



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2024 – 07:16 pm BST

PDB ID : 8BOX
Title : LSD1-CoREST in complex with AW4 and SNAG peptide
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2022-11-15
Resolution : 2.82 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 : 4.02b-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

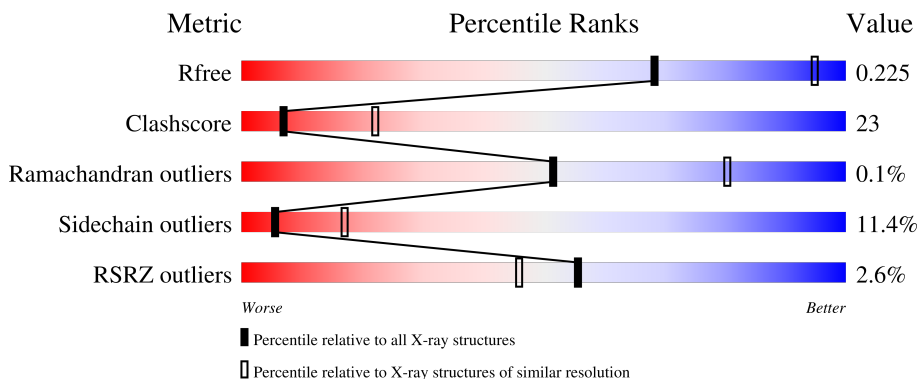
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	
2	B	144	
3	C	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6403 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

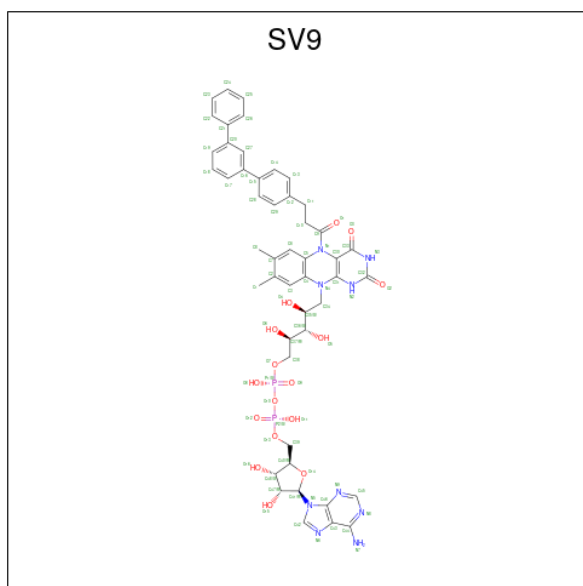
There are 8 discrepancies between the modelled and reference sequences:

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 a protein called Zinc finger protein SNAI1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	35	23	7	5	0	0	0

- Molecule 4 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: C₄₈H₅₁N₉O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	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, α , β , γ	118.98Å 177.89Å 234.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 2.82 48.34 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.34-2.82) 99.3 (48.34-2.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.220 , 0.229 0.223 , 0.225	Depositor DCC
R_{free} test set	1172 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtrriage
Anisotropy	0.480	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [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	0.69	0/5331	0.81	0/7232
2	B	0.58	0/1091	0.80	1/1471 (0.1%)
3	C	0.75	0/36	1.04	0/46
All	All	0.67	0/6458	0.81	1/8749 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	420	PHE	CB-CA-C	-8.38	93.64	110.40

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	236	1
2	B	1076	0	1091	84	1
3	C	35	0	34	1	0
4	A	75	0	0	8	0
All	All	6403	0	6377	294	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 23.

