Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2025 – 10:18 am BST

PDB ID	:	9F0A / pdb_00009f0a
Title	:	N5 Adduct of LSD1-CoREST in complex with MC4455
Authors	:	Barone, M.; Mattevi, A.
Deposited on	:	2024-04-15
Resolution	:	3.36 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:

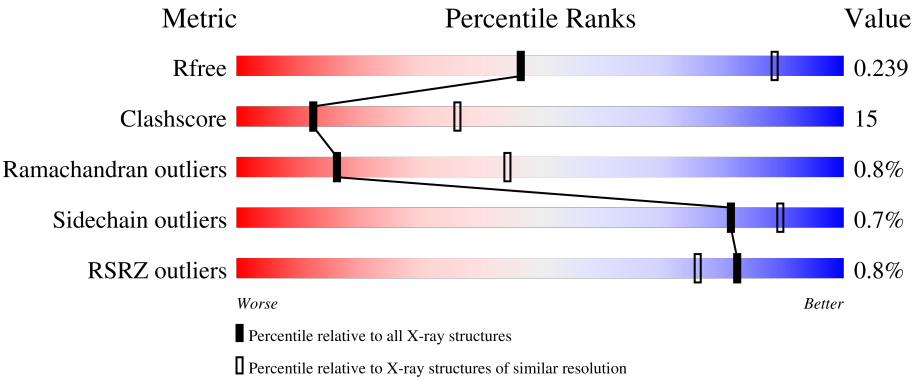
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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}	164625	1012 (3.40-3.32)
Clashscore	180529	1035 (3.40-3.32)
Ramachandran outliers	177936	1037 (3.40-3.32)
Sidechain outliers	177891	1037 (3.40-3.32)
RSRZ outliers	164620	1012 (3.40-3.32)

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 <=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	730	% 63% 26% . 9%
2	B	178	% 48% 23% . . 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6380 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.

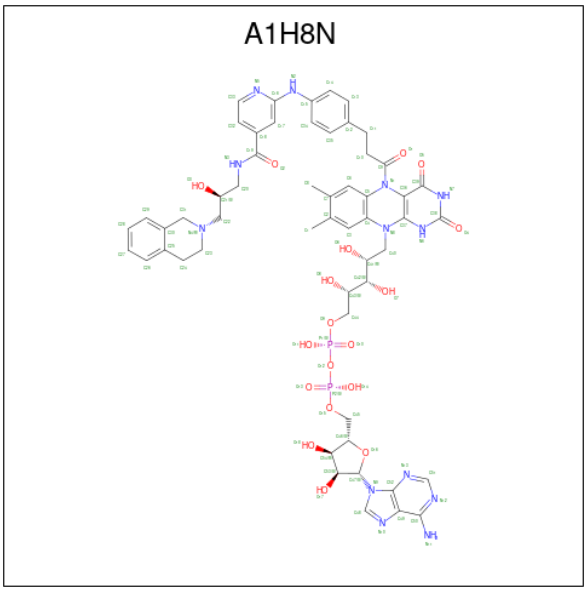
- Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

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

- 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			

- Molecule 3 is [[(2 {S},3 {R},4 {S},5 {S})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {S},3 {S},4 {R})-5-[5-[3-[4-[[4-[[(2 {S})-3-(3,4-dihydro-1 {H}-isoquinolin-2-yl)-2-oxidanyl-propyl]carbamoyl]pyridin-2-yl]amino]phenyl]propanoyl]-7,8 -dimethyl-2,4-bis(oxidanylidene)-4 {a} {H}-benzo[g]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] hydrogen phosphate (CCD ID: A1H8N) (formula: $C_{54}H_{63}N_{13}O_{18}P_2$) (labeled as "Ligand of Interest" by depositor).

