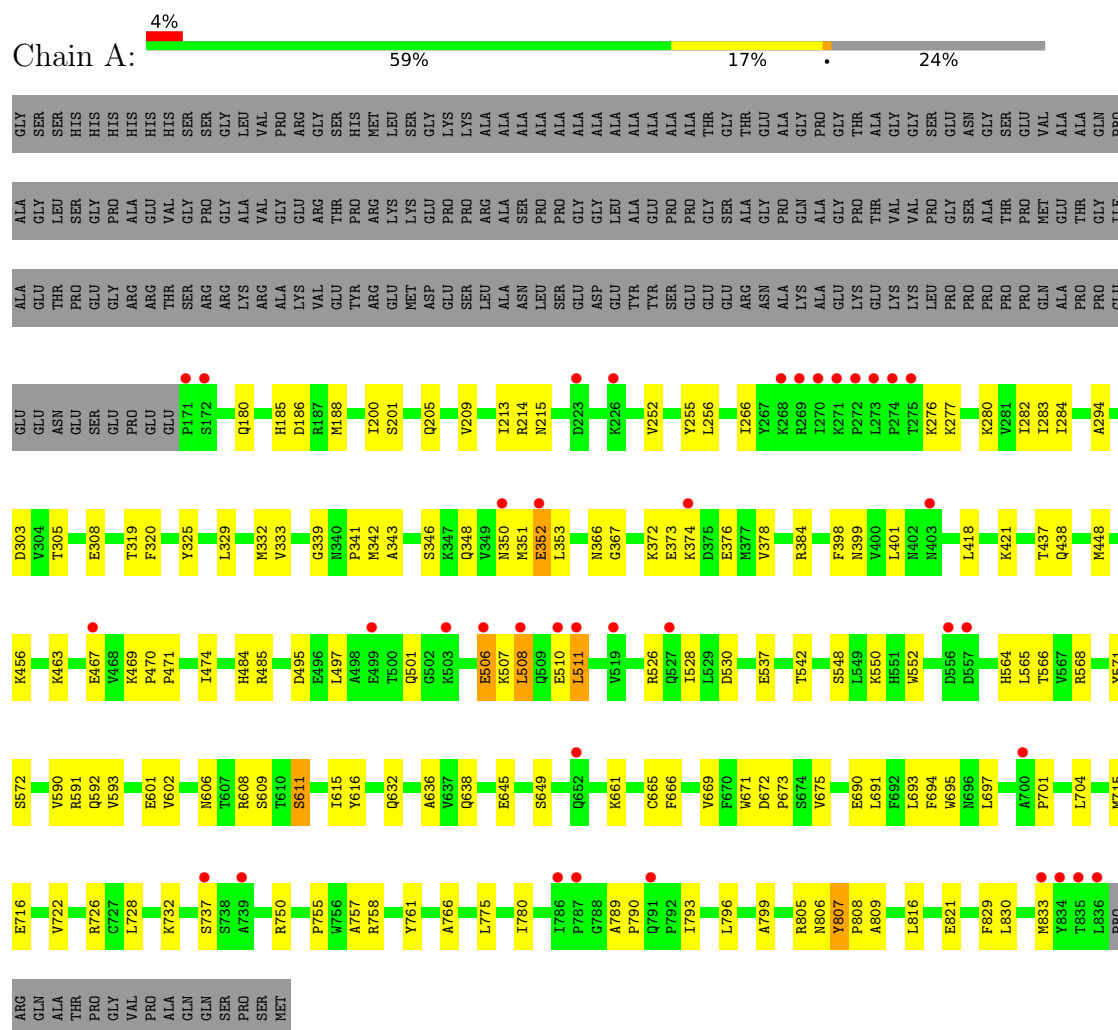


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			67	38	10	17	2	

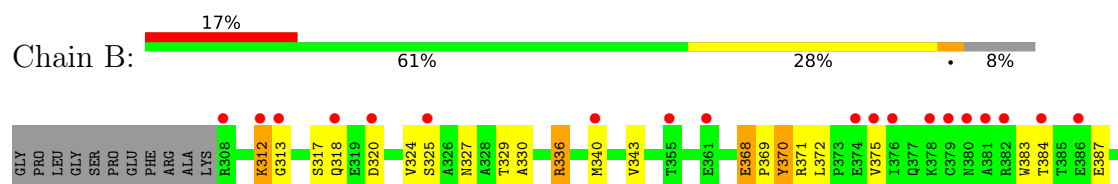
3 Residue-property plots

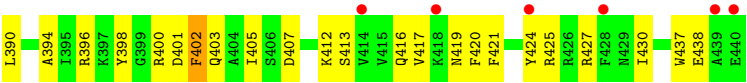
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lysine-specific histone demethylase 1A



• Molecule 2: REST corepressor 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.32Å 178.42Å 234.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.74 48.38 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.38-2.74) 96.5 (48.38-2.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.217 , 0.241 0.223 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6360	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: ZSI

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	0.52	0/5331	0.76	1/7232 (0.0%)
2	B	0.65	0/1091	1.01	4/1471 (0.3%)
All	All	0.54	0/6422	0.81	5/8703 (0.1%)

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
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	833	MET	CB-CG-SD	6.65	132.64	112.70
2	B	401	ASP	CA-C-N	-5.41	111.03	121.58
2	B	401	ASP	C-N-CA	-5.41	111.03	121.58
2	B	318	GLN	N-CA-C	-5.34	104.70	111.11
2	B	336	ARG	CG-CD-NE	5.02	123.04	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	402	PHE	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	5217	0	5252	135	1
2	B	1076	0	1091	53	0
3	A	67	0	0	2	0
All	All	6360	0	6343	165	1

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 (165) 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:266:ILE:N	1:A:348:GLN:OE1	1.78	1.17
1:A:456:LYS:HG2	2:B:370:TYR:CE1	1.84	1.12
