



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2024 – 07:34 pm BST

PDB ID : 8BOP  
Title : LSD1-CoREST in complex with AW4, long soaking  
Authors : Caroli, J.; Mattevi, A.  
Deposited on : 2022-11-15  
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](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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

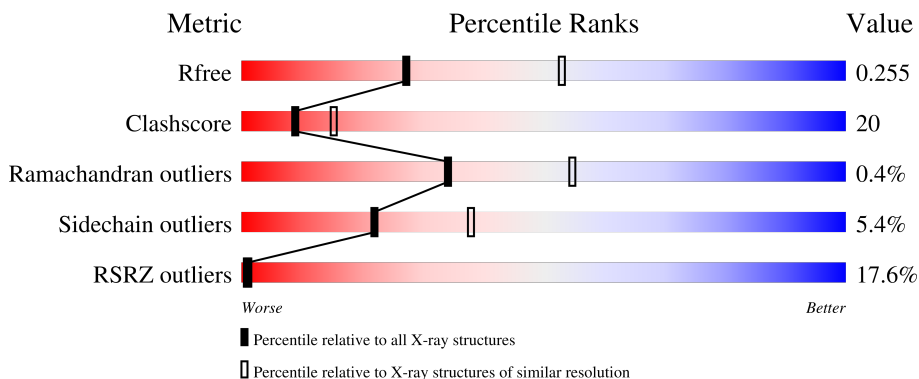
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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  $\geq 3$ , 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	871	
2	B	144	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6368 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
			Total	C	N	O	S			
1	A	666	5217	3324	906	967	20	0	0	0

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

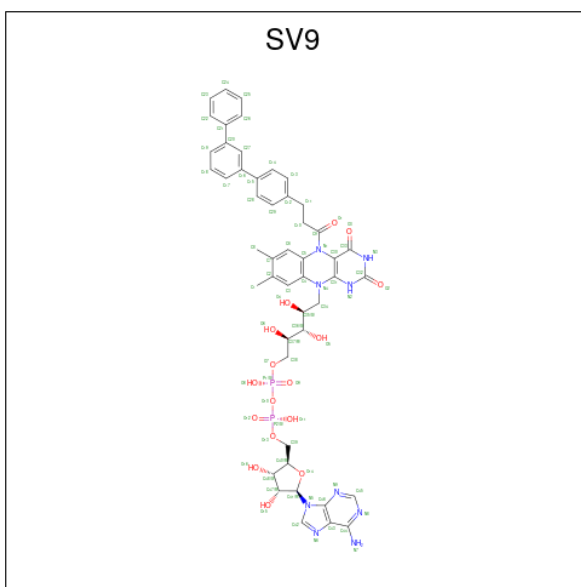
- Molecule 2 is a protein called REST corepressor 1.

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

There are 8 discrepancies between the modelled and reference sequences:

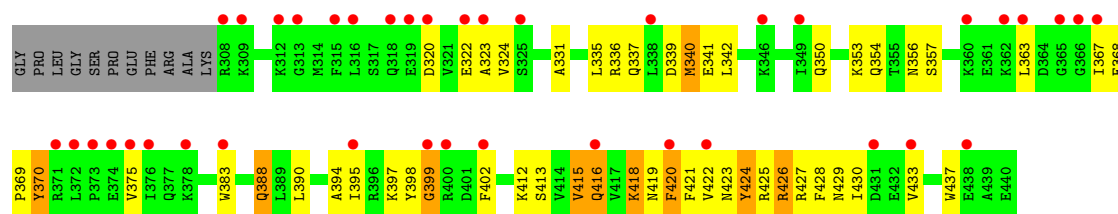
Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag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

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {S})-5-[7,8-dimethyl-2,4-bis(oxidanylidene)-5-[3-[4-(3-phenylphenyl)phenyl]propanoyl]-1 {H}-benzo[g]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] hydrogen phosphate (three-letter code: SV9) (formula: C<sub>48</sub>H<sub>51</sub>N<sub>9</sub>O<sub>16</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	75	48	9	16	2	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.82Å 177.60Å 234.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 2.74 47.22 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.22-2.74) 98.2 (47.22-2.74)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.18.2	Depositor
R, $R_{free}$	0.241 , 0.262 0.245 , 0.255	Depositor DCC
$R_{free}$ test set	1963 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.6	Xtrriage
Anisotropy	0.576	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 85.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: SV9

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	0.70	5/5331 (0.1%)	0.80	3/7232 (0.0%)
2	B	0.64	0/1091	0.86	0/1471
All	All	0.69	5/6422 (0.1%)	0.81	3/8703 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	GLU	CD-OE2	-7.44	1.17	1.25
1	A	821	GLU	CD-OE1	-6.46	1.18	1.25
1	A	308	GLU	CD-OE1	-6.25	1.18	1.25
1	A	801	GLU	CD-OE2	-5.86	1.19	1.25
1	A	821	GLU	CD-OE2	-5.29	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ASN	CB-CA-C	5.96	122.32	110.40
1	A	216	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	591	ARG	CB-CG-CD	5.06	124.75	111.60

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	5217	0	5252	198	0
2	B	1076	0	1091	81	0
3	A	75	0	0	6	0
All	All	6368	0	6343	258	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 20.