All (294) 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:435:VAL:HG12	2:B:349:ILE:CD1	1.76	1.16
1:A:654:MET:HE1	1:A:776:MET:CG	1.77	1.15
1:A:654:MET:CE	1:A:776:MET:HG3	1.82	1.10
1:A:793:ILE:HD12	1:A:793:ILE:H	1.22	1.04
1:A:754:ASP:OD1	1:A:755:PRO:HD2	1.59	1.01
1:A:654:MET:HE1	1:A:776:MET:HG3	0.98	0.96
1:A:654:MET:CE	1:A:776:MET:CG	2.41	0.95
1:A:485:ARG:NH1	2:B:407:ASP:OD2	2.01	0.92
1:A:435:VAL:HG12	2:B:349:ILE:HD11	1.53	0.91
1:A:457:GLU:O	1:A:461:GLN:HG3	1.71	0.91
2:B:403:GLN:O	2:B:406:SER:HB3	1.70	0.91
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.05	0.90
1:A:758:ARG:HG2	1:A:758:ARG:HH11	1.35	0.88
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.55	0.88
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.55	0.88
2:B:419:ASN:HD22	2:B:419:ASN:H	1.19	0.87
1:A:374:LYS:HD2	1:A:525:ASP:OD1	1.73	0.86
1:A:345:VAL:O	1:A:349:VAL:HG12	1.76	0.85
1:A:427:GLN:NE2	1:A:518:ASP:HA	1.94	0.83
1:A:435:VAL:CG1	2:B:349:ILE:HD11	2.09	0.82
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.61	0.82
1:A:325:TYR:HE2	1:A:665:CYS:HB3	1.42	0.81
1:A:346:SER:HA	1:A:351:MET:HE2	1.63	0.81
1:A:518:ASP:OD1	1:A:518:ASP:N	2.12	0.81
2:B:382:ARG:C	2:B:412:LYS:HZ1	1.84	0.80
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.11	0.80
2:B:368:GLU:HA	2:B:368:GLU:OE1	1.82	0.80
1:A:485:ARG:HG2	1:A:485:ARG:HH11	1.47	0.79
1:A:569:ASN:OD1	1:A:569:ASN:N	2.13	0.78
1:A:465:ALA:HB2	1:A:479:LEU:HD23	1.67	0.77
1:A:346:SER:HA	1:A:351:MET:CE	2.14	0.77
1:A:468:VAL:O	1:A:472:ARG:NH1	2.16	0.77
1:A:188:MET:HE3	1:A:200:ILE:HG12	1.65	0.77
1:A:435:VAL:HG12	2:B:349:ILE:CG1	2.15	0.77
1:A:188:MET:CE	1:A:200:ILE:HG12	2.16	0.75
1:A:434:ILE:HG22	2:B:349:ILE:CD1	2.16	0.75
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.69	0.74
1:A:435:VAL:HG12	2:B:349:ILE:HD13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.70	0.73
1:A:754:ASP:OD1	1:A:755:PRO:CD	2.35	0.72
1:A:511:LEU:N	1:A:511:LEU:HD23	2.03	0.72
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.55	0.72
2:B:425:ARG:NH1	2:B:425:ARG:HG2	2.05	0.71
1:A:438:GLN:HB3	2:B:352:ILE:HG21	1.70	0.71
1:A:332:MET:SD	1:A:661:LYS:NZ	2.65	0.70
1:A:467:GLU:HA	1:A:467:GLU:OE1	1.91	0.69
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.73	0.68
1:A:815:LEU:C	1:A:815:LEU:HD23	2.13	0.68
1:A:321:ARG:HG2	1:A:326:VAL:HG12	1.74	0.68
1:A:487:LEU:C	1:A:487:LEU:HD23	2.13	0.68
1:A:592:GLN:HG2	1:A:638:GLN:HB3	1.76	0.68
2:B:327:ASN:OD1	2:B:330:ALA:N	2.27	0.67
1:A:427:GLN:HE22	1:A:518:ASP:HA	1.60	0.67
1:A:346:SER:HB3	1:A:351:MET:HE3	1.77	0.66
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.26	0.66
2:B:425:ARG:HG2	2:B:425:ARG:HH11	1.61	0.66
1:A:445:LEU:N	1:A:445:LEU:HD23	2.08	0.66
1:A:758:ARG:HH11	1:A:758:ARG:CG	2.08	0.66
1:A:188:MET:CE	1:A:200:ILE:CG1	2.73	0.66
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.78	0.66
1:A:485:ARG:HH11	1:A:485:ARG:CG	2.09	0.65
2:B:418:LYS:O	2:B:421:PHE:HB2	1.96	0.65
2:B:403:GLN:OE1	2:B:407:ASP:OD1	2.14	0.65
1:A:188:MET:HE1	1:A:200:ILE:CA	2.27	0.65
1:A:601:GLU:HB3	1:A:617:LYS:HD3	1.78	0.64
1:A:455:ILE:HD11	1:A:490:LEU:CB	2.27	0.64
1:A:510:GLU:HG2	1:A:511:LEU:HD23	1.78	0.64
1:A:455:ILE:HD11	1:A:490:LEU:HB3	1.79	0.64
1:A:188:MET:HE1	1:A:200:ILE:HA	1.79	0.63
2:B:340:MET:O	2:B:343:VAL:HG23	1.98	0.63
1:A:266:ILE:HA	1:A:295:ARG:HH22	1.63	0.63
1:A:266:ILE:HD11	1:A:578:LEU:HD23	1.81	0.63