1:A:456:LYS:CG	2:B:370:TYR:HE1	1.68	1.07
1:A:456:LYS:HG2	2:B:370:TYR:HE1	1.11	1.05
1:A:456:LYS:CG	2:B:370:TYR:CE1	2.51	0.89
1:A:495:ASP:OD2	2:B:371:ARG:NH2	2.04	0.89
1:A:346:SER:HA	1:A:351:MET:HE2	1.56	0.88
1:A:384:ARG:HH22	2:B:313:GLY:HA3	1.41	0.86
1:A:346:SER:HA	1:A:351:MET:CE	2.05	0.85
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.54	0.85
1:A:384:ARG:NH1	2:B:312:LYS:O	2.12	0.82
1:A:276:LYS:HD3	1:A:277:LYS:H	1.45	0.82
1:A:352:GLU:HG2	1:A:568:ARG:HB2	1.65	0.79
1:A:506:GLU:N	1:A:506:GLU:OE1	2.16	0.78
2:B:425:ARG:HA	2:B:430:ILE:HD13	1.65	0.77
1:A:495:ASP:CG	2:B:371:ARG:NH2	2.43	0.76
2:B:317:SER:OG	2:B:320:ASP:CG	2.29	0.76
1:A:511:LEU:HD23	1:A:511:LEU:N	2.03	0.73
1:A:255:TYR:HD2	1:A:256:LEU:HD22	1.56	0.71
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.26	0.71
1:A:448:MET:HE2	1:A:497:LEU:HB3	1.73	0.70
1:A:384:ARG:HH22	2:B:313:GLY:CA	2.04	0.69
2:B:327:ASN:OD1	2:B:330:ALA:N	2.25	0.69
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.75	0.67
2:B:413:SER:OG	2:B:416:GLN:OE1	2.14	0.64
1:A:693:LEU:HD12	1:A:694:PHE:H	1.63	0.64
1:A:346:SER:CA	1:A:351:MET:CE	2.77	0.63
1:A:448:MET:HE1	1:A:501:GLN:HB2	1.80	0.63
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.81	0.61
1:A:438:GLN:NE2	1:A:508:LEU:CD1	2.63	0.61
1:A:437:THR:OG1	1:A:508:LEU:HD21	2.01	0.61
1:A:469:LYS:HA	1:A:469:LYS:HE2	1.82	0.61
1:A:645:GLU:OE1	1:A:649:SER:OG	2.15	0.61
1:A:384:ARG:NH2	2:B:313:GLY:HA3	2.13	0.60
1:A:806:ASN:C	1:A:807:TYR:HD1	2.09	0.60
2:B:384:THR:HG22	2:B:387:GLU:CD	2.25	0.60
1:A:266:ILE:CA	1:A:348:GLN:OE1	2.48	0.59
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.65	0.59
