



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:52 AM UTC

PDB ID : 8BOP / pdb_00008bop
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

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

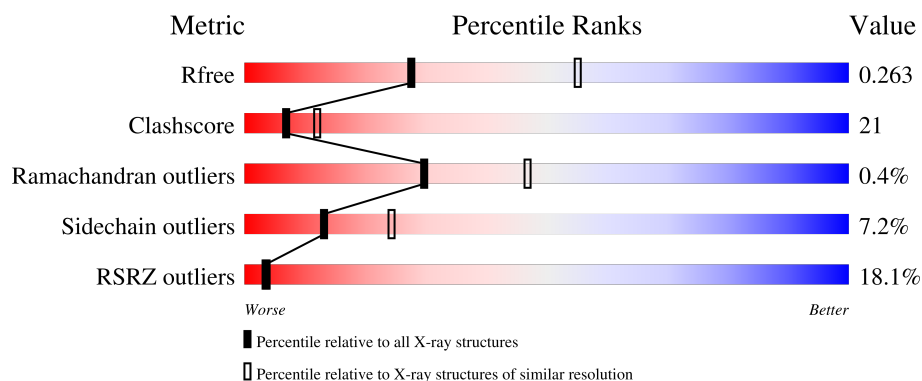
1 Overall quality at a glance

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	11% 54% 20% • 24%
2	B	144	33% 53% 30% 10% 8%

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
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

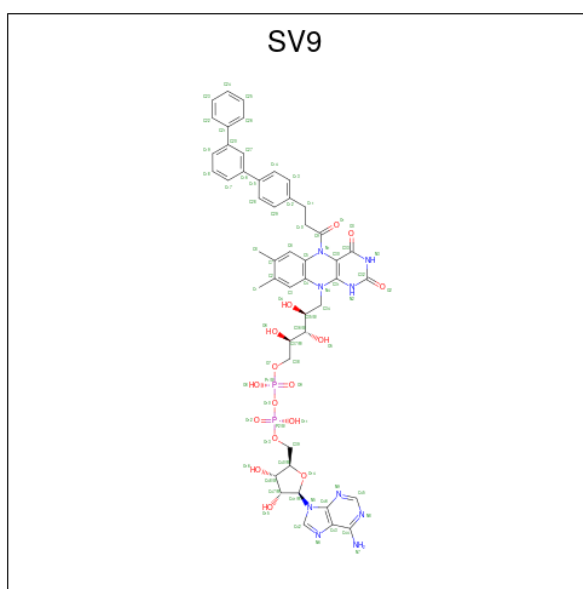
- Molecule 2 is a protein called REST corepressor 1.

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:

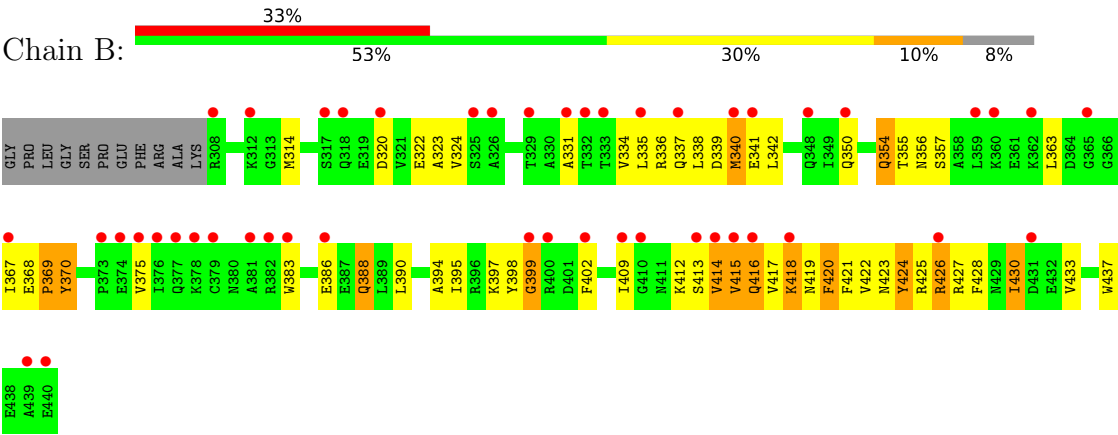
Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag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

- Molecule 3 is [[(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 (CCD ID: SV9) (formula: C₄₈H₅₁N₉O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