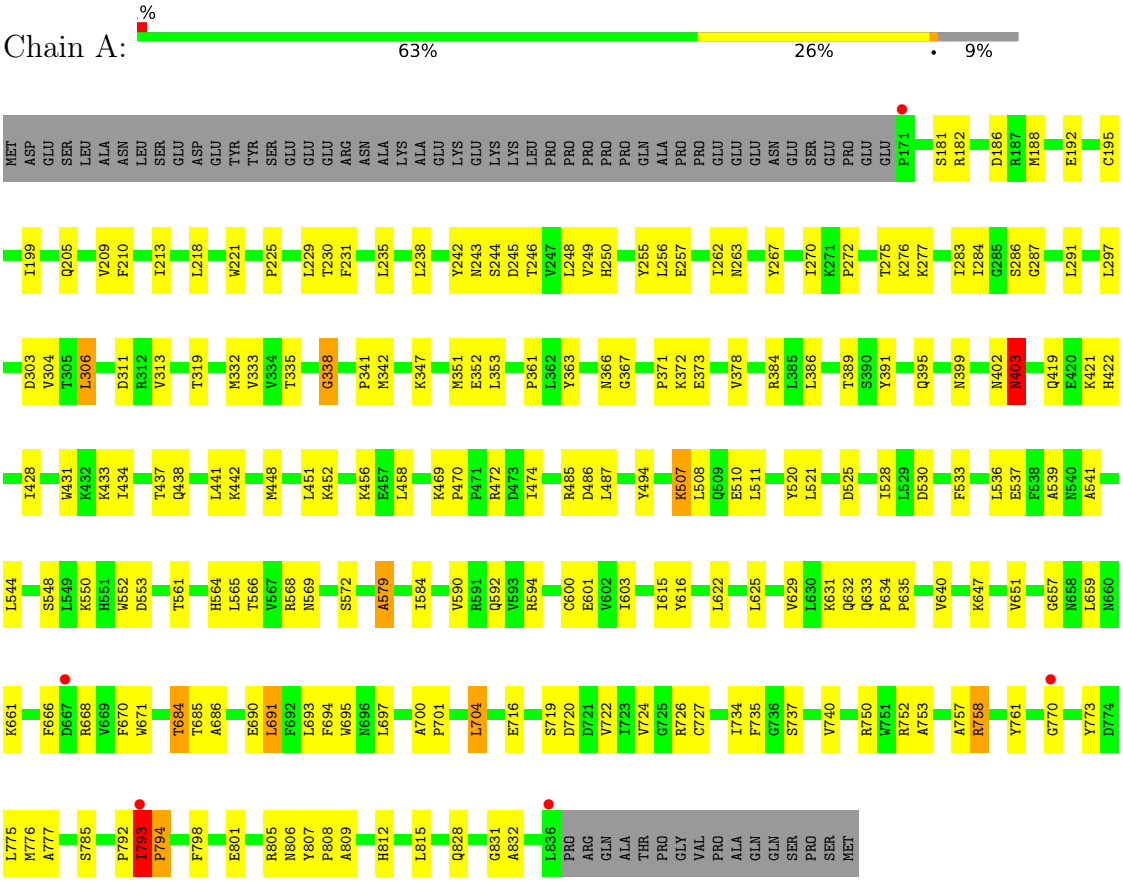


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			87	54	13	18	2		

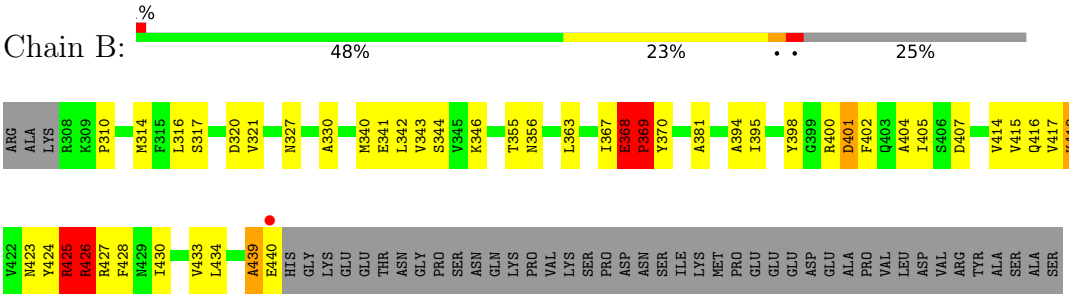
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lysine-specific histone demethylase 1A