1:A:438:GLN:HE21	1:A:508:LEU:CD1	2.15	0.59
1:A:456:LYS:HG3	2:B:370:TYR:CE1	2.38	0.59
2:B:370:TYR:N	2:B:370:TYR:HD2	2.00	0.59
1:A:438:GLN:HE21	1:A:508:LEU:HD11	1.68	0.58
1:A:806:ASN:C	1:A:807:TYR:CD1	2.81	0.58
2:B:383:TRP:CD2	2:B:412:LYS:HE2	2.38	0.58
2:B:424:TYR:HE1	2:B:427:ARG:HH22	1.50	0.58
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.85	0.58
1:A:456:LYS:HG2	2:B:370:TYR:CZ	2.35	0.58
1:A:564:HIS:C	1:A:565:LEU:HD12	2.27	0.58
2:B:370:TYR:N	2:B:370:TYR:CD2	2.70	0.58
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.69	0.58
1:A:438:GLN:NE2	1:A:508:LEU:HD12	2.18	0.58
1:A:185:HIS:CD2	1:A:186:ASP:HB3	2.40	0.57
1:A:255:TYR:CD2	1:A:256:LEU:HD22	2.39	0.57
1:A:320:PHE:HB2	1:A:329:LEU:HD21	1.87	0.56
1:A:384:ARG:NH2	2:B:312:LYS:O	2.38	0.56
1:A:606:ASN:HD22	1:A:609:SER:H	1.53	0.56
1:A:463:LYS:O	1:A:467:GLU:HG2	2.06	0.55
2:B:317:SER:OG	2:B:320:ASP:HB2	2.06	0.55
2:B:317:SER:OG	2:B:320:ASP:CB	2.54	0.55
2:B:340:MET:HA	2:B:343:VAL:HG12	1.89	0.55
2:B:424:TYR:HE1	2:B:427:ARG:NH2	2.05	0.54
1:A:384:ARG:CZ	2:B:312:LYS:O	2.56	0.53
1:A:728:LEU:O	1:A:732:LYS:HG2	2.07	0.53
2:B:416:GLN:HA	2:B:419:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:HG11	1:A:528:ILE:HG22	1.91	0.52
1:A:510:GLU:HG2	1:A:511:LEU:HD23	1.91	0.52
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.91	0.52
1:A:511:LEU:N	1:A:511:LEU:CD2	2.73	0.52
1:A:592:GLN:HG2	1:A:638:GLN:HB3	1.91	0.52
1:A:401:LEU:HD11	2:B:325:SER:HB2	1.92	0.52
1:A:526:ARG:NH1	1:A:530:ASP:OD1	2.42	0.51
1:A:200:ILE:HG22	1:A:201:SER:N	2.23	0.51
1:A:308:GLU:OE2	3:A:901:ZSI:O15	2.28	0.51
1:A:672:ASP:HB3	1:A:675:VAL:HG22	1.92	0.51
1:A:807:TYR:HD1	1:A:807:TYR:N	2.09	0.51