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

● 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	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) 98.3 (47.22-2.74)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.241 , 0.262 0.253 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6368	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage'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.*

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: 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	0.88	8/5331 (0.2%)	1.06	12/7232 (0.2%)
2	B	0.90	1/1091 (0.1%)	1.40	8/1471 (0.5%)
All	All	0.88	9/6422 (0.1%)	1.12	20/8703 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	PRO	C-O	-6.96	1.15	1.23
1	A	361	PRO	C-O	-6.85	1.16	1.23
1	A	543	PRO	C-O	-6.17	1.16	1.23
1	A	405	PRO	C-O	-5.98	1.17	1.23
1	A	637	VAL	C-O	-5.46	1.18	1.24
1	A	782	PRO	C-O	-5.26	1.16	1.23
2	B	369	PRO	C-O	-5.25	1.17	1.24
1	A	819	LEU	C-O	-5.15	1.18	1.24
1	A	823	GLY	C-O	-5.04	1.17	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	VAL	N-CA-C	-8.05	102.69	110.42
1	A	361	PRO	CB-CA-C	-7.42	102.43	111.11
1	A	324	ASN	CB-CA-C	6.96	122.32	110.56
1	A	438	GLN	N-CA-C	-6.72	104.03	111.36
2	B	354	GLN	CB-CA-C	-6.34	100.93	110.88
2	B	338	LEU	N-CA-C	-6.23	105.70	113.55
1	A	475	THR	CA-CB-OG1	-6.20	100.30	109.60
1	A	591	ARG	N-CA-C	-5.98	106.59	114.31
1	A	591	ARG	CB-CG-CD	5.85	124.75	111.30
1	A	793	ILE	N-CA-CB	-5.55	103.43	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	ILE	CA-C-N	-5.55	113.32	120.65
2	B	430	ILE	C-N-CA	-5.55	113.32	120.65
2	B	414	VAL	N-CA-C	-5.46	103.64	111.17
1	A	359	LYS	CA-C-N	-5.45	116.27	122.26
1	A	359	LYS	C-N-CA	-5.45	116.27	122.26
1	A	800	GLY	CA-C-O	-5.31	118.62	122.45
2	B	355	THR	CB-CA-C	-5.21	102.47	110.81
1	A	381	GLU	N-CA-C	-5.21	105.68	111.36
2	B	386	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	543	PRO	N-CA-CB	-5.12	98.90	103.35

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	208	0
2	B	1076	0	1091	83	0
3	A	75	0	0	6	0
All	All	6368	0	6343	269	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 21.

All (269) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:671:TRP:NE1	1:A:696:ASN:HD22	1.74	0.85
2:B:368:GLU:H	2:B:369:PRO:HD3	1.40	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:815:LEU:HD12	1:A:815:LEU:C	2.11	0.74
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
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:364:GLU:CD	1:A:524:ARG:NH2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:ARG:HD3	1:A:485:ARG:C	2.25	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:526:ARG:HH11	1:A:530:ASP:CG	2.10	0.59
1:A:188:MET:HE1	1:A:200:ILE:HA	1.84	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
1:A:651:VAL:HA	1:A:776:MET:HE1	1.85	0.58
2:B:383:TRP:CZ3	2:B:420:PHE:CD1	2.92	0.58
1:A:526:ARG:NH1	1:A:530:ASP:CG	2.58	0.57
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:384:ARG:HB3	2:B:314:MET:HE3	1.86	0.57
2:B:423:ASN:C	2:B:425:ARG:H	2.12	0.57
1:A:777:ALA:CB	1:A:820:ARG:HH12	2.17	0.57
1:A:537:GLU:CD	1:A:544:LEU:HD13	2.30	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
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:651:VAL:HG22	1:A:776:MET:HE1	1.89	0.55
1:A:205:GLN:O	1:A:209:VAL:HG23	2.06	0.55
2:B:420:PHE:CD2	2:B:420:PHE:C	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:520:TYR:CD1	1:A:520:TYR:C	2.84	0.51
1:A:291:LEU:HD12	1:A:291:LEU:H	1.76	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:448:MET:HE3	1:A:448:MET:HB3	1.76	0.48
2:B:413:SER:OG	2:B:413:SER:O	2.30	0.48
1:A:522:SER:C	1:A:524:ARG:N	2.71	0.48
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: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:420:PHE:C	2:B:420:PHE:HD2	2.22	0.47
2:B:416:GLN:HA	2:B:419:ASN:ND2	2.30	0.47
1:A:522:SER:C	1:A:524:ARG:H	2.22	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
1:A:484:HIS:ND1	1:A:484:HIS:C	2.73	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:188:MET:HE3	1:A:200:ILE:HD12	1.98	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: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
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:714:ILE:HG22	1:A:715:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:HA	1:A:474:ILE:HD12	1.71	0.43
1:A:188:MET:HE1	1:A:200:ILE:CA	2.46	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: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:422:HIS:O	1:A:422:HIS:CG	2.70	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
2:B:413:SER:C	2:B:415:VAL:N	2.74	0.42
1:A:789:ALA:HB1	1:A:790:PRO:HD2	2.02	0.42
2:B:423:ASN:C	2:B:425:ARG:N	2.73	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: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
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
1:A:696:ASN:OD1	1:A:696:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:485:ARG:C	1:A:485:ARG:CD	2.94	0.40
1:A:651:VAL:CA	1:A:776:MET:HE1	2.51	0.40
1:A:771:ASN:OD1	1:A:771:ASN:C	2.64	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%)	43	62
2	B	131/144 (91%)	120 (92%)	9 (7%)	2 (2%)	8	14
All	All	795/1015 (78%)	751 (94%)	41 (5%)	3 (0%)	30	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	399	GLY
2	B	424	TYR