All (258) 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:537:GLU:HG3	1:A:544:LEU:CD1	1.51	1.39
1:A:325:TYR:CE1	1:A:665:CYS:HB3	1.62	1.35
1:A:428:ILE:HG12	2:B:342:LEU:CD1	1.69	1.20
1:A:449:VAL:CG2	2:B:363:LEU:HD21	1.72	1.20
1:A:428:ILE:CG1	2:B:342:LEU:CD1	2.20	1.18
1:A:526:ARG:NH1	1:A:530:ASP:OD1	1.76	1.18
1:A:449:VAL:HG23	2:B:363:LEU:HD21	1.20	1.15
1:A:428:ILE:HG13	2:B:342:LEU:HD13	1.26	1.09
1:A:428:ILE:CG1	2:B:342:LEU:HD12	1.82	1.08
1:A:537:GLU:HG3	1:A:544:LEU:HD13	1.29	1.05
1:A:325:TYR:HE1	1:A:665:CYS:HB3	0.87	1.04
1:A:537:GLU:HG3	1:A:544:LEU:HD11	1.36	1.04
1:A:325:TYR:HD1	1:A:665:CYS:SG	1.82	1.02
1:A:428:ILE:HG12	2:B:342:LEU:HD12	1.02	1.01
1:A:537:GLU:CG	1:A:544:LEU:CD1	2.39	1.00
1:A:428:ILE:CG1	2:B:342:LEU:HD13	1.86	0.99
1:A:671:TRP:HA	1:A:735:PHE:HE1	1.27	0.98
1:A:786:ILE:H	1:A:786:ILE:HD12	1.27	0.98
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.01	0.96
1:A:537:GLU:CG	1:A:544:LEU:HD13	1.96	0.95
2:B:418:LYS:HZ2	2:B:418:LYS:HB2	1.31	0.95
1:A:671:TRP:HE1	1:A:696:ASN:HD22	1.00	0.94
1:A:232:GLU:O	1:A:236:GLN:HG2	1.69	0.93
2:B:426:ARG:H	2:B:426:ARG:HD2	1.35	0.92
1:A:363:TYR:CG	1:A:734:ILE:HD13	2.06	0.91
1:A:325:TYR:CE1	1:A:665:CYS:CB	2.53	0.89
2:B:418:LYS:N	2:B:418:LYS:HE3	1.87	0.89
1:A:325:TYR:CD1	1:A:665:CYS:SG	2.62	0.89
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.56	0.87
1:A:456:LYS:HG2	2:B:370:TYR:HE1	1.40	0.87
2:B:368:GLU:H	2:B:369:PRO:HD3	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:TYR:HD1	1:A:665:CYS:HG	0.86	0.84
1:A:815:LEU:HD12	1:A:815:LEU:O	1.77	0.84
1:A:591:ARG:HE	1:A:605:VAL:HG21	1.42	0.83
1:A:428:ILE:HG13	2:B:342:LEU:CD1	1.94	0.83
1:A:671:TRP:HE1	1:A:696:ASN:ND2	1.77	0.83
1:A:449:VAL:HG22	2:B:363:LEU:HD21	1.61	0.81
1:A:311:ASP:OD1	1:A:311:ASP:N	2.08	0.81
1:A:374:LYS:O	1:A:378:VAL:HG12	1.80	0.81
2:B:418:LYS:HB2	2:B:418:LYS:NZ	1.93	0.81
1:A:449:VAL:CG2	2:B:363:LEU:CD2	2.58	0.79
1:A:383:ASN:N	1:A:383:ASN:OD1	2.15	0.79
2:B:418:LYS:HE3	2:B:418:LYS:H	1.47	0.79
1:A:592:GLN:NE2	1:A:638:GLN:OE1	2.17	0.78
1:A:591:ARG:HE	1:A:605:VAL:CG2	1.95	0.77
2:B:413:SER:HB2	2:B:415:VAL:HG13	1.64	0.77
1:A:456:LYS:HG2	2:B:370:TYR:CE1	2.20	0.77
1:A:363:TYR:CB	1:A:734:ILE:CD1	2.62	0.77
1:A:456:LYS:CG	2:B:370:TYR:HE1	1.98	0.77
1:A:363:TYR:CG	1:A:734:ILE:CD1	2.67	0.76
2:B:341:GLU:HG3	2:B:341:GLU:O	1.85	0.76
2:B:368:GLU:N	2:B:369:PRO:HD3	2.01	0.76
2:B:368:GLU:N	2:B:369:PRO:CD	2.48	0.75
1:A:456:LYS:CG	2:B:370:TYR:CE1	2.70	0.75
1:A:364:GLU:OE1	1:A:524:ARG:NH2	2.20	0.73
1:A:591:ARG:HE	1:A:605:VAL:HG11	1.53	0.73
1:A:591:ARG:NE	1:A:605:VAL:HG21	2.03	0.73
1:A:213:ILE:HG22	1:A:238:LEU:HD11	1.71	0.72
1:A:325:TYR:HE1	1:A:665:CYS:CB	1.83	0.72
1:A:591:ARG:HE	1:A:605:VAL:CG1	2.02	0.72
2:B:426:ARG:H	2:B:426:ARG:CD	2.03	0.72
1:A:363:TYR:CB	1:A:734:ILE:HD11	2.21	0.71
1:A:786:ILE:HD12	1:A:786:ILE:N	2.03	0.71
1:A:363:TYR:HB2	1:A:734:ILE:HD11	1.73	0.70
1:A:431:TRP:O	1:A:434:ILE:N	2.24	0.69
1:A:449:VAL:HG23	2:B:363:LEU:CD2	2.13	0.69
1:A:363:TYR:CD2	1:A:734:ILE:HD13	2.28	0.69
1:A:591:ARG:HH21	1:A:605:VAL:HG21	1.56	0.69
1:A:449:VAL:HG22	2:B:363:LEU:CD2	2.22	0.68
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.59	0.68
1:A:591:ARG:NE	1:A:605:VAL:HG11	2.07	0.68
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:LEU:HD12	1:A:815:LEU:C	2.11	0.67
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.75	0.67
2:B:416:GLN:HB2	2:B:419:ASN:HB2	1.77	0.66
1:A:325:TYR:CD1	1:A:665:CYS:HB3	2.26	0.66
1:A:591:ARG:NH2	1:A:605:VAL:HG21	2.11	0.66
1:A:287:GLY:HA3	3:A:901:SV9:O13	1.95	0.65
1:A:777:ALA:HB1	1:A:820:ARG:HH12	1.62	0.64
1:A:472:ARG:NE	1:A:477:GLU:OE1	2.21	0.64
1:A:821:GLU:HA	1:A:821:GLU:OE1	1.97	0.64
1:A:225:PRO:O	1:A:348:GLN:NE2	2.31	0.63
1:A:606:ASN:HD21	1:A:608:ARG:HH21	1.47	0.63
1:A:456:LYS:HG3	2:B:370:TYR:CE1	2.34	0.63
1:A:633:GLN:HA	1:A:633:GLN:NE2	2.14	0.63
2:B:418:LYS:HE3	2:B:418:LYS:CA	2.29	0.63
1:A:379:GLU:O	1:A:383:ASN:OD1	2.16	0.62
1:A:647:LYS:O	1:A:651:VAL:HG23	1.99	0.62
1:A:591:ARG:HD2	1:A:605:VAL:CG1	2.30	0.62
1:A:364:GLU:OE2	1:A:524:ARG:NH2	2.34	0.61
