



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:41 AM UTC

PDB ID : 9EL7 / pdb_00009el7
Title : LSD1-CoREST in complex with T105 enantiomer (1R,2S)
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2024-12-04
Resolution : 2.87 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

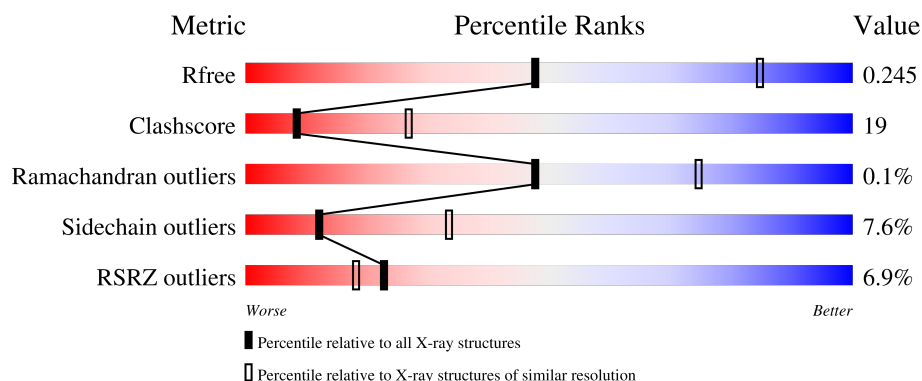
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	871	4% 55% 18% • 24%
2	B	144	12% 54% 29% 9% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6365 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

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

There are 19 discrepancies between the modelled and reference sequences:

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

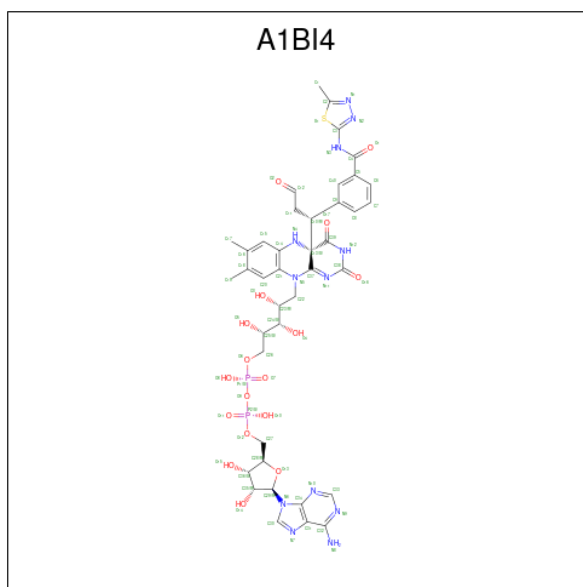
- Molecule 2 is a protein called REST corepressor 1.

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2S,3S,4R)-5-[(4aS)-7,8-dimethyl-4a-[(1R)-1-{3-[(5-methyl-1,3,4-thiadiazol-2-yl)carbamoyl]phenyl}-3-oxopropyl]-2,4-dioxo-3,4,4a,5-tetrahydrobenzo[g]pteridin-10(2H)-yl]-2,3,4-trihydroxypentyl dihydrogen diphosphate (non-preferred name) (CCD ID: A1BI4) (formula: C₄₀H₄₆N₁₂O₁₇P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			72	40	12	17	2	1		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.10Å 179.77Å 235.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.87 49.19 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.19-2.87) 99.5 (49.19-2.87)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.216 , 0.242 0.221 , 0.245	Depositor DCC
R_{free} test set	2000 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6365	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: A1BI4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.79	6/5331 (0.1%)	0.97	5/7232 (0.1%)
2	B	0.73	1/1091 (0.1%)	1.10	1/1471 (0.1%)
All	All	0.78	7/6422 (0.1%)	0.99	6/8703 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	PRO	C-O	-7.38	1.18	1.24
2	B	310	PRO	C-O	-6.65	1.17	1.24
1	A	782	PRO	C-O	-6.15	1.15	1.23
1	A	755	PRO	C-O	-6.00	1.16	1.24
1	A	405	PRO	C-O	-5.99	1.17	1.23
1	A	794	PRO	C-O	-5.77	1.17	1.23
1	A	792	PRO	C-O	-5.11	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	LEU	N-CA-C	-6.11	106.46	114.04
1	A	736	GLY	CA-C-O	-5.75	117.40	121.88
1	A	469	LYS	CA-C-N	5.62	123.70	119.66
1	A	469	LYS	C-N-CA	5.62	123.70	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	PRO	CB-CA-C	-5.31	103.27	110.60
2	B	421	PHE	CB-CA-C	-5.30	102.55	110.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	571	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5217	0	5252	195	0
2	B	1076	0	1091	67	0
3	A	72	0	0	3	0
All	All	6365	0	6343	243	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 19.