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Mol	Chain	Res	Type
1	A	792	PRO

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%)	534 (94%)	32 (6%)	18	34
2	B	117/125 (94%)	100 (86%)	17 (14%)	3	4
All	All	683/840 (81%)	634 (93%)	49 (7%)	13	24

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LEU
1	A	247	VAL
1	A	269	ARG
1	A	308	GLU
1	A	311	ASP
1	A	351	MET
1	A	356	ILE
1	A	383	ASN
1	A	422	HIS
1	A	429	GLU
1	A	432	LYS
1	A	440	GLU
1	A	442	LYS
1	A	443	GLU
1	A	445	LEU
1	A	448	MET
1	A	449	VAL
1	A	466	SER
1	A	469	LYS
1	A	474	ILE
1	A	487	LEU
1	A	488	THR

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Mol	Chain	Res	Type
1	A	523	SER
1	A	524	ARG
1	A	543	PRO
1	A	633	GLN
1	A	714	ILE
1	A	734	ILE
1	A	740	VAL
1	A	786	ILE
1	A	815	LEU
1	A	820	ARG
2	B	322	GLU
2	B	334	VAL
2	B	335	LEU
2	B	336	ARG
2	B	339	ASP
2	B	340	MET
2	B	370	TYR
2	B	388	GLN
2	B	397	LYS
2	B	409	ILE
2	B	414	VAL
2	B	415	VAL
2	B	416	GLN
2	B	418	LYS
2	B	420	PHE
2	B	422	VAL
2	B	426	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	207	GLN
1	A	236	GLN
1	A	259	HIS
1	A	298	GLN
1	A	402	ASN
1	A	427	GLN
1	A	438	GLN
1	A	592	GLN
1	A	606	ASN
1	A	633	GLN

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Mol	Chain	Res	Type
1	A	638	GLN
1	A	696	ASN
2	B	337	GLN
2	B	348	GLN
2	B	388	GLN
2	B	419	ASN
2	B	429	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z > 2$
3	SV9	A	901	-	82,83,83	1.30	8 (9%)	110,124,124	0.88	6 (5%)

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	-	-	19/51/67/67	0/9/9/9

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	SV9	C5-N1	-6.41	1.34	1.42
3	A	901	SV9	P1-O10	-3.37	1.55	1.59
3	A	901	SV9	C30-C33	-3.25	1.35	1.43
3	A	901	SV9	P2-O10	-3.15	1.56	1.59
3	A	901	SV9	O4-C35	-2.80	1.37	1.43
3	A	901	SV9	C6-C7	-2.63	1.36	1.39
3	A	901	SV9	C5-C4	-2.17	1.37	1.41
3	A	901	SV9	O5-C36	-2.05	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	SV9	C30-C33-N3	3.22	116.60	110.94
3	A	901	SV9	O11-P2-O12	2.51	124.13	112.44
3	A	901	SV9	C6-C5-N1	-2.32	119.22	122.70
3	A	901	SV9	O7-C38-C37	2.30	115.49	109.36
3	A	901	SV9	O15-C47-C41	-2.16	102.65	110.10
3	A	901	SV9	C40-O14-C41	-2.04	104.97	109.47

There are no chirality outliers.