1:A:807:TYR:CD1	1:A:807:TYR:N	2.79	0.51
1:A:341:PRO:HG3	1:A:816:LEU:HD21	1.92	0.50
2:B:327:ASN:OD1	2:B:329:THR:N	2.43	0.50
1:A:372:LYS:O	1:A:376:GLU:HG3	2.12	0.50
1:A:606:ASN:ND2	1:A:608:ARG:HB2	2.26	0.50
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.44	0.50
1:A:352:GLU:O	1:A:352:GLU:HG3	2.10	0.49
1:A:398:PHE:CZ	1:A:401:LEU:HD12	2.47	0.49
1:A:276:LYS:HD3	1:A:277:LYS:N	2.22	0.49
1:A:485:ARG:C	1:A:485:ARG:HD3	2.38	0.49
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.48	0.49
1:A:421:LYS:NZ	2:B:320:ASP:OD2	2.46	0.48
1:A:209:VAL:O	1:A:213:ILE:HG13	2.13	0.48
2:B:387:GLU:HA	2:B:390:LEU:HD12	1.96	0.47
1:A:332:MET:HG3	1:A:333:VAL:HG23	1.95	0.47
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.29	0.47
1:A:793:ILE:HD12	1:A:793:ILE:H	1.78	0.47
2:B:394:ALA:HB1	2:B:405:ILE:HG12	1.95	0.47
1:A:732:LYS:HD2	1:A:737:SER:HA	1.97	0.47
2:B:421:PHE:O	2:B:425:ARG:HB2	2.15	0.47
1:A:185:HIS:HD2	1:A:186:ASP:HB3	1.80	0.46
1:A:280:LYS:HD2	1:A:303:ASP:O	2.15	0.46
2:B:420:PHE:CD1	2:B:424:TYR:HD2	2.32	0.46
1:A:346:SER:CB	1:A:351:MET:CE	2.92	0.46
1:A:284:ILE:HD13	1:A:590:VAL:HG11	1.98	0.46
1:A:319:THR:HB	1:A:572:SER:HB3	1.96	0.46
1:A:205:GLN:O	1:A:209:VAL:HG23	2.15	0.46
1:A:352:GLU:HG2	1:A:568:ARG:CB	2.41	0.46
1:A:438:GLN:NE2	1:A:508:LEU:HD11	2.28	0.46
1:A:456:LYS:HA	2:B:370:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:CA	2:B:370:TYR:HE1	2.28	0.46
2:B:317:SER:HG	2:B:320:ASP:CG	2.22	0.46
2:B:400:ARG:HB3	2:B:402:PHE:CZ	2.50	0.46
1:A:805:ARG:O	1:A:808:PRO:HD3	2.15	0.46
1:A:669:VAL:HG13	1:A:671:TRP:CE2	2.51	0.46
1:A:537:GLU:HG2	1:A:542:THR:O	2.15	0.46