2:B:396:ARG:HD2	2:B:396:ARG:O	1.97	0.63
2:B:419:ASN:HD22	2:B:419:ASN:N	1.94	0.63
1:A:435:VAL:CG1	2:B:349:ILE:CD1	2.61	0.63
1:A:793:ILE:HD12	1:A:793:ILE:N	2.05	0.63
2:B:416:GLN:CD	2:B:416:GLN:H	2.00	0.62
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.16	0.61
1:A:346:SER:CA	1:A:351:MET:CE	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:PHE:HE2	2:B:421:PHE:CE2	2.19	0.60
1:A:442:LYS:CG	2:B:356:ASN:HD21	2.13	0.60
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.81	0.60
2:B:370:TYR:HD2	2:B:370:TYR:N	1.99	0.60
1:A:465:ALA:HB2	1:A:479:LEU:CD2	2.32	0.59
1:A:835:THR:O	1:A:835:THR:HG22	2.03	0.59
2:B:426:ARG:HD3	2:B:427:ARG:HG2	1.83	0.59
1:A:346:SER:HB3	1:A:351:MET:CE	2.32	0.59
2:B:419:ASN:H	2:B:419:ASN:ND2	1.96	0.59
1:A:804:ILE:HG23	1:A:804:ILE:O	2.01	0.59
1:A:820:ARG:NH1	1:A:820:ARG:HG2	2.16	0.59
1:A:325:TYR:CD2	1:A:665:CYS:SG	2.96	0.59
1:A:449:VAL:HA	2:B:363:LEU:HD21	1.85	0.58
1:A:434:ILE:CG2	2:B:349:ILE:HD12	2.33	0.58
1:A:820:ARG:HG2	1:A:820:ARG:HH11	1.68	0.58
1:A:665:CYS:HB2	1:A:745:GLU:O	2.04	0.58
2:B:424:TYR:HE2	2:B:427:ARG:NH2	2.01	0.58
1:A:355:LYS:HD3	1:A:355:LYS:H	1.69	0.57
1:A:654:MET:CE	1:A:776:MET:HG2	2.31	0.57
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.86	0.57
1:A:557:ASP:OD2	1:A:557:ASP:N	2.31	0.57
1:A:461:GLN:OE1	1:A:483:LYS:HE3	2.05	0.57
2:B:407:ASP:OD1	2:B:407:ASP:N	2.37	0.57
1:A:245:ASP:OD1	1:A:247:VAL:HG22	2.05	0.57
1:A:355:LYS:HD3	1:A:355:LYS:N	2.19	0.57
1:A:188:MET:HE1	1:A:200:ILE:CG1	2.34	0.57
1:A:258:ARG:HD2	1:A:826:ALA:HB3	1.86	0.57
2:B:359:LEU:HD23	2:B:359:LEU:N	2.20	0.56
2:B:403:GLN:O	2:B:407:ASP:OD1	2.23	0.56
1:A:434:ILE:CG2	2:B:349:ILE:CD1	2.82	0.56
2:B:370:TYR:N	2:B:370:TYR:CD2	2.70	0.56
1:A:830:LEU:N	1:A:830:LEU:HD23	2.19	0.56
2:B:403:GLN:O	2:B:406:SER:CB	2.50	0.56
1:A:345:VAL:O	1:A:349:VAL:CG1	2.52	0.56
1:A:424:LYS:NZ	2:B:339:ASP:OD2	2.38	0.56
1:A:758:ARG:HG2	1:A:758:ARG:NH1	2.15	0.56
2:B:402:PHE:CE2	2:B:421:PHE:CE2	2.94	0.56
1:A:435:VAL:CG1	2:B:349:ILE:HG12	2.36	0.56
1:A:465:ALA:HB1	1:A:479:LEU:HD23	1.85	0.56
1:A:684:THR:HG23	1:A:687:SER:H	1.71	0.55
1:A:719:SER:HB3	1:A:722:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:GLY:O	1:A:762:SER:HB2	2.05	0.55
1:A:487:LEU:HD23	1:A:487:LEU:O	2.06	0.55
1:A:667:ASP:HB3	1:A:744:LYS:HE2	1.87	0.55
1:A:793:ILE:H	1:A:793:ILE:CD1	1.95	0.55
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.89	0.54
1:A:695:TRP:HE1	1:A:706:LEU:HD13	1.72	0.54
1:A:504:LEU:N	1:A:504:LEU:HD23	2.21	0.54
1:A:451:LEU:HD21	1:A:493:GLU:HG2	1.87	0.54
1:A:676:ASN:HB2	1:A:677:LEU:HD22	1.89	0.54
1:A:286:SER:HB2	1:A:291:LEU:HD11	1.90	0.54
2:B:339:ASP:O	2:B:343:VAL:HG22	2.08	0.54
2:B:348:GLN:OE1	2:B:348:GLN:HA	2.08	0.54
2:B:382:ARG:O	2:B:412:LYS:NZ	2.33	0.54
1:A:308:GLU:HG3	1:A:310:ARG:O	2.07	0.53
1:A:238:LEU:HD22	1:A:239:GLU:H	1.73	0.53
1:A:325:TYR:HD2	1:A:665:CYS:SG	2.32	0.53
4:A:901:SV9:C11	4:A:901:SV9:C30	2.87	0.53
1:A:198:ASP:OD1	1:A:198:ASP:N	2.42	0.52
1:A:474:ILE:HG22	2:B:393:GLN:OE1	2.09	0.52
1:A:335:THR:O	1:A:335:THR:OG1	2.21	0.52
1:A:217:THR:HG22	1:A:234:THR:HG21	1.92	0.52
1:A:442:LYS:HG3	2:B:356:ASN:HD21	1.73	0.52
1:A:654:MET:HE2	1:A:776:MET:HG2	1.92	0.52
2:B:311:PRO:HG2	2:B:314:MET:CG	2.35	0.52
1:A:341:PRO:HG3	1:A:816:LEU:CD1	2.40	0.51
1:A:724:VAL:O	1:A:728:LEU:HG	2.10	0.51
2:B:317:SER:O	2:B:321:VAL:HG23	2.11	0.51