All (243) 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:424:LYS:HE3	2:B:339:ASP:OD1	1.29	1.24
1:A:438:GLN:CG	1:A:508:LEU:HD11	1.72	1.19
1:A:438:GLN:HG3	1:A:508:LEU:HD11	1.16	1.15
1:A:276:LYS:HE2	1:A:276:LYS:HA	1.29	1.13
2:B:414:VAL:HG12	2:B:418:LYS:NZ	1.69	1.06
1:A:363:TYR:CD2	1:A:734:ILE:HG23	1.91	1.05
1:A:793:ILE:HD12	1:A:793:ILE:H	1.21	1.04
1:A:794:PRO:HD2	1:A:828:GLN:OE1	1.59	1.02
2:B:414:VAL:HG12	2:B:418:LYS:HZ3	0.87	1.02
1:A:438:GLN:HG3	1:A:508:LEU:CD1	1.89	1.01
1:A:503:LYS:O	1:A:506:GLU:HG2	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:HG23	1:A:508:LEU:HD21	1.41	0.99
2:B:414:VAL:CG1	2:B:418:LYS:HZ3	1.79	0.95
1:A:463:LYS:O	1:A:467:GLU:HG2	1.65	0.95
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.51	0.93
1:A:666:PHE:O	1:A:701:PRO:CG	2.17	0.92
1:A:665:CYS:HA	1:A:702:ILE:HD13	1.48	0.92
1:A:363:TYR:CD2	1:A:734:ILE:CG2	2.53	0.92
1:A:438:GLN:CG	1:A:508:LEU:CD1	2.46	0.92
1:A:380:GLN:HG2	1:A:384:ARG:HD2	1.51	0.91
1:A:424:LYS:CE	2:B:339:ASP:OD1	2.19	0.90
1:A:380:GLN:O	1:A:384:ARG:HD3	1.70	0.90
1:A:276:LYS:HA	1:A:276:LYS:CE	1.97	0.89
1:A:378:VAL:HG11	1:A:528:ILE:HG22	1.54	0.89
2:B:425:ARG:HG3	2:B:425:ARG:HH11	1.37	0.89
1:A:524:ARG:HH21	1:A:524:ARG:HG3	1.35	0.88
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.08	0.88
1:A:325:TYR:OH	1:A:744:LYS:HD2	1.74	0.87
1:A:363:TYR:HD2	1:A:734:ILE:HG23	1.40	0.84
1:A:665:CYS:SG	1:A:702:ILE:HD11	2.18	0.84
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.59	0.84
1:A:325:TYR:OH	1:A:744:LYS:CD	2.27	0.83
2:B:403:GLN:NE2	2:B:403:GLN:O	2.13	0.82
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.45	0.81
1:A:755:PRO:HA	1:A:758:ARG:HE	1.48	0.79
1:A:174:VAL:HG12	1:A:219:GLN:OE1	1.81	0.79
1:A:380:GLN:O	1:A:384:ARG:CD	2.31	0.78
1:A:666:PHE:O	1:A:701:PRO:HG3	1.82	0.78
1:A:456:LYS:HE2	2:B:370:TYR:OH	1.84	0.78
1:A:665:CYS:HA	1:A:702:ILE:CD1	2.14	0.77
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.49	0.76
2:B:327:ASN:OD1	2:B:330:ALA:N	2.19	0.76
1:A:418:LEU:HD21	2:B:324:VAL:HG21	1.66	0.76
1:A:437:THR:HG23	1:A:508:LEU:CD2	2.15	0.76
2:B:338:LEU:N	2:B:338:LEU:HD23	2.01	0.76
2:B:400:ARG:HG3	2:B:400:ARG:HH11	1.52	0.75
1:A:695:TRP:CD1	1:A:697:LEU:HD21	2.21	0.74
1:A:363:TYR:CE2	1:A:734:ILE:CG2	2.68	0.74
1:A:680:HIS:CE1	1:A:730:ILE:CD1	2.71	0.73
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.66	0.73
2:B:341:GLU:HG3	2:B:341:GLU:O	1.88	0.73
1:A:372:LYS:O	1:A:376:GLU:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLN:HE21	1:A:508:LEU:HD12	1.54	0.72
1:A:366:ASN:OD1	1:A:367:GLY:N	2.22	0.72
1:A:475:THR:HA	2:B:393:GLN:HE22	1.54	0.71
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.03	0.71
1:A:232:GLU:OE2	1:A:232:GLU:N	2.17	0.71
1:A:671:TRP:HE1	1:A:696:ASN:ND2	1.89	0.71
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.20	0.71
1:A:380:GLN:HG2	1:A:384:ARG:CD	2.21	0.71
1:A:666:PHE:O	1:A:701:PRO:HG2	1.91	0.71
2:B:425:ARG:HG3	2:B:425:ARG:NH1	1.98	0.71
1:A:670:PHE:CE2	1:A:740:VAL:HG22	2.26	0.70
2:B:406:SER:OG	2:B:412:LYS:O	2.06	0.70
1:A:232:GLU:H	1:A:232:GLU:CD	2.00	0.69
1:A:524:ARG:HG3	1:A:524:ARG:NH2	1.99	0.69
1:A:366:ASN:OD1	1:A:368:GLN:N	2.26	0.68
1:A:685:THR:O	1:A:688:ARG:HG2	1.93	0.68
2:B:340:MET:O	2:B:343:VAL:HG22	1.94	0.68
1:A:669:VAL:HG11	1:A:673:PRO:HG3	1.75	0.67
1:A:463:LYS:O	1:A:467:GLU:CG	2.41	0.67
2:B:380:ASN:OD1	2:B:381:ALA:N	2.28	0.67
1:A:257:GLU:HG3	1:A:263:ASN:HD22	1.60	0.67
1:A:380:GLN:CG	1:A:384:ARG:HD2	2.22	0.66
1:A:680:HIS:NE2	1:A:730:ILE:HD13	2.11	0.66
2:B:414:VAL:CG1	2:B:418:LYS:NZ	2.48	0.65
1:A:236:GLN:OE1	1:A:236:GLN:HA	1.95	0.65
1:A:438:GLN:NE2	1:A:508:LEU:HD12	2.12	0.64
2:B:308:ARG:HG3	2:B:308:ARG:O	1.98	0.64
1:A:332:MET:HE1	1:A:695:TRP:CE3	2.32	0.64
2:B:416:GLN:OE1	2:B:416:GLN:N	2.28	0.64
1:A:235:LEU:O	1:A:235:LEU:HD12	1.99	0.63
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.81	0.62