1:A:373:GLU:HG3	1:A:374:LYS:N	2.27	0.45
1:A:282:ILE:HD13	1:A:305:THR:HB	1.97	0.45
1:A:829:PHE:O	1:A:830:LEU:HD23	2.15	0.45
2:B:368:GLU:N	2:B:369:PRO:CD	2.79	0.45
2:B:383:TRP:CZ2	2:B:420:PHE:HB2	2.52	0.45
1:A:252:VAL:O	1:A:256:LEU:HD23	2.16	0.45
1:A:343:ALA:O	1:A:346:SER:OG	2.28	0.45
1:A:799:ALA:HB2	1:A:821:GLU:HG3	1.98	0.45
1:A:346:SER:HB3	1:A:351:MET:CE	2.47	0.44
1:A:601:GLU:HA	1:A:616:TYR:O	2.17	0.44
1:A:188:MET:CE	1:A:200:ILE:HG12	2.47	0.44
1:A:366:ASN:OD1	1:A:367:GLY:N	2.51	0.44
1:A:548:SER:O	1:A:552:TRP:HB3	2.18	0.44
1:A:606:ASN:HD21	1:A:608:ARG:HB2	1.82	0.43
1:A:722:VAL:O	1:A:726:ARG:HG3	2.18	0.43
1:A:757:ALA:O	1:A:758:ARG:HB2	2.18	0.43
1:A:775:LEU:HA	1:A:775:LEU:HD23	1.78	0.43
1:A:325:TYR:CE1	1:A:665:CYS:HB3	2.54	0.43
1:A:691:LEU:HD23	1:A:691:LEU:HA	1.90	0.43
1:A:346:SER:HB3	1:A:351:MET:HE1	1.99	0.43
1:A:606:ASN:HD21	1:A:608:ARG:HE	1.66	0.43
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.53	0.43
1:A:666:PHE:O	1:A:701:PRO:HG2	2.19	0.43
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.01	0.43
2:B:394:ALA:O	2:B:398:TYR:N	2.51	0.43
1:A:308:GLU:OE1	3:A:901:ZSI:O14	2.37	0.42
1:A:632:GLN:OE1	1:A:636:ALA:HB2	2.18	0.42
1:A:353:LEU:HD13	1:A:565:LEU:HD22	2.01	0.42
1:A:506:GLU:OE1	1:A:506:GLU:CA	2.67	0.42
1:A:548:SER:HB2	1:A:766:ALA:HA	2.01	0.42
1:A:690:GLU:OE1	1:A:715:MET:HE3	2.20	0.42
1:A:283:ILE:HD12	1:A:294:ALA:HB2	2.01	0.42
2:B:396:ARG:O	2:B:437:TRP:HD1	2.02	0.42
1:A:448:MET:CE	1:A:497:LEU:HB3	2.48	0.42
1:A:789:ALA:HB1	1:A:790:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:SER:O	2:B:417:VAL:HG23	2.20	0.42
1:A:399:ASN:ND2	1:A:550:LYS:HE2	2.35	0.42
1:A:484:HIS:ND1	2:B:372:LEU:HD13	2.35	0.42