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.93	0.51
1:A:434:ILE:HG21	2:B:349:ILE:HD12	1.92	0.51
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.40	0.51
1:A:188:MET:HE3	1:A:200:ILE:CG1	2.38	0.51
1:A:458:LEU:HD21	1:A:486:ASP:HB3	1.92	0.51
1:A:695:TRP:NE1	1:A:706:LEU:HD13	2.26	0.51
1:A:601:GLU:OE1	1:A:617:LYS:HE2	2.12	0.50
1:A:474:ILE:CG2	2:B:393:GLN:OE1	2.59	0.50
1:A:458:LEU:HD21	1:A:486:ASP:CB	2.41	0.50
1:A:374:LYS:CD	1:A:525:ASP:OD1	2.53	0.50
1:A:346:SER:CB	1:A:351:MET:HE3	2.41	0.50
1:A:435:VAL:HG13	2:B:349:ILE:HD11	1.92	0.50
1:A:701:PRO:HG2	1:A:701:PRO:O	2.11	0.50
1:A:442:LYS:CB	2:B:356:ASN:HD21	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:NH2	2:B:404:ALA:HB2	2.27	0.50
2:B:415:VAL:O	2:B:419:ASN:ND2	2.44	0.50
2:B:425:ARG:HH11	2:B:425:ARG:CG	2.25	0.50
1:A:291:LEU:HD23	1:A:578:LEU:HB2	1.94	0.49
1:A:485:ARG:NH1	1:A:485:ARG:CG	2.72	0.49
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.94	0.49
1:A:451:LEU:CD2	1:A:493:GLU:HG2	2.42	0.49
1:A:438:GLN:HA	1:A:438:GLN:OE1	2.11	0.49
1:A:286:SER:HB2	1:A:291:LEU:CD1	2.42	0.49
1:A:213:ILE:HD11	1:A:248:LEU:HD23	1.95	0.49
1:A:693:LEU:HD12	1:A:694:PHE:H	1.78	0.49
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.48	0.49
1:A:332:MET:CE	1:A:661:LYS:NZ	2.75	0.49
1:A:776:MET:HE3	1:A:776:MET:HA	1.95	0.49
2:B:383:TRP:CZ2	2:B:420:PHE:HB2	2.48	0.49
1:A:438:GLN:O	1:A:441:LEU:HB3	2.13	0.48
1:A:446:ASN:ND2	2:B:359:LEU:HD11	2.27	0.48
1:A:455:ILE:HD11	1:A:490:LEU:HB2	1.94	0.48
1:A:540:ASN:O	1:A:542:THR:HG22	2.14	0.48
1:A:776:MET:HE3	1:A:776:MET:CA	2.44	0.48
1:A:392:LEU:HD23	1:A:398:PHE:CD1	2.49	0.48
1:A:632:GLN:NE2	1:A:636:ALA:HB2	2.29	0.47
1:A:676:ASN:O	1:A:696:ASN:N	2.33	0.47
2:B:340:MET:HA	2:B:343:VAL:CG2	2.44	0.47
1:A:329:LEU:HD12	1:A:749:SER:HB3	1.97	0.47
2:B:369:PRO:HB2	2:B:370:TYR:HD2	1.78	0.47
1:A:331:ALA:HB2	4:A:901:SV9:C31	2.44	0.47
1:A:520:TYR:C	1:A:520:TYR:CD2	2.86	0.47
1:A:346:SER:CB	1:A:351:MET:CE	2.92	0.47
1:A:383:ASN:O	1:A:387:GLU:HG3	2.15	0.47
1:A:568:ARG:HH21	1:A:699:LYS:HA	1.80	0.47
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.96	0.47
2:B:318:GLN:O	2:B:322:GLU:HG3	2.15	0.47
2:B:394:ALA:O	2:B:398:TYR:HB2	2.14	0.47
2:B:394:ALA:O	2:B:398:TYR:N	2.48	0.47
1:A:280:LYS:HD2	1:A:303:ASP:O	2.15	0.47
2:B:420:PHE:CD2	2:B:420:PHE:C	2.88	0.47
1:A:308:GLU:HG2	1:A:586:LEU:HD22	1.96	0.46
1:A:320:PHE:CZ	1:A:322:LYS:HB2	2.50	0.46
1:A:378:VAL:HG11	1:A:528:ILE:HG21	1.96	0.46
1:A:601:GLU:HA	1:A:616:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:GLN:OE1	1:A:635:PRO:HD3	2.16	0.46
1:A:820:ARG:HH11	1:A:820:ARG:CG	2.28	0.46
1:A:316:ARG:NH1	1:A:656:PHE:HZ	2.13	0.46
1:A:455:ILE:HG22	2:B:370:TYR:HD1	1.79	0.46
1:A:603:ILE:HG12	1:A:615:ILE:HD13	1.96	0.46
1:A:793:ILE:HG22	1:A:794:PRO:CD	2.46	0.46
2:B:404:ALA:C	2:B:406:SER:N	2.69	0.46
1:A:232:GLU:OE1	1:A:232:GLU:N	2.45	0.46
1:A:209:VAL:O	1:A:213:ILE:HG12	2.14	0.46
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.51	0.45
2:B:379:CYS:SG	2:B:413:SER:OG	2.60	0.45
1:A:217:THR:HG22	1:A:234:THR:CG2	2.46	0.45
1:A:647:LYS:NZ	1:A:778:GLN:O	2.49	0.45
2:B:426:ARG:H	2:B:426:ARG:HG3	1.47	0.45
1:A:266:ILE:N	1:A:348:GLN:OE1	2.31	0.45
1:A:564:HIS:ND1	1:A:564:HIS:N	2.62	0.45
1:A:793:ILE:N	1:A:793:ILE:CD1	2.72	0.45
1:A:286:SER:O	1:A:291:LEU:CD1	2.65	0.45
1:A:325:TYR:CD2	1:A:665:CYS:HB3	2.50	0.45