2:B:367:ILE:O	2:B:367:ILE:HG13	2.01	0.60
1:A:326:VAL:HG23	1:A:326:VAL:O	2.02	0.60
1:A:363:TYR:CB	1:A:734:ILE:HD13	2.27	0.60
1:A:366:ASN:OD1	1:A:368:GLN:N	2.35	0.60
1:A:468:VAL:HG12	1:A:468:VAL:O	2.02	0.60
2:B:337:GLN:HA	2:B:337:GLN:NE2	2.17	0.59
1:A:325:TYR:CD1	1:A:665:CYS:CB	2.84	0.59
1:A:364:GLU:CD	1:A:524:ARG:NH2	2.56	0.58
1:A:379:GLU:O	1:A:382:PHE:HB3	2.03	0.58
2:B:383:TRP:CH2	2:B:420:PHE:CD1	2.91	0.58
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.68	0.58
2:B:383:TRP:CZ3	2:B:420:PHE:CD1	2.92	0.58
1:A:619:ASP:O	1:A:795:ARG:NH1	2.33	0.57
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.86	0.57
1:A:485:ARG:HD3	1:A:485:ARG:C	2.25	0.57
1:A:777:ALA:CB	1:A:820:ARG:HH12	2.17	0.57
2:B:418:LYS:H	2:B:418:LYS:CE	2.17	0.56
1:A:591:ARG:NE	1:A:605:VAL:CG2	2.64	0.56
1:A:591:ARG:CZ	1:A:605:VAL:HG21	2.36	0.56
1:A:740:VAL:O	1:A:740:VAL:HG22	2.05	0.56
2:B:370:TYR:N	2:B:370:TYR:CD2	2.73	0.56
1:A:231:PHE:HA	1:A:253:HIS:CD2	2.41	0.56
1:A:286:SER:O	1:A:291:LEU:HD11	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:HD2	1:A:605:VAL:HG13	1.87	0.55
1:A:313:VAL:HG23	1:A:313:VAL:O	2.06	0.55
1:A:329:LEU:HD12	1:A:749:SER:HB3	1.88	0.55
1:A:469:LYS:HD3	1:A:469:LYS:N	2.22	0.55
1:A:205:GLN:O	1:A:209:VAL:HG23	2.06	0.55
1:A:526:ARG:HH11	1:A:530:ASP:CG	2.10	0.55
2:B:354:GLN:OE1	2:B:354:GLN:HA	2.07	0.55
1:A:426:GLU:OE1	1:A:426:GLU:HA	2.06	0.54
1:A:777:ALA:HB1	1:A:820:ARG:NH1	2.21	0.54
2:B:402:PHE:CE2	2:B:418:LYS:HD3	2.41	0.54
1:A:366:ASN:OD1	1:A:367:GLY:N	2.40	0.54
3:A:901:SV9:C11	3:A:901:SV9:C30	2.85	0.54
1:A:427:GLN:NE2	1:A:518:ASP:HA	2.23	0.54
1:A:591:ARG:NE	1:A:605:VAL:CG1	2.67	0.54
2:B:402:PHE:CE1	2:B:421:PHE:CE2	2.97	0.53
2:B:363:LEU:HD23	2:B:363:LEU:N	2.22	0.53
1:A:526:ARG:NH1	1:A:530:ASP:CG	2.58	0.53
2:B:383:TRP:CH2	2:B:420:PHE:HD1	2.27	0.53
1:A:281:VAL:HB	1:A:304:VAL:HG12	1.90	0.52
1:A:409:GLY:N	1:A:544:LEU:O	2.41	0.52
2:B:423:ASN:C	2:B:425:ARG:H	2.12	0.52
1:A:428:ILE:HA	2:B:342:LEU:CD1	2.40	0.52
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.92	0.52
1:A:537:GLU:CD	1:A:544:LEU:HD13	2.30	0.52
2:B:399:GLY:CA	2:B:437:TRP:CD2	2.93	0.52
2:B:416:GLN:HA	2:B:419:ASN:HD22	1.73	0.52
2:B:424:TYR:CD2	2:B:427:ARG:NH2	2.78	0.52
1:A:282:ILE:HD13	1:A:305:THR:HB	1.92	0.52
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.43	0.52
2:B:375:VAL:HG23	2:B:375:VAL:O	2.09	0.52
1:A:341:PRO:HG3	1:A:816:LEU:CD1	2.40	0.51
2:B:324:VAL:HG12	2:B:324:VAL:O	2.09	0.51
1:A:544:LEU:CD1	1:A:544:LEU:N	2.73	0.51
1:A:291:LEU:HD12	1:A:291:LEU:H	1.76	0.50
1:A:188:MET:HE1	1:A:200:ILE:HA	1.93	0.50
2:B:420:PHE:CD2	2:B:420:PHE:C	2.85	0.50
1:A:544:LEU:N	1:A:544:LEU:HD12	2.26	0.50
1:A:435:VAL:O	1:A:439:GLU:HB2	2.12	0.50
1:A:341:PRO:HG3	1:A:816:LEU:HD13	1.94	0.50
2:B:426:ARG:CD	2:B:426:ARG:N	2.73	0.50
1:A:405:PRO:O	1:A:405:PRO:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:CD	1:A:605:VAL:CG1	2.89	0.49
1:A:669:VAL:HG13	1:A:671:TRP:CE2	2.47	0.49
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.94	0.49
1:A:666:PHE:O	1:A:701:PRO:HG2	2.13	0.49
1:A:235:LEU:HD13	1:A:249:VAL:HG21	1.95	0.49
1:A:829:PHE:O	1:A:830:LEU:HD23	2.13	0.49
1:A:235:LEU:HD21	1:A:246:THR:HG22	1.95	0.49
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.95	0.49
2:B:337:GLN:NE2	2:B:337:GLN:CA	2.73	0.49
1:A:209:VAL:O	1:A:213:ILE:HG12	2.13	0.49
2:B:423:ASN:O	2:B:425:ARG:N	2.43	0.48
2:B:369:PRO:HD2	2:B:370:TYR:HD2	1.78	0.48
1:A:296:GLN:O	1:A:299:SER:HB3	2.14	0.48
1:A:793:ILE:HD12	1:A:793:ILE:N	2.28	0.48
1:A:363:TYR:HB2	1:A:734:ILE:CD1	2.36	0.48
1:A:363:TYR:HB3	1:A:734:ILE:CD1	2.44	0.48
2:B:413:SER:OG	2:B:413:SER:O	2.30	0.48
1:A:188:MET:HE3	1:A:200:ILE:HD12	1.96	0.47
1:A:308:GLU:HB3	1:A:586:LEU:HA	1.96	0.47
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.95	0.47
1:A:520:TYR:CD1	1:A:520:TYR:C	2.84	0.47
1:A:633:GLN:NE2	1:A:633:GLN:CA	2.73	0.47
1:A:667:ASP:OD2	1:A:667:ASP:N	2.46	0.47
2:B:416:GLN:HA	2:B:419:ASN:ND2	2.30	0.47
1:A:591:ARG:CD	1:A:605:VAL:HG11	2.45	0.46
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.97	0.46