1:A:794:PRO:CD	1:A:828:GLN:OE1	2.43	0.61
1:A:325:TYR:OH	1:A:744:LYS:HD3	1.99	0.61
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.33	0.61
1:A:384:ARG:NH1	1:A:384:ARG:HG2	2.15	0.61
1:A:329:LEU:HD12	1:A:749:SER:HB3	1.83	0.60
1:A:700:ALA:HB1	1:A:701:PRO:CD	2.28	0.60
1:A:484:HIS:ND1	2:B:372:LEU:HD13	2.16	0.60
1:A:346:SER:HB3	1:A:351:MET:HE3	1.83	0.59
1:A:384:ARG:HG2	1:A:384:ARG:HH11	1.67	0.59
1:A:583:ASP:OD2	1:A:585:LYS:NZ	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:HG11	1:A:528:ILE:CG2	2.32	0.58
1:A:437:THR:CG2	1:A:508:LEU:CD2	2.80	0.58
1:A:671:TRP:NE1	1:A:696:ASN:ND2	2.51	0.58
1:A:391:TYR:CZ	2:B:310:PRO:HD3	2.39	0.58
1:A:437:THR:CG2	1:A:508:LEU:HD21	2.23	0.58
1:A:793:ILE:HD12	1:A:793:ILE:N	2.05	0.58
2:B:402:PHE:CD1	2:B:418:LYS:HD2	2.39	0.58
1:A:524:ARG:HH21	1:A:524:ARG:CG	2.12	0.57
1:A:332:MET:CE	1:A:695:TRP:CZ3	2.87	0.57
1:A:438:GLN:HE22	2:B:353:LYS:HD3	1.69	0.57
1:A:671:TRP:NE1	1:A:696:ASN:HD22	2.03	0.57
1:A:395:GLN:NE2	2:B:308:ARG:HA	2.20	0.57
1:A:680:HIS:CD2	1:A:730:ILE:HD13	2.39	0.56
1:A:670:PHE:HE2	1:A:740:VAL:HG22	1.66	0.56
1:A:363:TYR:CD2	1:A:734:ILE:HG21	2.39	0.56
1:A:419:GLN:NE2	2:B:314:MET:HA	2.20	0.56
1:A:448:MET:HE2	2:B:363:LEU:HD23	1.86	0.56
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.41	0.56
1:A:793:ILE:HG23	1:A:828:GLN:CD	2.31	0.55
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.71	0.55
2:B:425:ARG:CA	2:B:430:ILE:HD12	2.34	0.55
1:A:754:ASP:OD1	1:A:755:PRO:HD2	2.07	0.55
1:A:793:ILE:H	1:A:793:ILE:CD1	1.93	0.55
2:B:425:ARG:HH11	2:B:425:ARG:CG	2.12	0.55
1:A:603:ILE:HG12	1:A:615:ILE:HD13	1.89	0.54
1:A:755:PRO:HB3	1:A:758:ARG:HH21	1.73	0.54
1:A:568:ARG:HH21	1:A:699:LYS:CA	2.21	0.54
1:A:363:TYR:HD2	1:A:734:ILE:CG2	2.05	0.54
1:A:381:GLU:HA	1:A:384:ARG:HD3	1.90	0.54
1:A:391:TYR:CE1	2:B:310:PRO:HD3	2.42	0.53
1:A:374:LYS:CE	1:A:525:ASP:OD1	2.56	0.53
1:A:721:ASP:HA	1:A:724:VAL:HG22	1.89	0.53
1:A:690:GLU:HG3	1:A:715:MET:HE2	1.91	0.53
1:A:566:THR:HG21	1:A:697:LEU:HG	1.90	0.53
1:A:503:LYS:O	1:A:506:GLU:CG	2.45	0.52
1:A:695:TRP:CE3	1:A:706:LEU:HD11	2.44	0.52
1:A:427:GLN:NE2	1:A:518:ASP:HA	2.24	0.52
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.38	0.52
3:A:901:A1BI4:C6	3:A:901:A1BI4:N2	2.73	0.51
2:B:400:ARG:HG3	2:B:400:ARG:NH1	2.23	0.51
1:A:650:ALA:O	1:A:654:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:VAL:HA	2:B:418:LYS:HE2	1.93	0.51
1:A:438:GLN:NE2	1:A:508:LEU:CD1	2.74	0.51
1:A:456:LYS:HG3	2:B:370:TYR:CZ	2.46	0.51
1:A:198:ASP:OD1	1:A:199:ILE:N	2.44	0.51
1:A:424:LYS:HE3	2:B:339:ASP:CG	2.25	0.50
1:A:487:LEU:C	1:A:487:LEU:HD23	2.37	0.50
1:A:362:LEU:HD11	1:A:531:TRP:CD2	2.46	0.50
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.26	0.50
1:A:378:VAL:CG1	1:A:528:ILE:HG22	2.34	0.50
1:A:280:LYS:HD3	1:A:303:ASP:HB3	1.94	0.50
1:A:680:HIS:CE1	1:A:730:ILE:HD13	2.46	0.49
1:A:448:MET:HB3	2:B:363:LEU:HD21	1.94	0.49
1:A:723:ILE:O	1:A:727:CYS:SG	2.67	0.49
1:A:701:PRO:HG2	1:A:701:PRO:O	2.13	0.49
1:A:702:ILE:HG22	1:A:702:ILE:O	2.10	0.49
2:B:317:SER:O	2:B:321:VAL:HG23	2.13	0.48
2:B:402:PHE:HE2	2:B:421:PHE:CZ	2.31	0.48
1:A:438:GLN:CD	1:A:508:LEU:CD1	2.86	0.48
1:A:332:MET:HE1	1:A:695:TRP:CZ3	2.48	0.48
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.48	0.48
1:A:364:GLU:HA	1:A:681:VAL:HB	1.95	0.48
1:A:363:TYR:HD2	1:A:734:ILE:HG12	1.78	0.48
1:A:695:TRP:CD1	1:A:697:LEU:CD2	2.95	0.48
2:B:403:GLN:NE2	2:B:403:GLN:C	2.72	0.47
1:A:419:GLN:HE22	2:B:314:MET:HA	1.79	0.47
1:A:742:GLN:OE1	1:A:742:GLN:HA	2.15	0.47
1:A:273:LEU:HD22	1:A:274:PRO:HD2	1.96	0.47
1:A:296:GLN:O	1:A:299:SER:HB3	2.15	0.47
1:A:647:LYS:HE3	1:A:780:ILE:HD11	1.96	0.47
2:B:402:PHE:CB	2:B:414:VAL:HG13	2.45	0.47
1:A:183:LEU:HD13	1:A:214:ARG:HD2	1.95	0.47
1:A:684:THR:HG22	1:A:686:ALA:H	1.80	0.46
1:A:808:PRO:O	1:A:810:THR:HG23	2.16	0.46