• Molecule 2: REST corepressor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.44Å 179.77Å 234.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.67 – 3.36 71.67 – 3.36	Depositor EDS
% Data completeness (in resolution range)	98.8 (71.67-3.36) 98.9 (71.67-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.199 , 0.234 0.204 , 0.239	Depositor DCC
R_{free} test set	34071 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å^2)	114.6	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 101.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6380	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1H8N

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	0.61	3/5331 (0.1%)	0.91	19/7232 (0.3%)
2	B	0.57	1/1091 (0.1%)	0.92	6/1471 (0.4%)
All	All	0.60	4/6422 (0.1%)	0.91	25/8703 (0.3%)

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	6
2	B	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	794	PRO	N-CD	18.00	1.73	1.47
2	B	369	PRO	N-CD	9.42	1.61	1.47
1	A	600	CYS	CB-SG	-5.75	1.72	1.81
1	A	195	CYS	CB-SG	-5.37	1.73	1.81

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	831	GLY	N-CA-C	13.92	147.90	113.10
1	A	403	ASN	CB-CA-C	-13.01	84.39	110.40
1	A	793	ILE	CB-CA-C	-11.03	89.55	111.60
1	A	794	PRO	CA-N-CD	-10.55	96.73	111.50
2	B	368	GLU	CB-CA-C	-10.33	89.75	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	794	PRO	N-CA-CB	9.95	115.24	103.30
2	B	368	GLU	C-N-CD	-9.40	99.93	120.60
2	B	369	PRO	N-CA-C	-8.90	88.95	112.10
2	B	439	ALA	N-CA-C	-8.49	88.09	111.00
1	A	579	ALA	CB-CA-C	7.76	121.75	110.10
1	A	338	GLY	N-CA-C	-7.66	93.95	113.10
1	A	691	LEU	CA-CB-CG	-7.60	97.82	115.30
1	A	794	PRO	N-CA-C	-7.57	92.43	112.10
1	A	832	ALA	N-CA-CB	6.84	119.68	110.10
1	A	777	ALA	N-CA-C	6.70	129.08	111.00
1	A	737	SER	CB-CA-C	6.68	122.80	110.10
1	A	507	LYS	CB-CA-C	6.46	123.32	110.40
2	B	418	LYS	CD-CE-NZ	-6.09	97.68	111.70
1	A	777	ALA	N-CA-CB	-5.91	101.83	110.10
2	B	401	ASP	N-CA-C	-5.86	95.17	111.00
1	A	815	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	373	GLU	CB-CA-C	-5.35	99.71	110.40
1	A	704	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	539	ALA	N-CA-CB	5.07	117.19	110.10
1	A	306	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	403	ASN	Peptide
1	A	684	THR	Peptide
1	A	758	ARG	Sidechain
1	A	792	PRO	Peptide
1	A	793	ILE	Peptide,Mainchain
2	B	425	ARG	Sidechain
2	B	426	ARG	Sidechain

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	154	0
2	B	1076	0	1091	55	0
3	A	87	0	0	2	0
All	All	6380	0	6343	191	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 15.