2:B:320:ASP:O	2:B:323:ALA:HB3	2.15	0.46
1:A:591:ARG:HD2	1:A:605:VAL:HG11	1.97	0.46
1:A:670:PHE:O	1:A:735:PHE:CD1	2.69	0.46
1:A:601:GLU:HA	1:A:616:TYR:O	2.16	0.45
2:B:388:GLN:HE21	2:B:428:PHE:HZ	1.65	0.45
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.80	0.45
1:A:428:ILE:CA	2:B:342:LEU:CD1	2.95	0.45
1:A:786:ILE:H	1:A:786:ILE:CD1	2.06	0.45
1:A:232:GLU:N	1:A:232:GLU:OE1	2.50	0.45
1:A:817:SER:HB2	1:A:820:ARG:HH21	1.81	0.44
2:B:354:GLN:O	2:B:357:SER:HB3	2.17	0.44
1:A:422:HIS:O	1:A:422:HIS:CG	2.70	0.44
1:A:655:GLY:HA3	1:A:763:TYR:CZ	2.51	0.44
1:A:835:THR:O	1:A:835:THR:HG22	2.17	0.44
1:A:520:TYR:CD1	1:A:520:TYR:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:TYR:N	2:B:370:TYR:HD2	2.15	0.44
2:B:394:ALA:O	2:B:398:TYR:N	2.50	0.44
1:A:489:ALA:O	1:A:492:LYS:N	2.51	0.44
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.84	0.44
2:B:383:TRP:CZ2	2:B:420:PHE:HD1	2.36	0.43
1:A:294:ALA:CB	1:A:306:LEU:HD11	2.48	0.43
1:A:693:LEU:HD23	1:A:694:PHE:N	2.33	0.43
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.49	0.43
1:A:474:ILE:HA	1:A:474:ILE:HD12	1.71	0.43
1:A:331:ALA:HA	3:A:901:SV9:C5	2.49	0.43
1:A:548:SER:HB2	1:A:766:ALA:HA	2.01	0.43
1:A:691:LEU:HD23	1:A:691:LEU:HA	1.88	0.43
3:A:901:SV9:O3	3:A:901:SV9:C9	2.66	0.43
1:A:198:ASP:OD1	1:A:198:ASP:N	2.51	0.42
1:A:428:ILE:HA	2:B:342:LEU:HD11	2.00	0.42
1:A:522:SER:C	1:A:524:ARG:N	2.71	0.42
1:A:522:SER:C	1:A:524:ARG:H	2.22	0.42
1:A:601:GLU:HB3	1:A:617:LYS:HD3	2.01	0.42
1:A:710:GLU:OE2	1:A:710:GLU:HA	2.18	0.42
1:A:728:LEU:O	1:A:732:LYS:HG3	2.18	0.42
2:B:340:MET:N	2:B:340:MET:SD	2.90	0.42
1:A:210:PHE:CE1	1:A:252:VAL:HG22	2.54	0.42
1:A:383:ASN:O	1:A:387:GLU:HG3	2.19	0.42
1:A:441:LEU:HG	1:A:445:LEU:HD22	2.00	0.42
1:A:591:ARG:CD	1:A:605:VAL:HG13	2.48	0.42
1:A:742:GLN:OE1	1:A:743:PRO:HD2	2.19	0.42
1:A:732:LYS:O	1:A:736:GLY:N	2.43	0.42
2:B:412:LYS:HD3	2:B:412:LYS:HA	1.80	0.42
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.49	0.42
2:B:399:GLY:HA3	2:B:437:TRP:CD2	2.55	0.42
1:A:789:ALA:HB1	1:A:790:PRO:HD2	2.02	0.42
2:B:402:PHE:CZ	2:B:418:LYS:HD3	2.55	0.42
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.85	0.42
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.49	0.42
1:A:548:SER:O	1:A:552:TRP:HB3	2.20	0.42
1:A:448:MET:HE3	1:A:448:MET:HB3	1.83	0.41
1:A:484:HIS:ND1	1:A:484:HIS:C	2.73	0.41
1:A:356:ILE:O	1:A:356:ILE:HG22	2.19	0.41
1:A:716:GLU:O	1:A:750:ARG:NH1	2.53	0.41
1:A:438:GLN:HE21	1:A:438:GLN:HB3	1.56	0.41
1:A:174:VAL:O	1:A:215:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:HE	1:A:605:VAL:CB	2.32	0.41
2:B:324:VAL:HG13	2:B:331:ALA:HB2	2.02	0.41
2:B:426:ARG:HD3	2:B:427:ARG:HG3	2.03	0.41
1:A:331:ALA:HA	3:A:901:SV9:N1	2.35	0.41
1:A:441:LEU:CD2	2:B:356:ASN:HD22	2.33	0.41
1:A:419:GLN:HB2	1:A:520:TYR:CE2	2.55	0.41
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.85	0.41
2:B:423:ASN:C	2:B:425:ARG:N	2.73	0.41
1:A:220:LEU:HD22	1:A:237:GLN:OE1	2.21	0.41
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.95	0.41
1:A:728:LEU:HD23	1:A:728:LEU:HA	1.87	0.41
2:B:350:GLN:O	2:B:354:GLN:HG2	2.21	0.41
2:B:420:PHE:C	2:B:420:PHE:HD2	2.22	0.41
2:B:430:ILE:O	2:B:430:ILE:HG22	2.21	0.41
1:A:321:ARG:HG2	1:A:326:VAL:HG12	2.03	0.40
2:B:383:TRP:CZ3	2:B:420:PHE:HD1	2.39	0.40
1:A:331:ALA:HA	3:A:901:SV9:C30	2.52	0.40
1:A:567:VAL:HG21	1:A:571:TYR:CD1	2.57	0.40
2:B:324:VAL:O	2:B:324:VAL:CG1	2.70	0.40
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.51	0.40
1:A:332:MET:HG3	1:A:333:VAL:HG23	2.03	0.40
1:A:361:PRO:O	1:A:361:PRO:HG2	2.22	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	664/871 (76%)	631 (95%)	32 (5%)	1 (0%)	47	69
2	B	131/144 (91%)	120 (92%)	9 (7%)	2 (2%)	10	18
All	All	795/1015 (78%)	751 (94%)	41 (5%)	3 (0%)	34	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	399	GLY
2	B	424	TYR
1	A	792	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/715 (79%)	545 (96%)	21 (4%)	34	54
2	B	117/125 (94%)	101 (86%)	16 (14%)	3	5
All	All	683/840 (81%)	646 (95%)	37 (5%)	22	38