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.97	0.46
1:A:568:ARG:HH21	1:A:699:LYS:HA	1.80	0.46
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.97	0.46
1:A:188:MET:CE	1:A:200:ILE:HB	2.46	0.46
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.98	0.46
1:A:362:LEU:C	1:A:363:TYR:HD1	2.24	0.46
1:A:374:LYS:NZ	1:A:525:ASP:OD1	2.48	0.46
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.56	0.45
2:B:395:ILE:CG2	2:B:433:VAL:CG1	2.93	0.45
1:A:448:MET:HE2	2:B:363:LEU:CD2	2.47	0.45
1:A:706:LEU:N	1:A:706:LEU:HD12	2.32	0.45
2:B:395:ILE:HG22	2:B:433:VAL:HG11	1.98	0.45
1:A:380:GLN:C	1:A:384:ARG:HD3	2.38	0.45
2:B:402:PHE:HB2	2:B:414:VAL:HG13	1.99	0.44
2:B:420:PHE:CD2	2:B:420:PHE:C	2.94	0.44
1:A:693:LEU:HD12	1:A:694:PHE:H	1.82	0.44
1:A:603:ILE:HG12	1:A:615:ILE:CD1	2.48	0.44
2:B:315:PHE:O	2:B:316:LEU:HD23	2.18	0.44
1:A:461:GLN:OE1	1:A:483:LYS:HE3	2.18	0.44
2:B:342:LEU:O	2:B:346:LYS:HG3	2.18	0.44
1:A:332:MET:CE	1:A:695:TRP:CE3	2.99	0.44
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.88	0.44
1:A:353:LEU:HB3	1:A:565:LEU:HD23	2.00	0.43
2:B:396:ARG:HE	2:B:436:GLU:HG2	1.82	0.43
2:B:429:ASN:HD22	2:B:432:GLU:HG3	1.83	0.43
1:A:834:TYR:C	1:A:834:TYR:CD2	2.95	0.43
2:B:400:ARG:NH1	2:B:400:ARG:CG	2.79	0.43
1:A:284:ILE:HD13	1:A:590:VAL:HG11	2.00	0.43
1:A:508:LEU:N	1:A:508:LEU:HD23	2.33	0.43
1:A:541:ALA:O	1:A:657:GLY:HA3	2.17	0.43
2:B:403:GLN:NE2	2:B:403:GLN:CA	2.81	0.43
1:A:364:GLU:HG2	1:A:365:ALA:H	1.84	0.43
1:A:468:VAL:O	1:A:468:VAL:HG12	2.18	0.43
2:B:312:LYS:HD2	2:B:312:LYS:HA	1.67	0.43
2:B:388:GLN:O	2:B:391:ALA:HB3	2.18	0.43
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.71	0.43
1:A:470:PRO:HA	1:A:472:ARG:HG2	2.01	0.43
1:A:793:ILE:CG2	1:A:828:GLN:CD	2.92	0.43
2:B:421:PHE:HA	2:B:430:ILE:HD13	2.00	0.43
1:A:665:CYS:CA	1:A:702:ILE:CD1	2.94	0.43
1:A:789:ALA:HB1	1:A:790:PRO:HD2	2.01	0.43
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.93	0.42
1:A:451:LEU:HA	1:A:451:LEU:HD12	1.66	0.42
2:B:368:GLU:N	2:B:369:PRO:CD	2.81	0.42
1:A:374:LYS:HE3	1:A:525:ASP:OD1	2.18	0.42
1:A:425:ASP:OD2	2:B:338:LEU:CD1	2.67	0.42
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.82	0.42
2:B:395:ILE:CG2	2:B:433:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD1	1:A:199:ILE:HG13	2.20	0.42
1:A:601:GLU:HA	1:A:616:TYR:O	2.20	0.42
1:A:654:MET:HB3	1:A:654:MET:HE2	1.70	0.42
1:A:174:VAL:CG1	1:A:219:GLN:OE1	2.61	0.42
1:A:189:THR:OG1	1:A:192:GLU:HG3	2.20	0.42
1:A:487:LEU:HD23	1:A:487:LEU:O	2.20	0.42
1:A:235:LEU:HD11	1:A:243:ASN:HB2	2.02	0.41
1:A:671:TRP:O	1:A:673:PRO:HD3	2.20	0.41
2:B:371:ARG:HE	2:B:371:ARG:HB2	1.67	0.41
1:A:702:ILE:HD13	1:A:702:ILE:HA	1.75	0.41
1:A:684:THR:HG22	1:A:685:THR:N	2.36	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.62	0.41
1:A:175:GLU:H	1:A:175:GLU:HG2	1.37	0.41
1:A:428:ILE:HD13	2:B:341:GLU:HG2	2.03	0.41
3:A:901:A1BI4:C8	3:A:901:A1BI4:N4	2.84	0.41
1:A:691:LEU:HA	1:A:706:LEU:O	2.22	0.41
2:B:403:GLN:C	2:B:403:GLN:HE21	2.27	0.41
1:A:695:TRP:HZ2	3:A:901:A1BI4:N1	2.19	0.40
1:A:800:GLY:O	1:A:803:THR:OG1	2.36	0.40
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.56	0.40
1:A:492:LYS:O	1:A:496:GLU:HG3	2.20	0.40
1:A:659:LEU:O	1:A:660:ASN:ND2	2.54	0.40
1:A:606:ASN:HD22	1:A:609:SER:H	1.68	0.40
1:A:680:HIS:CE1	1:A:730:ILE:HD11	2.53	0.40
2:B:418:LYS:HE2	2:B:418:LYS:HB2	1.87	0.40
1:A:474:ILE:HG23	2:B:393:GLN:OE1	2.21	0.40
1:A:666:PHE:CD2	1:A:670:PHE:HE1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/871 (76%)	641 (96%)	22 (3%)	1 (0%)	43	70
2	B	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
All	All	795/1015 (78%)	765 (96%)	29 (4%)	1 (0%)	48	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	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%)	530 (94%)	36 (6%)	16	42
2	B	117/125 (94%)	101 (86%)	16 (14%)	3	10
All	All	683/840 (81%)	631 (92%)	52 (8%)	12	33