All (191) 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:794:PRO:N	1:A:794:PRO:CD	1.73	1.26
1:A:507:LYS:O	1:A:510:GLU:HB3	1.48	1.12
2:B:439:ALA:O	2:B:440:GLU:HB2	1.69	0.91
1:A:243:ASN:O	1:A:243:ASN:OD1	1.91	0.88
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.63	0.79
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.67	0.77
1:A:366:ASN:OD1	1:A:367:GLY:N	2.18	0.76
2:B:340:MET:O	2:B:341:GLU:C	2.26	0.74
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.22	0.74
2:B:421:PHE:HE1	2:B:434:LEU:HD11	1.54	0.71
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.72	0.70
1:A:386:LEU:O	1:A:389:THR:OG1	2.07	0.69
1:A:371:PRO:O	1:A:372:LYS:C	2.31	0.68
1:A:494:TYR:CD1	2:B:367:ILE:HG12	2.30	0.67
1:A:647:LYS:HE3	1:A:798:PHE:CE2	2.29	0.67
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.76	0.67
2:B:426:ARG:HG3	2:B:427:ARG:N	2.11	0.66
1:A:335:THR:HA	1:A:564:HIS:CD2	2.31	0.65
2:B:418:LYS:HD2	2:B:418:LYS:N	2.12	0.64
1:A:287:GLY:HA3	3:A:901:A1H8N:O15	1.97	0.64
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.80	0.64
1:A:243:ASN:O	1:A:243:ASN:CG	2.36	0.63
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.15	0.63
1:A:437:THR:HG23	1:A:508:LEU:HD21	1.81	0.63
2:B:424:TYR:O	2:B:425:ARG:C	2.36	0.63
2:B:439:ALA:O	2:B:440:GLU:CB	2.47	0.63
1:A:657:GLY:HA2	1:A:752:ARG:HH22	1.64	0.62
1:A:750:ARG:HB3	1:A:753:ALA:HB3	1.80	0.62
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.82	0.62
1:A:230:THR:HG23	1:A:270:ILE:HD12	1.82	0.61
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HE3	1:A:661:LYS:HZ2	1.67	0.60
1:A:536:LEU:HB3	1:A:544:LEU:HD21	1.82	0.60
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.37	0.60
1:A:277:LYS:HE3	1:A:303:ASP:HA	1.84	0.59
1:A:594:ARG:HA	1:A:640:VAL:O	2.02	0.59
1:A:448:MET:HE1	2:B:363:LEU:HD13	1.85	0.59
2:B:368:GLU:H	2:B:369:PRO:CD	2.16	0.58
1:A:428:ILE:HD11	2:B:341:GLU:HB3	1.85	0.58
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.67	0.58
1:A:720:ASP:O	1:A:724:VAL:HG23	2.04	0.58
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.84	0.58
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.19	0.58
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.39	0.57
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.86	0.57
2:B:341:GLU:O	2:B:344:SER:HB3	2.04	0.57
1:A:275:THR:HG23	1:A:276:LYS:HE3	1.86	0.56
1:A:311:ASP:N	1:A:311:ASP:OD1	2.28	0.56
1:A:693:LEU:HD12	1:A:694:PHE:N	2.21	0.56
1:A:332:MET:CE	1:A:661:LYS:NZ	2.69	0.56
2:B:369:PRO:HD2	2:B:370:TYR:HD1	1.70	0.56
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.68	0.56
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.88	0.55
1:A:548:SER:O	1:A:552:TRP:HB3	2.06	0.55
1:A:332:MET:CE	1:A:661:LYS:HZ2	2.20	0.55
2:B:426:ARG:CG	2:B:427:ARG:N	2.70	0.54
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.43	0.54
1:A:530:ASP:OD2	1:A:685:THR:HA	2.08	0.53
1:A:458:LEU:HB3	1:A:487:LEU:HD13	1.90	0.53
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.72	0.53
2:B:368:GLU:N	2:B:369:PRO:CD	2.72	0.53
1:A:255:TYR:CD1	1:A:256:LEU:HD23	2.43	0.53
1:A:351:MET:HA	1:A:569:ASN:HD21	1.73	0.53