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LEU
1	A	269	ARG
1	A	308	GLU
1	A	311	ASP
1	A	351	MET
1	A	383	ASN
1	A	422	HIS
1	A	440	GLU
1	A	442	LYS
1	A	445	LEU
1	A	449	VAL
1	A	466	SER
1	A	487	LEU
1	A	488	THR
1	A	523	SER
1	A	524	ARG
1	A	714	ILE
1	A	734	ILE
1	A	740	VAL
1	A	786	ILE

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Mol	Chain	Res	Type
1	A	815	LEU
2	B	322	GLU
2	B	335	LEU
2	B	336	ARG
2	B	339	ASP
2	B	340	MET
2	B	353	LYS
2	B	370	TYR
2	B	388	GLN
2	B	397	LYS
2	B	415	VAL
2	B	416	GLN
2	B	418	LYS
2	B	420	PHE
2	B	422	VAL
2	B	426	ARG
2	B	429	ASN

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	207	GLN
1	A	236	GLN
1	A	394	HIS
1	A	399	ASN
1	A	402	ASN
1	A	438	GLN
1	A	540	ASN
1	A	592	GLN
1	A	633	GLN
1	A	638	GLN
2	B	337	GLN
2	B	348	GLN
2	B	416	GLN
2	B	419	ASN