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	GLU
1	A	235	LEU
1	A	237	GLN
1	A	238	LEU
1	A	239	GLU
1	A	271	LYS
1	A	275	THR
1	A	276	LYS
1	A	421	LYS
1	A	423	VAL
1	A	429	GLU
1	A	467	GLU
1	A	469	LYS
1	A	472	ARG
1	A	474	ILE

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Mol	Chain	Res	Type
1	A	482	SER
1	A	508	LEU
1	A	509	GLN
1	A	511	LEU
1	A	517	SER
1	A	524	ARG
1	A	526	ARG
1	A	528	ILE
1	A	659	LEU
1	A	696	ASN
1	A	697	LEU
1	A	699	LYS
1	A	702	ILE
1	A	719	SER
1	A	727	CYS
1	A	730	ILE
1	A	742	GLN
1	A	744	LYS
1	A	780	ILE
1	A	786	ILE
1	A	793	ILE
2	B	308	ARG
2	B	312	LYS
2	B	334	VAL
2	B	337	GLN
2	B	338	LEU
2	B	339	ASP
2	B	341	GLU
2	B	368	GLU
2	B	371	ARG
2	B	403	GLN
2	B	405	ILE
2	B	412	LYS
2	B	413	SER
2	B	425	ARG
2	B	433	VAL
2	B	440	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN