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.44	0.53
1:A:693:LEU:HD12	1:A:694:PHE:H	1.74	0.52
2:B:342:LEU:HD21	2:B:346:LYS:HD2	1.91	0.52
2:B:368:GLU:H	2:B:369:PRO:HD3	1.75	0.52
1:A:205:GLN:O	1:A:209:VAL:HG23	2.10	0.52
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.91	0.52
1:A:485:ARG:HG3	2:B:407:ASP:HB2	1.92	0.51
1:A:319:THR:HB	1:A:572:SER:HB3	1.92	0.51
1:A:428:ILE:HD13	2:B:341:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HG12	1:A:622:LEU:HB3	1.93	0.51
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.93	0.51
2:B:394:ALA:O	2:B:398:TYR:HB2	2.11	0.51
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.47	0.50
2:B:340:MET:O	2:B:343:VAL:N	2.44	0.50
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.94	0.50
1:A:243:ASN:OD1	1:A:243:ASN:C	2.50	0.50
1:A:684:THR:HG22	1:A:685:THR:N	2.27	0.50
2:B:369:PRO:HD2	2:B:370:TYR:CD1	2.47	0.49
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.93	0.49
1:A:297:LEU:HB2	1:A:304:VAL:HG21	1.93	0.49
1:A:399:ASN:ND2	1:A:550:LYS:HE2	2.26	0.49
1:A:456:LYS:HA	2:B:370:TYR:HE2	1.73	0.49
1:A:456:LYS:HA	2:B:370:TYR:CD2	2.47	0.49
1:A:485:ARG:HD2	2:B:404:ALA:HA	1.95	0.49
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.48	0.49
2:B:342:LEU:O	2:B:343:VAL:C	2.47	0.49
1:A:238:LEU:HD22	1:A:242:TYR:HB2	1.93	0.49
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.95	0.48
1:A:533:PHE:O	1:A:537:GLU:HG3	2.13	0.48
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.79	0.48
1:A:363:TYR:CD2	1:A:734:ILE:HG12	2.48	0.48
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.70	0.48
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.49	0.48
1:A:775:LEU:O	1:A:776:MET:C	2.53	0.48
2:B:368:GLU:HB2	2:B:369:PRO:HD3	1.96	0.48
1:A:521:LEU:HB3	1:A:525:ASP:HB2	1.95	0.47
1:A:719:SER:OG	1:A:722:VAL:HG23	2.15	0.47
1:A:793:ILE:O	1:A:793:ILE:HG22	2.12	0.47
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.50	0.47
1:A:494:TYR:CD1	1:A:494:TYR:O	2.68	0.47
2:B:317:SER:O	2:B:321:VAL:HG23	2.14	0.47
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.45	0.47
2:B:414:VAL:O	2:B:417:VAL:HB	2.15	0.47
1:A:235:LEU:HD21	1:A:246:THR:HG22	1.96	0.47
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.55	0.47
1:A:332:MET:HE3	1:A:661:LYS:NZ	2.27	0.46
1:A:378:VAL:HG11	1:A:528:ILE:HG22	1.97	0.46
1:A:632:GLN:O	1:A:633:GLN:NE2	2.48	0.46
2:B:367:ILE:HG13	2:B:367:ILE:O	2.15	0.46
1:A:625:LEU:HD22	1:A:629:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:PRO:HB3	2:B:316:LEU:HD12	1.98	0.46
1:A:352:GLU:HB3	1:A:568:ARG:HB2	1.97	0.46
1:A:647:LYS:O	1:A:651:VAL:HG23	2.16	0.45
2:B:400:ARG:O	2:B:401:ASP:C	2.53	0.45
1:A:441:LEU:HB3	2:B:356:ASN:ND2	2.31	0.45
1:A:770:GLY:O	1:A:773:TYR:HB2	2.16	0.45
1:A:770:GLY:O	1:A:805:ARG:HG3	2.16	0.45
1:A:333:VAL:HA	1:A:565:LEU:O	2.15	0.45
1:A:601:GLU:HA	1:A:616:TYR:O	2.17	0.45
1:A:801:GLU:HG2	1:A:809:ALA:H	1.82	0.45
2:B:425:ARG:O	2:B:428:PHE:N	2.49	0.44
1:A:255:TYR:CE1	1:A:256:LEU:HD23	2.52	0.44
2:B:415:VAL:HA	2:B:418:LYS:HG2	1.99	0.44
1:A:684:THR:HG22	1:A:685:THR:H	1.82	0.44
1:A:419:GLN:HB3	1:A:520:TYR:CE1	2.53	0.44