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.98	0.45
1:A:515:PRO:HA	1:A:516:PRO:HD3	1.82	0.44
1:A:520:TYR:CD2	1:A:520:TYR:O	2.70	0.44
1:A:317:VAL:HG13	1:A:571:TYR:HB3	1.98	0.44
2:B:336:ARG:O	2:B:340:MET:HG2	2.17	0.44
1:A:331:ALA:HA	4:A:901:SV9:C5	2.47	0.44
2:B:310:PRO:HB3	2:B:316:LEU:HD12	1.98	0.44
1:A:474:ILE:HD13	1:A:474:ILE:HA	1.56	0.44
1:A:591:ARG:HD2	1:A:605:VAL:HG13	1.99	0.44
2:B:430:ILE:HG22	2:B:434:LEU:HD12	1.99	0.44
1:A:255:TYR:CE1	1:A:259:HIS:HD2	2.36	0.44
2:B:421:PHE:HE1	2:B:434:LEU:HD11	1.82	0.44
1:A:627:LEU:HD21	1:A:654:MET:HB3	2.00	0.44
1:A:379:GLU:O	1:A:383:ASN:ND2	2.50	0.44
1:A:470:PRO:HA	1:A:472:ARG:HG2	2.00	0.44
1:A:776:MET:HE2	1:A:776:MET:HB3	1.65	0.44
1:A:541:ALA:O	1:A:657:GLY:HA3	2.18	0.44
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.99	0.44
1:A:815:LEU:HD23	1:A:815:LEU:O	2.17	0.44
1:A:265:GLY:O	1:A:295:ARG:NH2	2.51	0.43
1:A:801:GLU:O	1:A:801:GLU:HG2	2.14	0.43
1:A:487:LEU:C	1:A:487:LEU:CD2	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:HD2	1:A:605:VAL:CG1	2.49	0.43
1:A:656:PHE:CE2	1:A:759:GLY:HA3	2.54	0.43
2:B:327:ASN:OD1	2:B:329:THR:N	2.51	0.43
1:A:291:LEU:CD2	1:A:578:LEU:HB2	2.48	0.43
1:A:332:MET:CE	1:A:661:LYS:HZ3	2.31	0.43
1:A:364:GLU:HA	1:A:681:VAL:HB	2.01	0.43
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.84	0.43
1:A:401:LEU:HD12	1:A:402:ASN:N	2.34	0.43
1:A:434:ILE:HG22	2:B:349:ILE:HD11	1.99	0.43
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.99	0.43
1:A:828:GLN:HE21	1:A:828:GLN:HB2	1.63	0.43
1:A:287:GLY:HA3	4:A:901:SV9:O13	2.19	0.43
1:A:331:ALA:HA	4:A:901:SV9:N1	2.34	0.43
1:A:213:ILE:HG22	1:A:238:LEU:HD11	2.00	0.42
1:A:366:ASN:HD21	1:A:368:GLN:HB2	1.84	0.42
1:A:791:GLN:HE21	1:A:791:GLN:HB2	1.41	0.42
2:B:419:ASN:N	2:B:419:ASN:ND2	2.59	0.42
1:A:378:VAL:HG11	1:A:528:ILE:CG2	2.50	0.42
1:A:435:VAL:CG1	2:B:349:ILE:CG1	2.90	0.42
1:A:690:GLU:OE1	1:A:726:ARG:NH1	2.44	0.42
1:A:815:LEU:C	1:A:815:LEU:CD2	2.85	0.42
1:A:448:MET:HB2	2:B:363:LEU:HD11	2.01	0.42
1:A:463:LYS:HD2	1:A:463:LYS:HA	1.77	0.42
1:A:510:GLU:HG2	1:A:511:LEU:CD2	2.46	0.42
1:A:691:LEU:HA	1:A:691:LEU:HD23	1.77	0.42
1:A:732:LYS:HG2	1:A:740:VAL:HG11	2.01	0.42
4:A:901:SV9:O3	4:A:901:SV9:C9	2.68	0.42
1:A:807:TYR:O	1:A:813:GLY:HA3	2.20	0.42
1:A:312:ARG:NH1	1:A:312:ARG:HG3	2.35	0.41
1:A:606:ASN:HB3	1:A:609:SER:O	2.20	0.41
1:A:655:GLY:O	1:A:762:SER:CB	2.68	0.41
1:A:776:MET:CA	1:A:776:MET:CE	2.98	0.41
1:A:331:ALA:CB	4:A:901:SV9:C30	2.98	0.41
1:A:654:MET:HE2	1:A:776:MET:CG	2.38	0.41
2:B:368:GLU:N	2:B:369:PRO:CD	2.84	0.41
2:B:379:CYS:HA	2:B:411:ASN:O	2.20	0.41
1:A:458:LEU:HA	1:A:458:LEU:HD12	1.68	0.41
4:A:901:SV9:C22	3:C:67:ARG:H	2.33	0.41
1:A:311:ASP:OD2	1:A:311:ASP:N	2.49	0.41
1:A:455:ILE:HD12	1:A:455:ILE:HA	1.94	0.41
1:A:656:PHE:CD2	1:A:759:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:HA	1:A:694:PHE:O	2.20	0.41
2:B:418:LYS:O	2:B:421:PHE:CB	2.66	0.41
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.91	0.41
1:A:204:GLN:HE21	1:A:204:GLN:HB2	1.64	0.40
2:B:437:TRP:O	2:B:440:GLU:HG3	2.21	0.40
1:A:316:ARG:NH1	1:A:656:PHE:CZ	2.90	0.40
1:A:231:PHE:O	1:A:234:THR:HB	2.22	0.40
1:A:308:GLU:HG2	1:A:586:LEU:CD2	2.51	0.40
1:A:366:ASN:OD1	1:A:367:GLY:N	2.55	0.40
1:A:453:GLU:N	1:A:453:GLU:OE1	2.54	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:324:ASN:ND2	2:B:354:GLN:OE1[8_455]	1.26	0.94