1:A:342:MET:HE2	1:A:571:TYR:OH	2.21	0.41
1:A:180:GLN:HA	1:A:339:GLY:HA2	2.03	0.41
1:A:214:ARG:NH1	1:A:215:ASN:OD1	2.54	0.41
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.75	0.41
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.97	0.41
1:A:671:TRP:O	1:A:673:PRO:HD3	2.20	0.41
1:A:188:MET:HB2	1:A:200:ILE:HD11	2.03	0.41
2:B:403:GLN:NE2	2:B:407:ASP:OD1	2.54	0.41
1:A:418:LEU:HD21	2:B:324:VAL:HG21	2.03	0.40
2:B:425:ARG:HA	2:B:430:ILE:CD1	2.43	0.40
1:A:693:LEU:HD12	1:A:694:PHE:N	2.31	0.40
2:B:336:ARG:O	2:B:340:MET:HG2	2.22	0.40
1:A:282:ILE:HG21	1:A:602:VAL:HG21	2.04	0.40
1:A:470:PRO:HA	1:A:471:PRO:C	2.46	0.40
1:A:609:SER:O	1:A:609:SER:OG	2.27	0.40

All (1) 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:591:ARG:NH1	1:A:611:SER:CA[2_565]	2.04	0.16

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	664/871 (76%)	641 (96%)	23 (4%)	0	100	100
2	B	131/144 (91%)	127 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	795/1015 (78%)	768 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/715 (79%)	556 (98%)	10 (2%)	51	69
2	B	117/125 (94%)	112 (96%)	5 (4%)	26	46
All	All	683/840 (81%)	668 (98%)	15 (2%)	45	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	ASN
1	A	352	GLU
1	A	506	GLU
1	A	507	LYS
1	A	508	LEU
1	A	511	LEU
1	A	593	VAL
1	A	611	SER
1	A	615	ILE
1	A	807	TYR
2	B	312	LYS
2	B	368	GLU
2	B	370	TYR
2	B	375	VAL
2	B	438	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	228	GLN
1	A	296	GLN
1	A	298	GLN
1	A	395	GLN
1	A	399	ASN
1	A	427	GLN
1	A	438	GLN
1	A	514	ASN
1	A	606	ASN
1	A	638	GLN
1	A	742	GLN
2	B	356	ASN
2	B	403	GLN
2	B	419	ASN