2:B:402:PHE:CG	2:B:418:LYS:NZ	2.82	0.44
2:B:423:ASN:O	2:B:426:ARG:NH2	2.50	0.44
1:A:244:SER:OG	1:A:245:ASP:N	2.51	0.44
1:A:695:TRP:HB3	1:A:697:LEU:HG	1.99	0.44
1:A:181:SER:OG	1:A:218:LEU:HD22	2.17	0.44
1:A:438:GLN:OE1	1:A:508:LEU:HD13	2.17	0.44
1:A:448:MET:CE	2:B:363:LEU:HD13	2.47	0.44
1:A:541:ALA:HB2	1:A:659:LEU:HD23	2.00	0.43
1:A:670:PHE:CE1	1:A:740:VAL:HG22	2.53	0.43
2:B:430:ILE:HG22	2:B:434:LEU:HD12	1.98	0.43
1:A:552:TRP:CE2	1:A:553:ASP:HB3	2.52	0.43
1:A:284:ILE:HD13	1:A:590:VAL:HG11	1.99	0.43
1:A:391:TYR:CD2	1:A:395:GLN:HG3	2.54	0.43
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.34	0.43
1:A:494:TYR:CE1	2:B:367:ILE:HG12	2.54	0.43
1:A:209:VAL:HG12	1:A:213:ILE:HD11	2.01	0.43
1:A:257:GLU:HG3	1:A:263:ASN:HD22	1.84	0.43
2:B:381:ALA:HA	2:B:416:GLN:NE2	2.33	0.43
1:A:402:ASN:O	1:A:403:ASN:C	2.57	0.43
1:A:452:LYS:O	1:A:456:LYS:HB2	2.19	0.43
1:A:806:ASN:C	1:A:807:TYR:CD1	2.92	0.43
1:A:448:MET:HB3	1:A:448:MET:HE2	1.77	0.42
1:A:451:LEU:HD23	1:A:494:TYR:HB2	2.01	0.42
1:A:684:THR:HG22	1:A:686:ALA:H	1.84	0.42
1:A:186:ASP:N	1:A:186:ASP:OD1	2.52	0.42
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:PRO:HA	1:A:635:PRO:HD3	1.79	0.42
1:A:793:ILE:HA	1:A:794:PRO:HD3	2.01	0.42
1:A:633:GLN:HA	1:A:634:PRO:HA	1.74	0.42
1:A:793:ILE:C	1:A:794:PRO:CD	2.70	0.42
1:A:632:GLN:OE1	1:A:758:ARG:NH2	2.52	0.42
1:A:192:GLU:HG3	1:A:255:TYR:OH	2.19	0.42
1:A:270:ILE:O	1:A:272:PRO:HD3	2.20	0.42
1:A:286:SER:HB2	1:A:291:LEU:HD21	2.01	0.42
3:A:901:A1H8N:C17	3:A:901:A1H8N:C20	2.97	0.42
2:B:394:ALA:HB1	2:B:405:ILE:HG12	2.02	0.42
1:A:221:TRP:CZ3	1:A:225:PRO:HA	2.55	0.42
1:A:521:LEU:HB3	1:A:525:ASP:CB	2.50	0.42
1:A:794:PRO:HD2	1:A:828:GLN:OE1	2.20	0.42
1:A:451:LEU:HA	1:A:451:LEU:HD12	1.78	0.41
1:A:776:MET:HB3	1:A:776:MET:HE3	1.87	0.41
1:A:603:ILE:HG12	1:A:615:ILE:HD13	2.03	0.41
1:A:229:LEU:HD12	1:A:229:LEU:HA	1.89	0.41
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.56	0.41
1:A:666:PHE:O	1:A:701:PRO:CG	2.69	0.41
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.63	0.41
1:A:631:LYS:HE2	1:A:651:VAL:O	2.20	0.41
2:B:425:ARG:HA	2:B:430:ILE:CG1	2.51	0.41
1:A:433:LYS:O	1:A:437:THR:HG22	2.21	0.41
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.88	0.41
1:A:291:LEU:HD22	1:A:579:ALA:HB2	2.03	0.41
1:A:338:GLY:HA3	1:A:561:THR:O	2.21	0.41
1:A:421:LYS:NZ	2:B:320:ASP:OD1	2.54	0.41
1:A:472:ARG:H	1:A:472:ARG:HG2	1.72	0.41
1:A:225:PRO:HG2	1:A:347:LYS:HD3	2.02	0.41
2:B:415:VAL:O	2:B:418:LYS:HG2	2.21	0.41
2:B:425:ARG:HA	2:B:430:ILE:HG13	2.03	0.40
1:A:372:LYS:H	1:A:372:LYS:HG2	1.67	0.40
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.56	0.40
1:A:431:TRP:CE3	1:A:434:ILE:HD12	2.56	0.40
1:A:428:ILE:HD13	2:B:341:GLU:CG	2.50	0.40
1:A:419:GLN:NE2	2:B:314:MET:HA	2.37	0.40
1:A:566:THR:HG21	1:A:697:LEU:HD13	2.03	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	664/730 (91%)	605 (91%)	57 (9%)	2 (0%)	37 65
2	B	131/178 (74%)	111 (85%)	16 (12%)	4 (3%)	3 18
All	All	795/908 (88%)	716 (90%)	73 (9%)	6 (1%)	16 44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	369	PRO
2	B	425	ARG
1	A	785	SER
2	B	426	ARG
1	A	757	ALA
2	B	368	GLU