### 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 monosaccharides 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	SV9	A	901	-	77,83,83	1.27	7 (9%)	94,124,124	0.94	7 (7%)

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	SV9	A	901	-	-	22/47/67/67	0/9/9/9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	SV9	C5-N1	-6.53	1.34	1.42
3	A	901	SV9	C30-C33	-3.16	1.35	1.43
3	A	901	SV9	O4-C35	-2.78	1.37	1.43
3	A	901	SV9	C42-N6	-2.47	1.30	1.34
3	A	901	SV9	C6-C7	-2.41	1.36	1.39
3	A	901	SV9	C5-C4	-2.23	1.37	1.40
3	A	901	SV9	O5-C36	-2.16	1.37	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	SV9	C30-C33-N3	3.19	116.60	110.99
3	A	901	SV9	O14-C41-C47	-2.99	102.55	106.93
3	A	901	SV9	O11-P2-O12	2.40	124.13	112.24
3	A	901	SV9	O7-C38-C37	2.30	115.49	109.36
3	A	901	SV9	O15-C47-C41	-2.22	102.65	110.85
3	A	901	SV9	C43-C44-N7	2.22	123.73	120.35
3	A	901	SV9	C6-C5-N1	-2.21	119.22	122.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

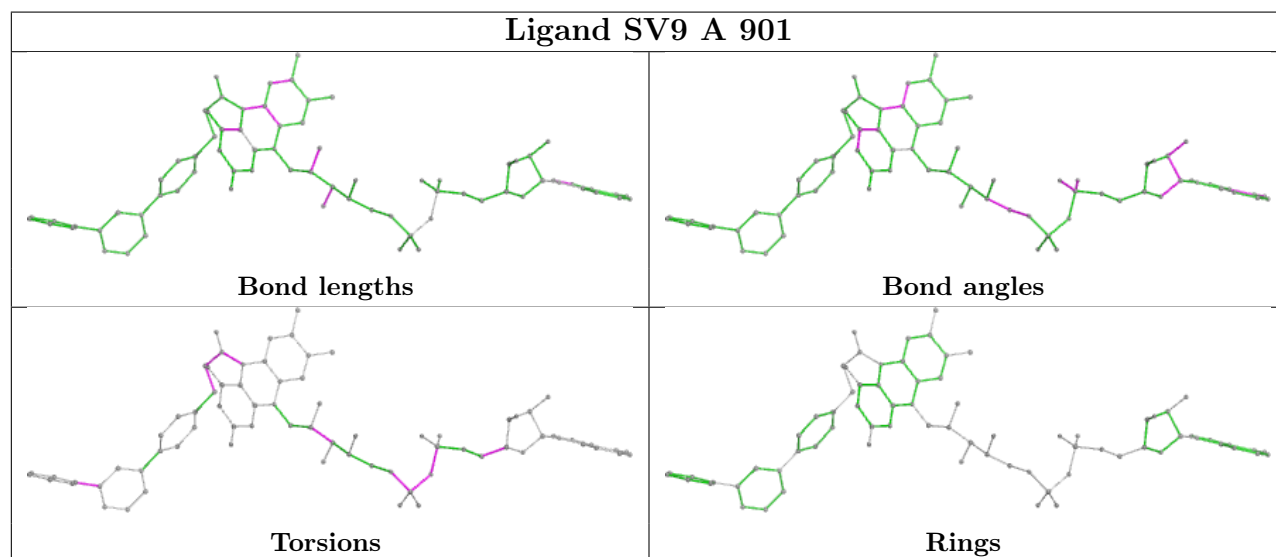
Mol	Chain	Res	Type	Atoms
3	A	901	SV9	C9-C10-C11-C12
3	A	901	SV9	C10-C9-N1-C5
3	A	901	SV9	C10-C9-N1-C30
3	A	901	SV9	O1-C9-N1-C5
3	A	901	SV9	O1-C9-N1-C30
3	A	901	SV9	C38-O7-P1-O9
3	A	901	SV9	C27-C20-C21-C22
3	A	901	SV9	C19-C20-C21-C22
3	A	901	SV9	C27-C20-C21-C26
3	A	901	SV9	C11-C10-C9-N1
3	A	901	SV9	C19-C20-C21-C26
3	A	901	SV9	C11-C10-C9-O1
3	A	901	SV9	O4-C35-C36-C37
3	A	901	SV9	P2-O10-P1-O7
3	A	901	SV9	O4-C35-C36-O5
3	A	901	SV9	P1-O10-P2-O11
3	A	901	SV9	C38-O7-P1-O10
3	A	901	SV9	P2-O10-P1-O9
3	A	901	SV9	P1-O10-P2-O12
3	A	901	SV9	C38-O7-P1-O8
3	A	901	SV9	O13-C39-C40-O14
3	A	901	SV9	C34-C35-C36-O5