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Mol	Chain	Res	Type
1	A	395	GLN
1	A	427	GLN
1	A	438	GLN
1	A	535	ASN
1	A	632	GLN
1	A	660	ASN
1	A	696	ASN
1	A	812	HIS
2	B	393	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A1BI4	A	901	-	77,79,79	0.98	3 (3%)	105,120,120	1.38	9 (8%)

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	A1BI4	A	901	-	-	15/53/104/104	0/8/8/8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	A1BI4	C13-C39	-5.83	1.52	1.54
3	A	901	A1BI4	C13-C10	2.37	1.60	1.55
3	A	901	A1BI4	C4-N3	2.23	1.41	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	A1BI4	C3-N3-C4	9.41	139.25	123.67
3	A	901	A1BI4	C5-C4-N3	3.86	121.81	116.25
3	A	901	A1BI4	N3-C3-N2	2.99	123.49	120.81
3	A	901	A1BI4	O1-C4-N3	-2.75	118.25	122.27
3	A	901	A1BI4	C13-N4-C14	2.63	124.92	119.43
3	A	901	A1BI4	C39-N12-C38	-2.43	121.75	125.42
3	A	901	A1BI4	C3-S1-C2	-2.43	86.62	88.39
3	A	901	A1BI4	O10-P2-O11	2.12	122.29	112.44
3	A	901	A1BI4	O13-C29-C35	-2.05	102.22	106.62

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	A1BI4	C5-C4-N3-C3
3	A	901	A1BI4	O1-C4-N3-C3
3	A	901	A1BI4	C13-C10-C9-C8
3	A	901	A1BI4	C13-C10-C9-C40
3	A	901	A1BI4	N2-C3-N3-C4
3	A	901	A1BI4	S1-C3-N3-C4
3	A	901	A1BI4	C23-C22-N5-C37
3	A	901	A1BI4	O3-C23-C24-O4
3	A	901	A1BI4	O3-C23-C24-C25
3	A	901	A1BI4	C23-C22-N5-C21
3	A	901	A1BI4	C11-C10-C9-C8