2	B	423	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](#)

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
3	ZSI	A	901	-	71,74,74	1.47	16 (22%)	97,115,115	1.53	10 (10%)

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
3	ZSI	A	901	-	-	2/44/112/112	0/7/8/8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ZSI	P2-O9	-3.58	1.55	1.59
3	A	901	ZSI	C36-N10	-3.38	1.32	1.37
3	A	901	ZSI	P1-O9	-3.34	1.55	1.59
3	A	901	ZSI	C35-N9	-3.10	1.29	1.36
3	A	901	ZSI	C27-N4	-3.04	1.32	1.37
3	A	901	ZSI	O3-C20	-2.79	1.37	1.43
3	A	901	ZSI	C11-N2	-2.60	1.36	1.41
3	A	901	ZSI	C10-N2	-2.42	1.43	1.46
3	A	901	ZSI	C26-N4	-2.30	1.40	1.46
3	A	901	ZSI	C18-C11	-2.22	1.37	1.41
3	A	901	ZSI	C12-C13	-2.18	1.36	1.39
3	A	901	ZSI	O16-C35	-2.16	1.20	1.24
3	A	901	ZSI	O2-C10	-2.11	1.37	1.41
3	A	901	ZSI	P1-O7	-2.08	1.45	1.55
3	A	901	ZSI	P2-O11	-2.07	1.45	1.55
3	A	901	ZSI	O4-C21	-2.02	1.38	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ZSI	C11-N2-C10	-6.70	108.56	123.92
3	A	901	ZSI	C37-C8-C7	6.34	125.93	116.08
3	A	901	ZSI	C36-C37-C34	-4.72	105.02	113.40
3	A	901	ZSI	C8-C9-C10	-3.70	96.79	104.25
3	A	901	ZSI	C6-C7-C8	-3.66	113.77	121.07
3	A	901	ZSI	C36-N10-C35	-3.14	120.69	125.42
3	A	901	ZSI	C4-C3-C2	-2.91	111.17	120.60
3	A	901	ZSI	C38-C7-C8	2.53	127.36	120.63
3	A	901	ZSI	C38-C3-C2	2.52	128.74	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ZSI	O11-P2-O10	2.16	122.51	112.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

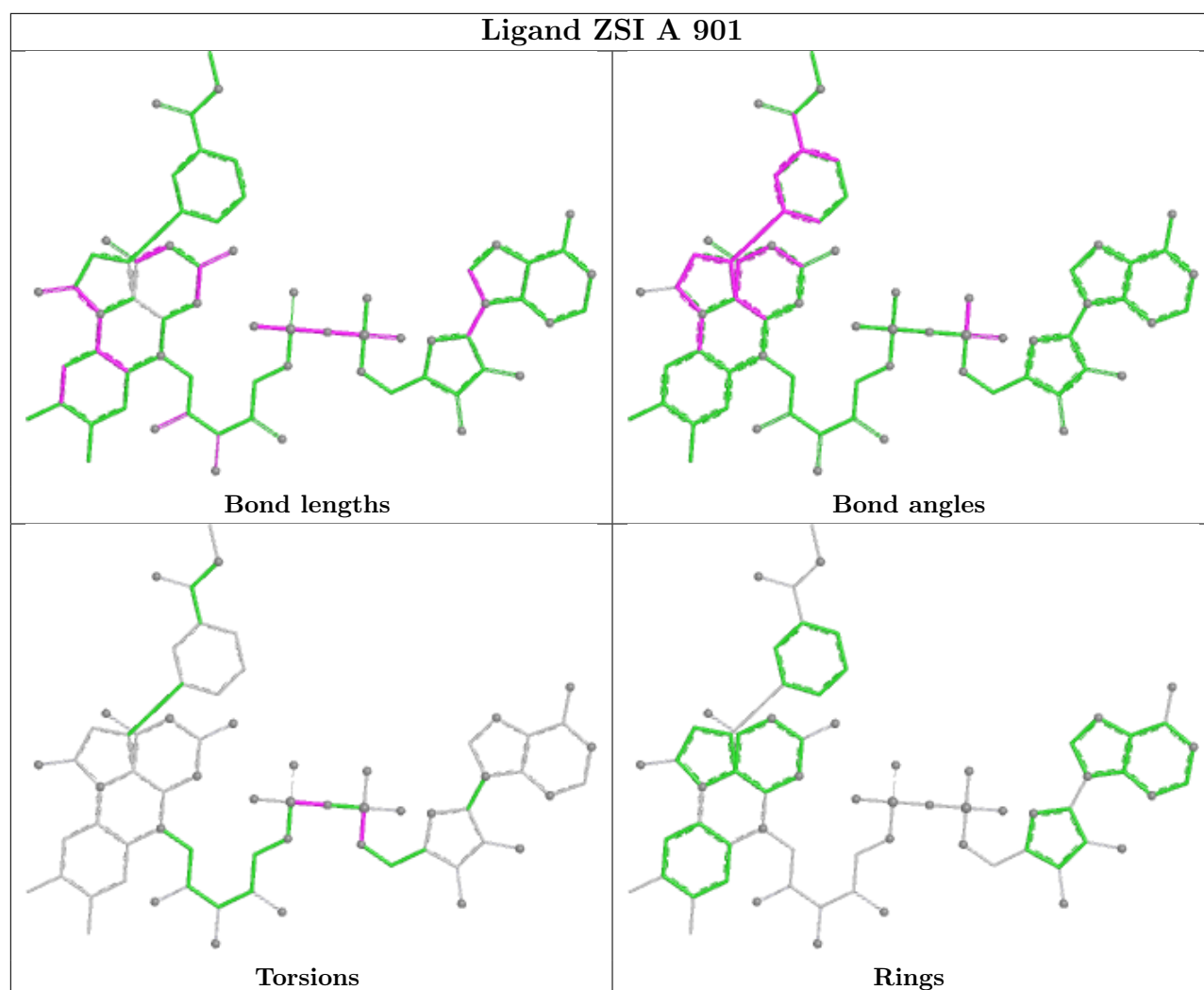
Mol	Chain	Res	Type	Atoms
3	A	901	ZSI	C24-O12-P2-O10