All (19) 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	C11-C10-C9-N1
3	A	901	SV9	C19-C20-C21-C22
3	A	901	SV9	C27-C20-C21-C26
3	A	901	SV9	C19-C20-C21-C26
3	A	901	SV9	C11-C10-C9-O1
3	A	901	SV9	O4-C35-C36-O5
3	A	901	SV9	O4-C35-C36-C37

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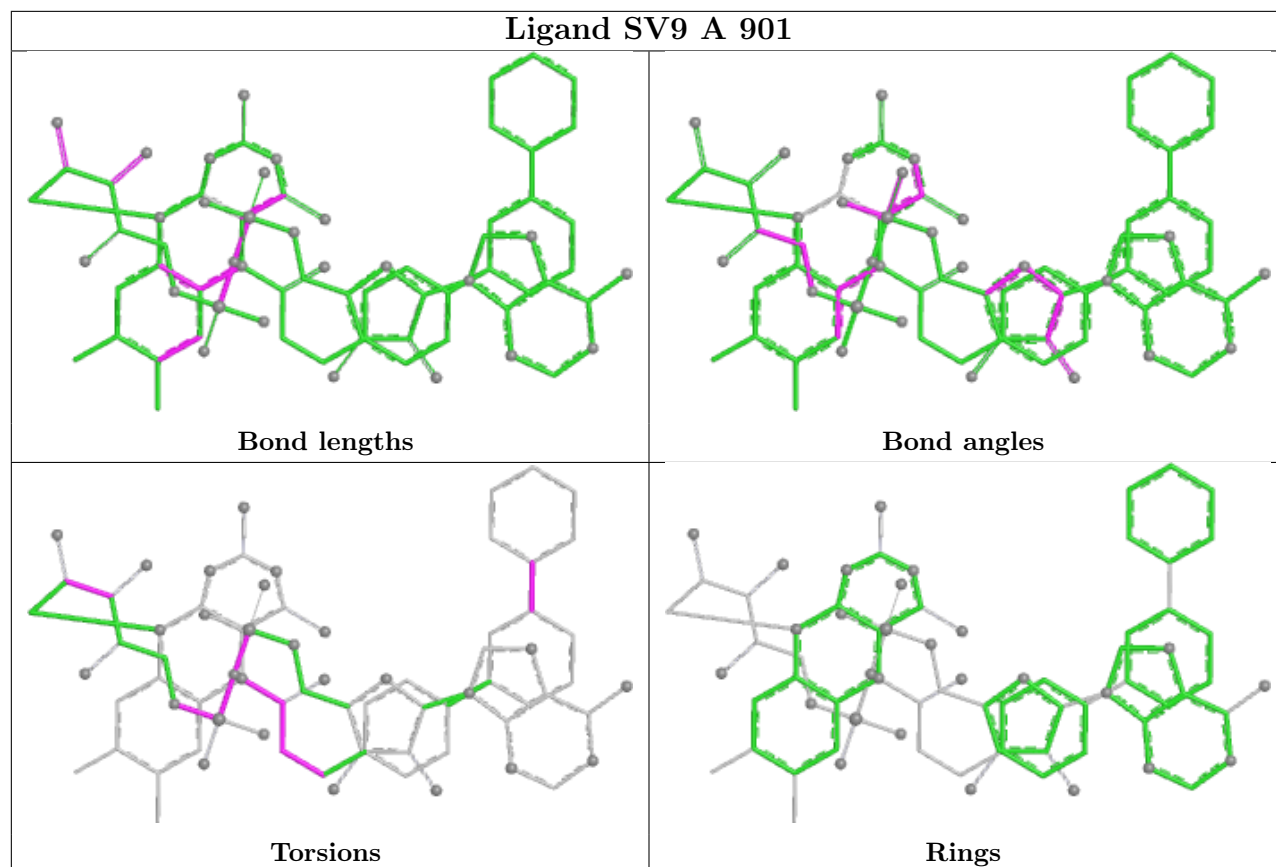
Mol	Chain	Res	Type	Atoms
3	A	901	SV9	P2-O10-P1-O7
3	A	901	SV9	P1-O10-P2-O11
3	A	901	SV9	C34-C35-C36-O5
3	A	901	SV9	P2-O10-P1-O9
3	A	901	SV9	P1-O10-P2-O12