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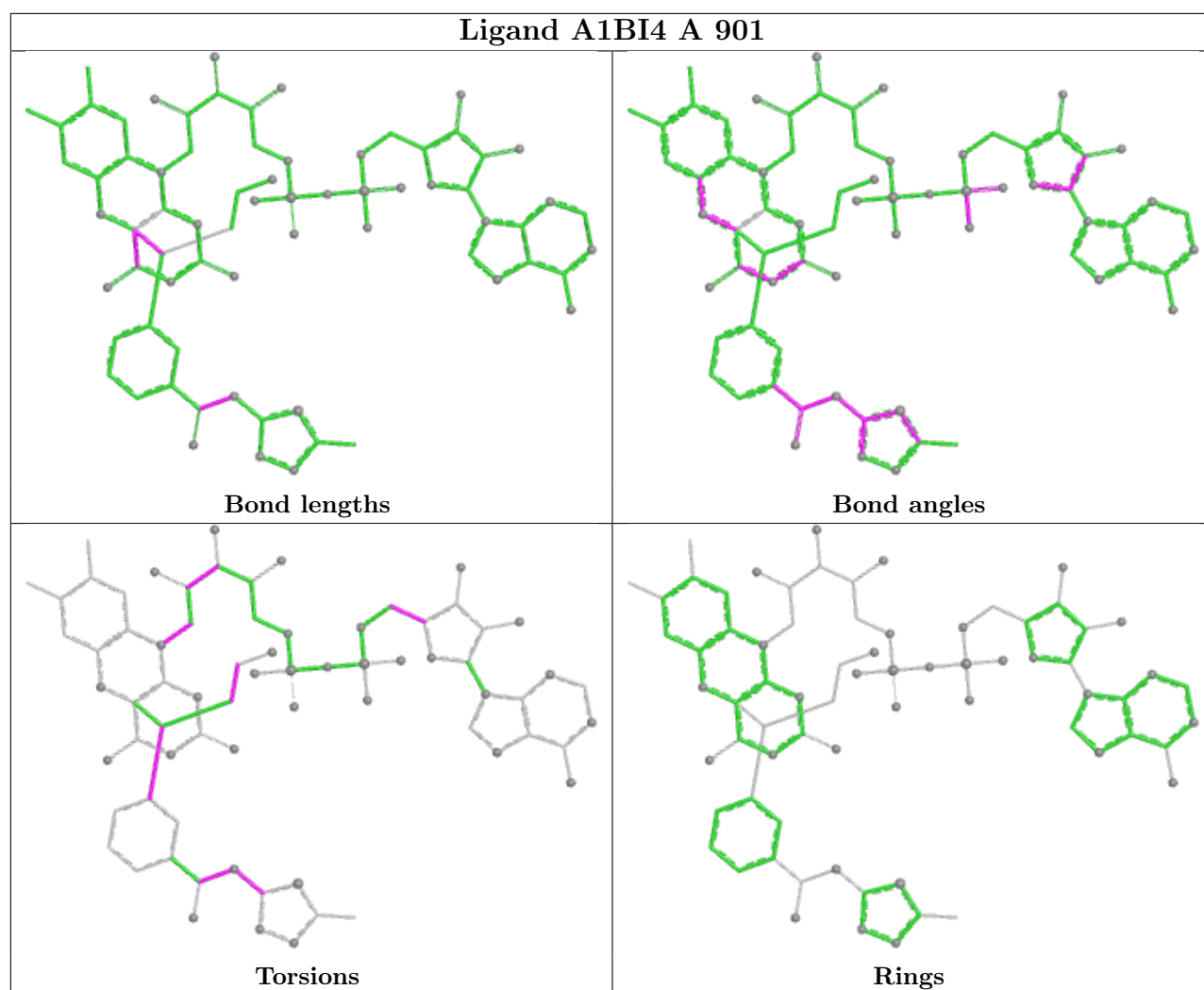
Mol	Chain	Res	Type	Atoms
3	A	901	A1BI4	C11-C10-C9-C40
3	A	901	A1BI4	C10-C11-C12-O2
3	A	901	A1BI4	C22-C23-C24-O4
3	A	901	A1BI4	O12-C27-C28-O13