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	SV9	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 [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	666/871 (76%)	1.10	102 (15%) <b>2</b>   <b>2</b>	60, 88, 120, 139	0
2	B	133/144 (92%)	1.49	39 (29%) <b>0</b>   <b>0</b>	89, 118, 138, 146	0
All	All	799/1015 (78%)	1.17	141 (17%) <b>1</b>   <b>1</b>	60, 94, 126, 146	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	LEU	6.7
2	B	376	ILE	6.6
2	B	308	ARG	6.0
1	A	519	VAL	5.8
1	A	373	GLU	5.7
2	B	378	LYS	5.7
1	A	509	GLN	5.5
2	B	312	LYS	5.3
2	B	374	GLU	5.3
1	A	174	VAL	5.2
2	B	366	GLY	5.1
1	A	514	ASN	4.8
1	A	511	LEU	4.7
1	A	235	LEU	4.6
1	A	242	TYR	4.5
2	B	365	GLY	4.4
1	A	455	ILE	4.3
1	A	239	GLU	4.3
2	B	402	PHE	4.2
2	B	360	LYS	4.1
2	B	367	ILE	4.1
1	A	504	LEU	4.0
2	B	349	ILE	4.0
1	A	273	LEU	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	510	GLU	4.0
1	A	497	LEU	3.9
1	A	238	LEU	3.8
2	B	372	LEU	3.7
2	B	438	GLU	3.7
2	B	400	ARG	3.7
1	A	503	LYS	3.7
1	A	703	LEU	3.6
1	A	487	LEU	3.6
2	B	399	GLY	3.6
1	A	241	PRO	3.6
1	A	507	LYS	3.5
2	B	309	LYS	3.5
1	A	435	VAL	3.5
1	A	451	LEU	3.5
2	B	422	VAL	3.4
1	A	398	PHE	3.4
1	A	493	GLU	3.4
1	A	172	SER	3.3
2	B	371	ARG	3.3
2	B	395	ILE	3.3
2	B	373	PRO	3.3
1	A	492	LYS	3.2
1	A	506	GLU	3.2
1	A	762	SER	3.2
1	A	433	LYS	3.2
2	B	318	GLN	3.2
1	A	212	PHE	3.1
2	B	375	VAL	3.1
1	A	449	VAL	3.1
2	B	315	PHE	3.0
1	A	499	GLU	2.8
1	A	377	MET	2.7
1	A	208	LYS	2.7
1	A	763	TYR	2.7
1	A	512	GLU	2.7
1	A	542	THR	2.7
1	A	274	PRO	2.7
1	A	276	LYS	2.7
2	B	316	LEU	2.7
1	A	244	SER	2.6
2	B	313	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	808	PRO	2.6
1	A	655	GLY	2.6
1	A	270	ILE	2.6
1	A	436	LYS	2.6
1	A	411	ALA	2.5
2	B	383	TRP	2.5
1	A	490	LEU	2.5
2	B	420	PHE	2.5
1	A	400	VAL	2.5
1	A	458	LEU	2.5
1	A	706	LEU	2.5
1	A	428	ILE	2.5
1	A	362	LEU	2.5
2	B	325	SER	2.5
1	A	810	THR	2.4
1	A	355	LYS	2.4
1	A	391	TYR	2.4
1	A	626	PRO	2.4
2	B	431	ASP	2.4
1	A	256	LEU	2.4
1	A	707	VAL	2.4
1	A	500	THR	2.3
1	A	764	VAL	2.3
1	A	671	TRP	2.3
1	A	364	GLU	2.3
1	A	395	GLN	2.3
1	A	275	THR	2.3
2	B	323	ALA	2.3
1	A	359	LYS	2.3
1	A	380	GLN	2.3
2	B	416	GLN	2.3
1	A	544	LEU	2.3
1	A	800	GLY	2.3
1	A	765	ALA	2.3
1	A	811	VAL	2.3
1	A	175	GLU	2.3
1	A	171	PRO	2.3
1	A	447	LYS	2.3
1	A	444	LEU	2.3
1	A	705	ALA	2.3
2	B	319	GLU	2.3
1	A	231	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	454	LYS	2.3
1	A	538	PHE	2.3
2	B	363	LEU	2.2
1	A	496	GLU	2.2
1	A	179	PHE	2.2
1	A	396	LEU	2.2
1	A	657	GLY	2.2
1	A	591	ARG	2.2
2	B	346	LYS	2.2
1	A	809	ALA	2.2
1	A	240	ALA	2.2
1	A	568	ARG	2.2
1	A	693	LEU	2.2
2	B	322	GLU	2.2
1	A	374	LYS	2.1
2	B	362	LYS	2.1
1	A	761	TYR	2.1
2	B	338	LEU	2.1
1	A	229	LEU	2.1
1	A	331	ALA	2.1
1	A	445	LEU	2.1
1	A	372	LYS	2.1
2	B	320	ASP	2.1
1	A	232	GLU	2.1
1	A	429	GLU	2.1
1	A	691	LEU	2.1
1	A	426	GLU	2.0
1	A	431	TRP	2.0
1	A	659	LEU	2.0
1	A	731	LEU	2.0
1	A	836	LEU	2.0
1	A	534	ALA	2.0
2	B	433	VAL	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 monosaccharides in this entry.