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, 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%)	1.09	98 (14%) 6 6	60, 88, 120, 139	0
2	B	133/144 (92%)	1.81	47 (35%) 1 1	89, 118, 138, 146	0
All	All	799/1015 (78%)	1.21	145 (18%) 3 4	60, 94, 126, 146	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	375	VAL	6.5
2	B	376	ILE	5.6
1	A	171	PRO	5.3
1	A	509	GLN	5.1
1	A	836	LEU	5.0
1	A	611	SER	4.9
1	A	239	GLU	4.5
1	A	591	ARG	4.5
2	B	332	THR	4.2
2	B	373	PRO	4.1
2	B	308	ARG	4.1
2	B	340	MET	4.1
1	A	833	MET	4.0
2	B	439	ALA	4.0
1	A	377	MET	4.0
2	B	416	GLN	4.0
2	B	415	VAL	4.0
1	A	373	GLU	3.9
2	B	378	LYS	3.8
1	A	492	LYS	3.7
2	B	381	ALA	3.7
2	B	414	VAL	3.7
1	A	374	LYS	3.6
1	A	273	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	499	GLU	3.3
2	B	382	ARG	3.3
1	A	508	LEU	3.3
2	B	379	CYS	3.3
1	A	519	VAL	3.2
1	A	274	PRO	3.1
2	B	400	ARG	3.1
2	B	440	GLU	3.1
1	A	786	ILE	3.1
2	B	402	PHE	3.1
1	A	467	GLU	3.0
2	B	386	GLU	3.0
1	A	314	GLY	3.0
1	A	172	SER	3.0
1	A	527	GLN	3.0
2	B	337	GLN	2.9
1	A	240	ALA	2.9
1	A	699	LYS	2.9
2	B	317	SER	2.9
1	A	518	ASP	2.9
1	A	465	ALA	2.9
1	A	422	HIS	2.9
2	B	374	GLU	2.9
1	A	237	GLN	2.8
1	A	792	PRO	2.8
1	A	205	GLN	2.8
2	B	312	LYS	2.8
1	A	682	GLY	2.8
2	B	320	ASP	2.8
1	A	834	TYR	2.8
1	A	413	GLU	2.8
1	A	506	GLU	2.8
1	A	269	ARG	2.8
1	A	835	THR	2.8
2	B	326	ALA	2.8
2	B	410	GLY	2.8
1	A	353	LEU	2.7
1	A	303	ASP	2.7
2	B	333	THR	2.7
1	A	683	SER	2.6
2	B	325	SER	2.6
1	A	241	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	244	SER	2.6
2	B	377	GLN	2.6
1	A	291	LEU	2.6
2	B	335	LEU	2.6
2	B	399	GLY	2.6
1	A	350	ASN	2.6
2	B	383	TRP	2.5
1	A	359	LYS	2.5
1	A	432	LYS	2.5
2	B	418	LYS	2.5
1	A	242	TYR	2.5
2	B	431	ASP	2.5
1	A	421	LYS	2.5
1	A	232	GLU	2.5
1	A	364	GLU	2.4
1	A	454	LYS	2.4
1	A	668	ARG	2.4
2	B	426	ARG	2.4
2	B	360	LYS	2.4
1	A	777	ALA	2.4
1	A	175	GLU	2.4
1	A	247	VAL	2.4
1	A	696	ASN	2.3
1	A	426	GLU	2.3
1	A	672	ASP	2.3
1	A	787	PRO	2.3
1	A	450	ASN	2.3
1	A	671	TRP	2.3
1	A	173	GLY	2.3
1	A	608	ARG	2.3
1	A	741	PRO	2.3
1	A	612	GLN	2.3
1	A	740	VAL	2.3
1	A	451	LEU	2.3
1	A	369	ALA	2.3
2	B	409	ILE	2.3
1	A	493	GLU	2.3
2	B	329	THR	2.2
1	A	514	ASN	2.2
1	A	583	ASP	2.2
1	A	539	ALA	2.2
2	B	331	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	275	THR	2.2
2	B	348	GLN	2.2
1	A	556	ASP	2.2
1	A	271	LYS	2.2
2	B	362	LYS	2.2
2	B	367	ILE	2.2
1	A	638	GLN	2.2
1	A	213	ILE	2.2
1	A	510	GLU	2.2
1	A	580	GLU	2.2
1	A	395	GLN	2.2
1	A	259	HIS	2.2
1	A	206	THR	2.1
1	A	255	TYR	2.1
1	A	463	LYS	2.1
2	B	365	GLY	2.1
1	A	453	GLU	2.1
2	B	341	GLU	2.1
2	B	350	GLN	2.1
1	A	315	GLY	2.1
1	A	433	LYS	2.1
1	A	223	ASP	2.1
1	A	245	ASP	2.1
1	A	563	SER	2.1
1	A	674	SER	2.1
1	A	645	GLU	2.1
1	A	503	LYS	2.1
1	A	461	GLN	2.1
1	A	430	HIS	2.1
1	A	200	ILE	2.1
1	A	280	LYS	2.0
2	B	318	GLN	2.0
1	A	669	VAL	2.0
1	A	375	ASP	2.0
2	B	413	SER	2.0
1	A	437	THR	2.0
2	B	359	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