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	76
2	B	131/144 (91%)	121 (92%)	10 (8%)	0	100	100
3	C	2/9 (22%)	2 (100%)	0	0	100	100
All	All	797/1024 (78%)	754 (95%)	42 (5%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASN

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%)	517 (91%)	49 (9%)	10	28
2	B	117/125 (94%)	89 (76%)	28 (24%)	0	2
3	C	4/9 (44%)	3 (75%)	1 (25%)	0	1
All	All	687/849 (81%)	609 (89%)	78 (11%)	5	17

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ILE
1	A	237	GLN
1	A	238	LEU
1	A	277	LYS
1	A	291	LEU
1	A	295	ARG
1	A	349	VAL
1	A	351	MET
1	A	404	LYS
1	A	424	LYS
1	A	429	GLU
1	A	436	LYS
1	A	442	LYS
1	A	445	LEU
1	A	449	VAL
1	A	452	LYS
1	A	453	GLU
1	A	455	ILE
1	A	466	SER
1	A	467	GLU
1	A	472	ARG
1	A	474	ILE
1	A	479	LEU
1	A	485	ARG
1	A	488	THR
1	A	504	LEU

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Mol	Chain	Res	Type
1	A	506	GLU
1	A	507	LYS
1	A	508	LEU
1	A	511	LEU
1	A	518	ASP
1	A	523	SER
1	A	526	ARG
1	A	554	GLN
1	A	557	ASP
1	A	564	HIS
1	A	568	ARG
1	A	569	ASN
1	A	571	TYR
1	A	612	GLN
1	A	645	GLU
1	A	659	LEU
1	A	696	ASN
1	A	697	LEU
1	A	758	ARG
1	A	791	GLN
1	A	801	GLU
1	A	805	ARG
1	A	836	LEU
2	B	343	VAL
2	B	344	SER
2	B	346	LYS
2	B	347	ARG
2	B	353	LYS
2	B	354	GLN
2	B	356	ASN
2	B	359	LEU
2	B	368	GLU
2	B	370	TYR
2	B	375	VAL
2	B	396	ARG
2	B	397	LYS
2	B	403	GLN
2	B	405	ILE
2	B	407	ASP
2	B	411	ASN
2	B	412	LYS
2	B	413	SER

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Mol	Chain	Res	Type
2	B	415	VAL
2	B	416	GLN
2	B	419	ASN
2	B	421	PHE
2	B	422	VAL
2	B	425	ARG
2	B	426	ARG
2	B	427	ARG
2	B	430	ILE
3	C	67	ARG

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	204	GLN
1	A	259	HIS
1	A	383	ASN
1	A	402	ASN
1	A	427	GLN
1	A	446	ASN
1	A	632	GLN
1	A	696	ASN
1	A	791	GLN
1	A	806	ASN
1	A	828	GLN
2	B	419	ASN
2	B	423	ASN
2	B	429	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 monosaccharides in this entry.