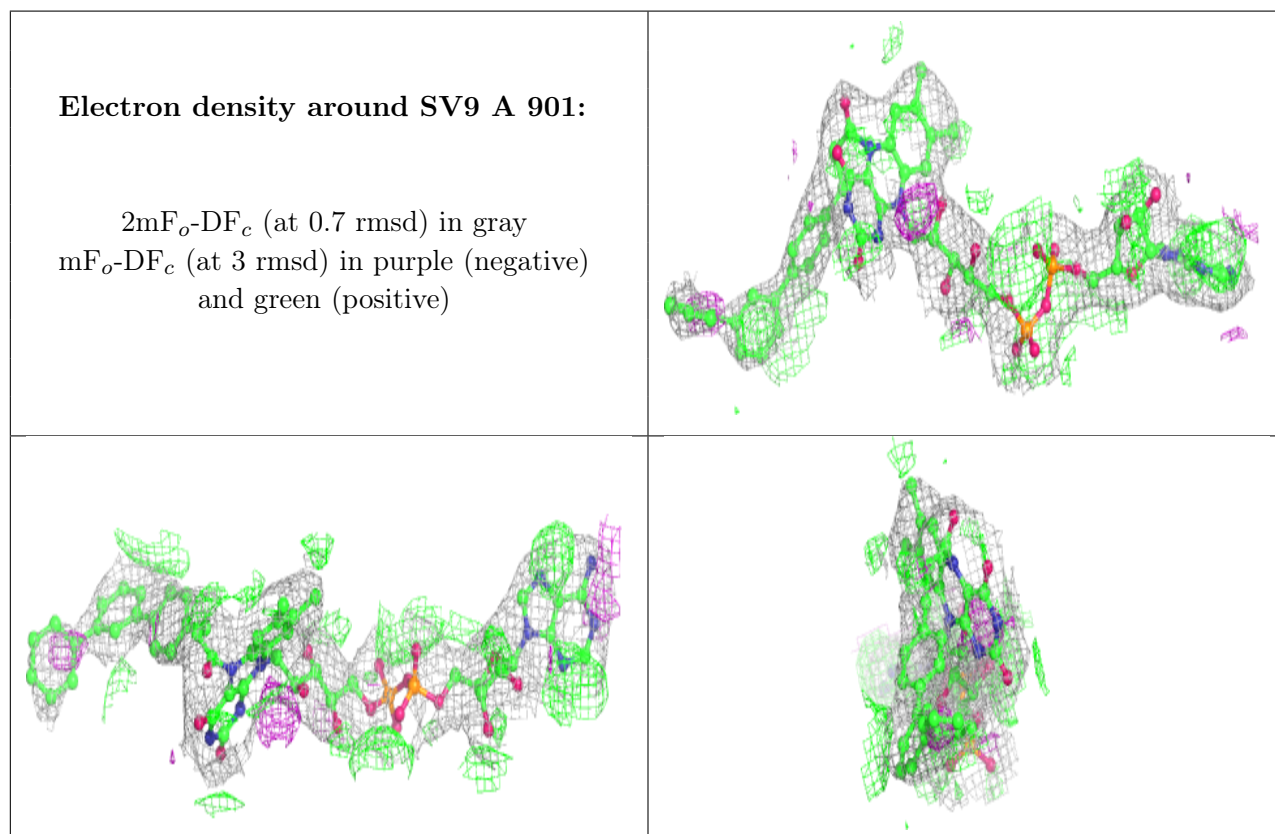


## 6.4 Ligands [i](#)

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
3	SV9	A	901	75/75	0.95	0.25	49,75,114,116	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.