3	A	901	ZSI	P2-O9-P1-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ZSI	2	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	666/871 (76%)	0.57	38 (5%)	29 29	54, 81, 111, 133	0
2	B	133/144 (92%)	1.20	25 (18%)	3 3	77, 108, 130, 144	0
All	All	799/1015 (78%)	0.67	63 (7%)	18 19	54, 87, 119, 144	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	7.3
1	A	171	PRO	4.5
1	A	269	ARG	4.5
2	B	308	ARG	4.2
1	A	833	MET	4.1
2	B	376	ILE	3.8
1	A	272	PRO	3.7
1	A	275	THR	3.7
1	A	273	LEU	3.4
1	A	786	ILE	3.2
2	B	382	ARG	3.2
1	A	835	THR	3.1
1	A	352	GLU	3.0
1	A	556	ASP	3.0
2	B	375	VAL	3.0
1	A	403	ASN	2.9
2	B	428	PHE	2.9
2	B	418	LYS	2.8
1	A	508	LEU	2.8
2	B	381	ALA	2.8
1	A	271	LYS	2.7
2	B	440	GLU	2.6
1	A	274	PRO	2.6
1	A	834	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	374	GLU	2.6
2	B	380	ASN	2.6
1	A	737	SER	2.5
1	A	506	GLU	2.5
2	B	355	THR	2.5
1	A	557	ASP	2.5
2	B	320	ASP	2.5
2	B	386	GLU	2.5
2	B	379	CYS	2.4
1	A	268	LYS	2.4
2	B	439	ALA	2.4
1	A	374	LYS	2.4
2	B	312	LYS	2.4
2	B	414	VAL	2.4
1	A	511	LEU	2.3
1	A	739	ALA	2.3
1	A	503	LYS	2.3
2	B	340	MET	2.3
2	B	361	GLU	2.3
1	A	787	PRO	2.3
1	A	652	GLN	2.3
2	B	318	GLN	2.3
1	A	510	GLU	2.2
2	B	378	LYS	2.2
1	A	226	LYS	2.2
1	A	467	GLU	2.1
1	A	499	GLU	2.1
1	A	527	GLN	2.1
2	B	424	TYR	2.1
2	B	313	GLY	2.1
1	A	519	VAL	2.1
2	B	325	SER	2.1
1	A	700	ALA	2.1
1	A	172	SER	2.1
1	A	791	GLN	2.1
1	A	270	ILE	2.1
1	A	223	ASP	2.0
1	A	350	ASN	2.0
2	B	384	THR	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](#)

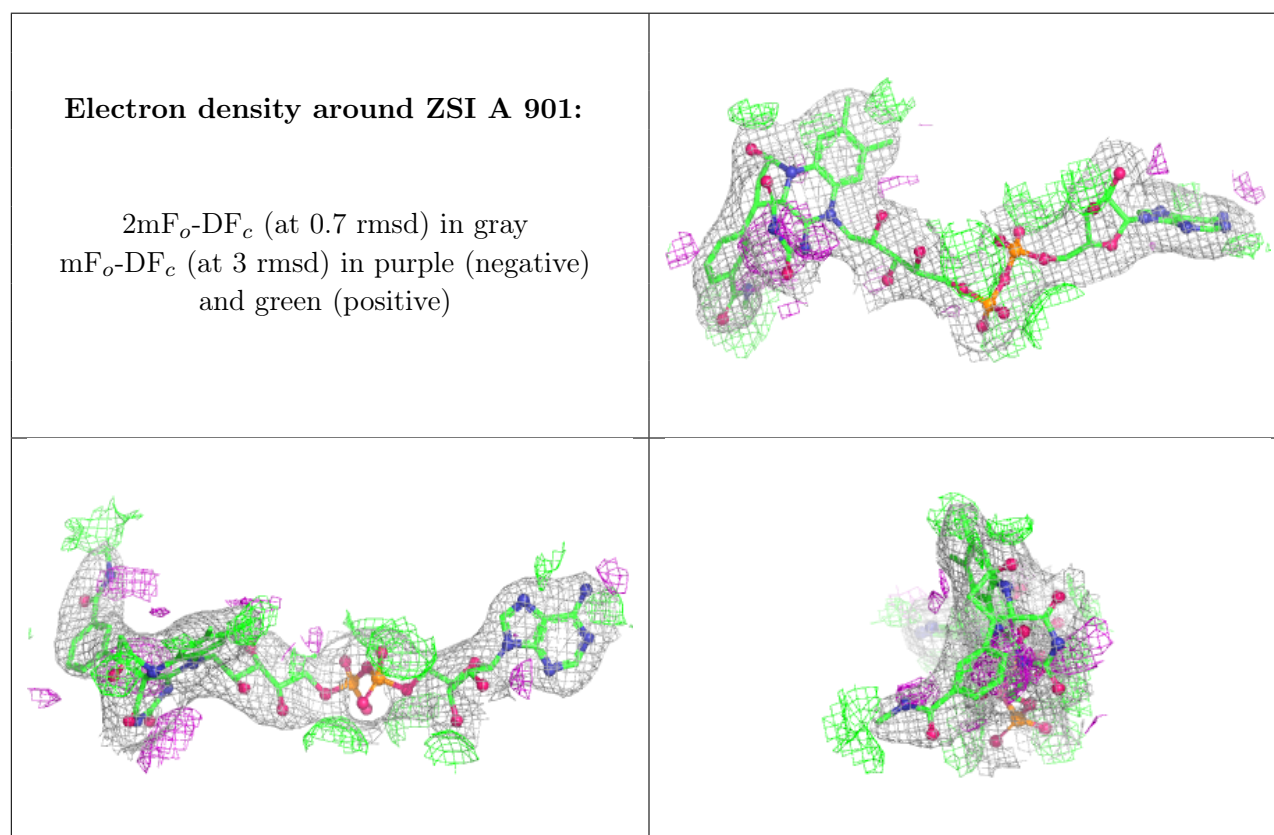
There are no oligosaccharides in this entry.

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
3	ZSI	A	901	67/67	0.96	0.10	40,63,78,84	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.