5.6 Ligand geometry

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
4	SV9	A	901	-	77,83,83	1.28	6 (7%)	94,124,124	0.98	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
4	SV9	A	901	-	-	29/47/67/67	0/9/9/9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	SV9	C5-N1	-6.29	1.34	1.42
4	A	901	SV9	C30-C33	-3.29	1.34	1.43
4	A	901	SV9	O4-C35	-2.69	1.37	1.43
4	A	901	SV9	C42-N6	-2.44	1.30	1.34
4	A	901	SV9	O5-C36	-2.34	1.37	1.43
4	A	901	SV9	C6-C7	-2.28	1.36	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	SV9	C30-C33-N3	3.38	116.94	110.99
4	A	901	SV9	C48-C47-C41	-3.18	96.20	100.98
4	A	901	SV9	O14-C41-C47	-2.95	102.61	106.93
4	A	901	SV9	C43-C44-N7	2.50	124.15	120.35
4	A	901	SV9	C6-C5-N1	-2.12	119.38	122.83
4	A	901	SV9	O4-C35-C34	-2.08	104.77	109.80
4	A	901	SV9	O16-C48-C47	-2.03	105.26	111.82

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	SV9	C9-C10-C11-C12
4	A	901	SV9	C10-C9-N1-C5
4	A	901	SV9	C10-C9-N1-C30
4	A	901	SV9	O1-C9-N1-C5
4	A	901	SV9	O1-C9-N1-C30
4	A	901	SV9	O6-C37-C38-O7
4	A	901	SV9	C38-O7-P1-O9
4	A	901	SV9	C19-C20-C21-C26
4	A	901	SV9	C27-C20-C21-C22
4	A	901	SV9	C19-C20-C21-C22
4	A	901	SV9	C27-C20-C21-C26
4	A	901	SV9	C11-C10-C9-N1
4	A	901	SV9	C11-C10-C9-O1
4	A	901	SV9	C14-C15-C16-C17
4	A	901	SV9	C14-C15-C16-C27
4	A	901	SV9	C28-C15-C16-C17
4	A	901	SV9	C36-C37-C38-O7
4	A	901	SV9	C28-C15-C16-C27
4	A	901	SV9	P2-O10-P1-O7
4	A	901	SV9	C38-O7-P1-O10
4	A	901	SV9	C39-O13-P2-O12
4	A	901	SV9	C38-O7-P1-O8
4	A	901	SV9	O4-C35-C36-C37
4	A	901	SV9	P1-O10-P2-O11
4	A	901	SV9	P1-O10-P2-O12
4	A	901	SV9	C10-C11-C12-C13
4	A	901	SV9	C10-C11-C12-C29
4	A	901	SV9	O13-C39-C40-O14
4	A	901	SV9	C39-O13-P2-O10

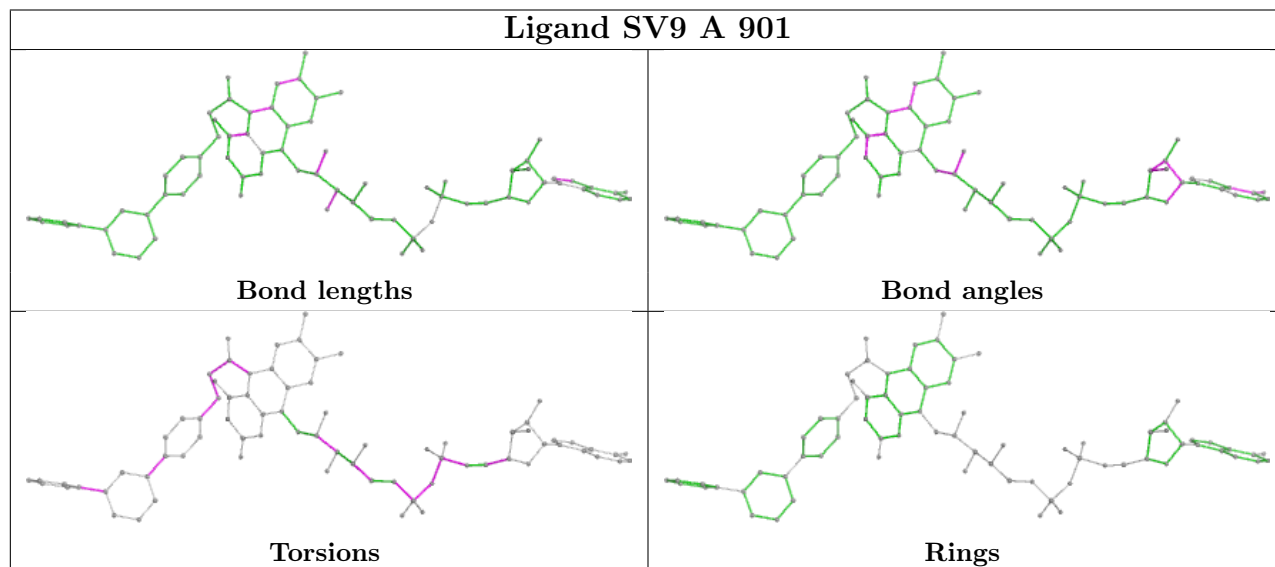
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	SV9	8	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%)	0.41	12 (1%) 68 61	63, 98, 132, 147	0
2	B	133/144 (92%)	0.55	8 (6%) 21 14	95, 127, 148, 159	0
3	C	4/9 (44%)	1.27	1 (25%) 0 0	120, 125, 131, 137	0
All	All	803/1024 (78%)	0.44	21 (2%) 56 46	63, 105, 136, 159	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	4.4
2	B	312	LYS	3.8
2	B	308	ARG	3.5
2	B	374	GLU	3.4
2	B	420	PHE	3.0
2	B	375	VAL	3.0
3	C	66	PRO	2.9
2	B	376	ILE	2.8
1	A	508	LEU	2.8
1	A	506	GLU	2.7
1	A	273	LEU	2.7
2	B	413	SER	2.7
1	A	174	VAL	2.7
1	A	454	LYS	2.5
2	B	378	LYS	2.4
1	A	242	TYR	2.3
1	A	275	THR	2.2
1	A	238	LEU	2.1
1	A	494	TYR	2.1
1	A	655	GLY	2.1
1	A	455	ILE	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](#)