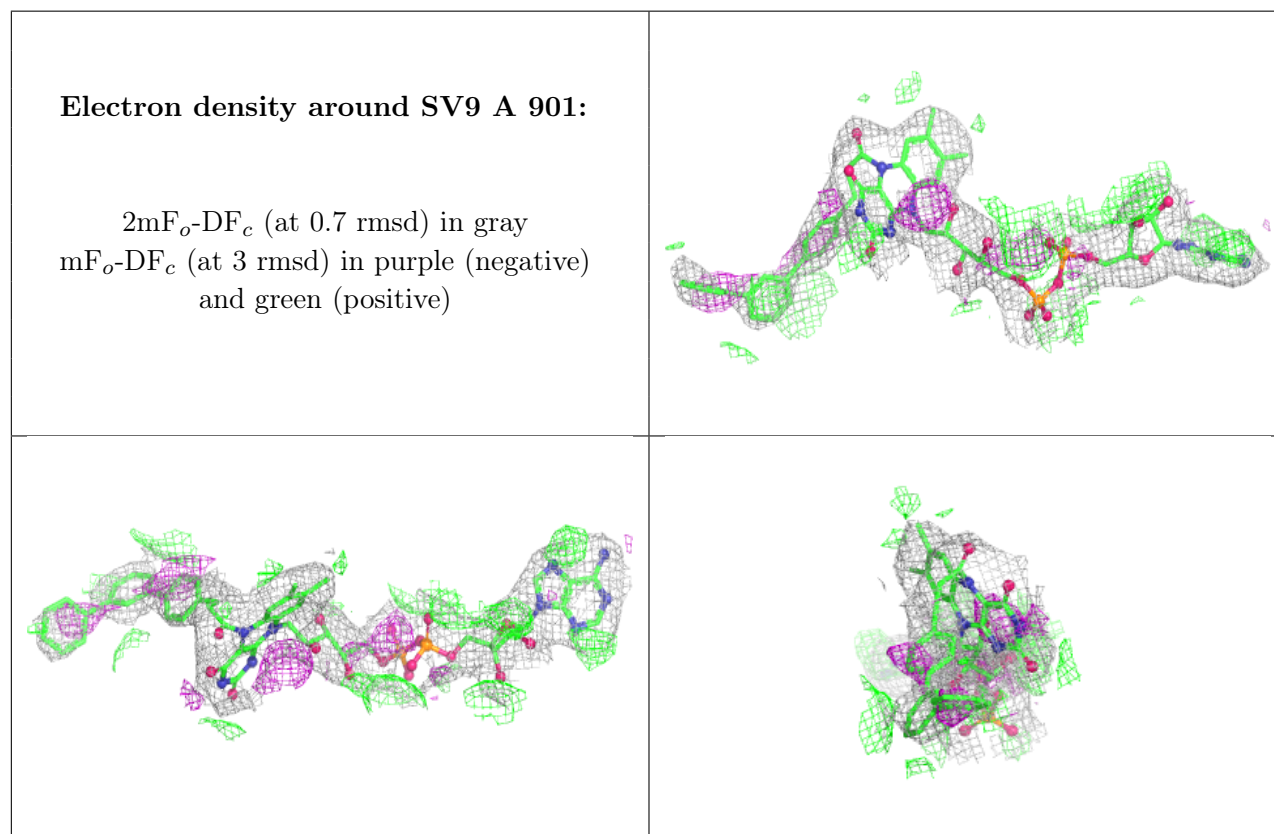
There are no oligosaccharides in this entry.

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	SV9	A	901	75/75	0.93	0.14	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.