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	A1BI4	3	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%)	0.43	37 (5%) 30 23	47, 79, 112, 128	0
2	B	133/144 (92%)	1.04	18 (13%) 7 5	75, 107, 130, 142	0
All	All	799/1015 (78%)	0.53	55 (6%) 23 18	47, 85, 118, 142	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	6.6
1	A	171	PRO	4.8
1	A	667	ASP	4.4
1	A	700	ALA	4.4
1	A	275	THR	4.1
2	B	376	ILE	4.0
2	B	374	GLU	3.9
1	A	833	MET	3.8
1	A	350	ASN	3.7
1	A	373	GLU	3.7
1	A	785	SER	3.5
1	A	744	LYS	3.4
2	B	375	VAL	3.3
1	A	698	TYR	3.2
2	B	440	GLU	3.2
2	B	382	ARG	3.2
1	A	739	ALA	3.1
1	A	695	TRP	2.9
2	B	378	LYS	2.9
2	B	312	LYS	2.8
2	B	337	GLN	2.8
2	B	439	ALA	2.8
1	A	660	ASN	2.7
1	A	580	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	699	LYS	2.5
2	B	427	ARG	2.5
1	A	270	ILE	2.4
1	A	269	ARG	2.4
1	A	272	PRO	2.4
1	A	669	VAL	2.4
1	A	358	GLN	2.4
1	A	740	VAL	2.3
1	A	507	LYS	2.3
2	B	329	THR	2.3
1	A	508	LEU	2.2
1	A	563	SER	2.2
1	A	670	PHE	2.2
2	B	315	PHE	2.2
1	A	443	GLU	2.2
1	A	363	TYR	2.2
1	A	467	GLU	2.2
1	A	668	ARG	2.2
2	B	383	TRP	2.2
2	B	317	SER	2.2
1	A	786	ILE	2.1
2	B	379	CYS	2.1
1	A	364	GLU	2.1
1	A	696	ASN	2.1
1	A	741	PRO	2.1
1	A	273	LEU	2.1
2	B	336	ARG	2.1
2	B	309	LYS	2.1
2	B	308	ARG	2.1
1	A	673	PRO	2.0
1	A	325	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

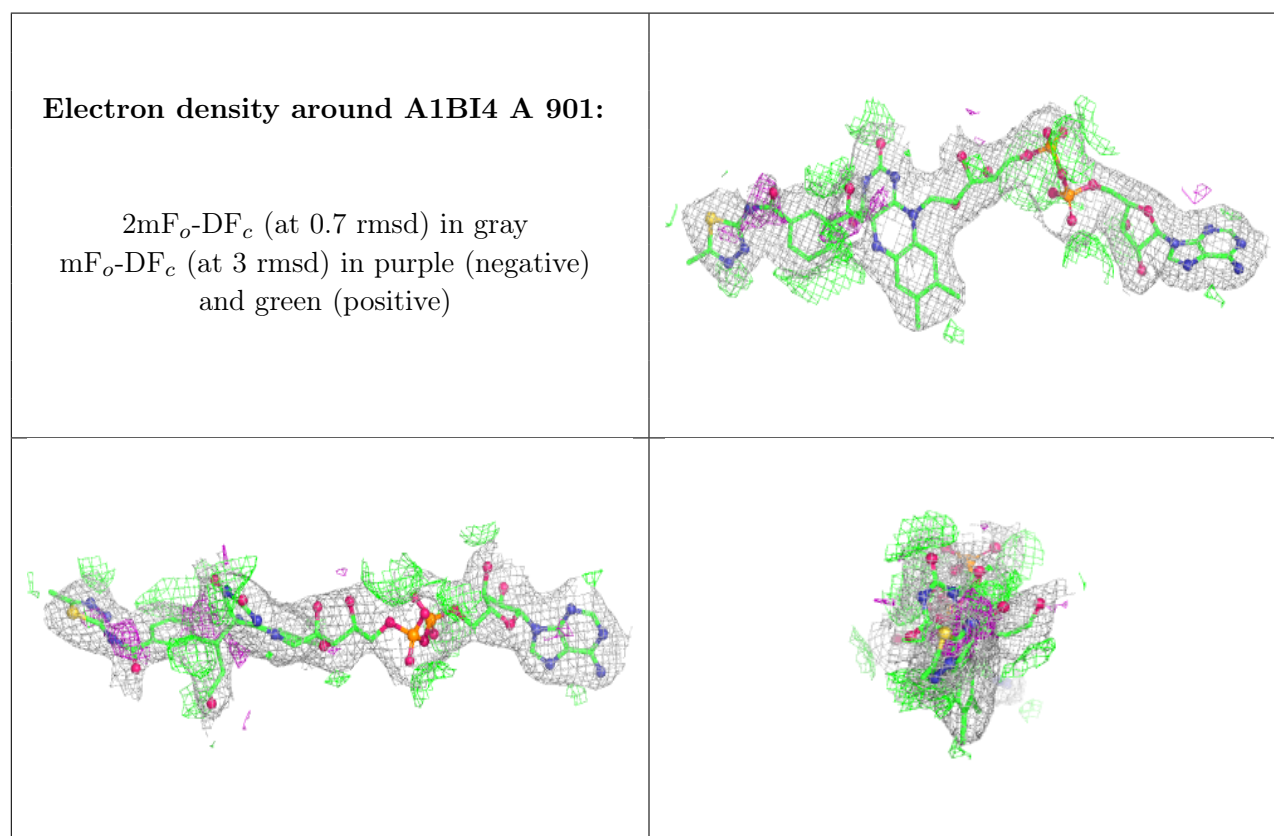
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1BI4	A	901	72/72	0.96	0.10	45,61,112,127	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.