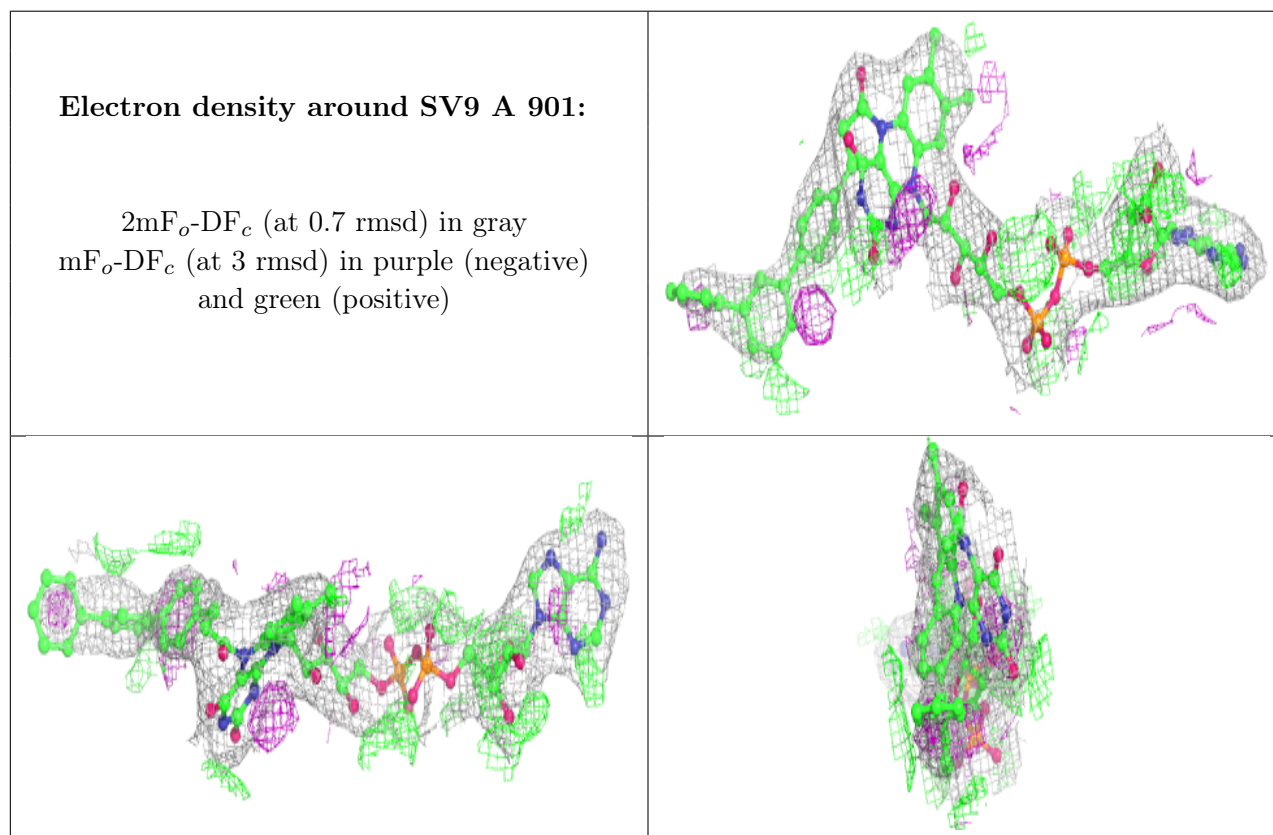
There are no monosaccharides in this entry.

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, 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(Å ²)	Q<0.9
4	SV9	A	901	75/75	0.97	0.25	55,79,124,131	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.