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	566/623 (91%)	561 (99%)	5 (1%)	75 87
2	B	117/156 (75%)	117 (100%)	0	100 100
All	All	683/779 (88%)	678 (99%)	5 (1%)	81 89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	HIS
1	A	267	TYR
1	A	313	VAL
1	A	422	HIS
1	A	668	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	ASN
1	A	564	HIS

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	A1H8N	A	901	-	90,96,96	0.72	1 (1%)	111,142,142	1.50	13 (11%)

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	A1H8N	A	901	-	-	20/56/85/85	0/10/10/10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	A1H8N	C38-N6	2.38	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	A1H8N	C21-C20-N3	6.10	129.30	111.37
3	A	901	A1H8N	N2-C16-N5	4.65	131.02	116.81
3	A	901	A1H8N	C11-C10-C9	4.36	117.54	112.34
3	A	901	A1H8N	C17-C16-N2	-4.13	107.13	120.24
3	A	901	A1H8N	C36-C39-N7	3.83	117.74	110.99
3	A	901	A1H8N	C10-C11-C12	-3.34	100.49	112.70
3	A	901	A1H8N	C30-C31-N4	3.26	115.98	112.14
3	A	901	A1H8N	C47-N9-C52	3.00	131.91	126.64
3	A	901	A1H8N	O18-C54-C46	2.75	118.99	111.05
3	A	901	A1H8N	O16-C46-C54	-2.35	100.47	105.11
3	A	901	A1H8N	C21-C22-N4	2.16	116.15	112.23
3	A	901	A1H8N	C32-C18-C19	2.14	127.56	120.62
3	A	901	A1H8N	O1-C9-N1	2.04	122.63	120.31

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	A1H8N	C10-C9-N1-C5
3	A	901	A1H8N	C10-C9-N1-C36
3	A	901	A1H8N	O1-C9-N1-C5
3	A	901	A1H8N	O1-C9-N1-C36
3	A	901	A1H8N	O2-C19-N3-C20
3	A	901	A1H8N	C20-C21-C22-N4
3	A	901	A1H8N	O3-C21-C22-N4
3	A	901	A1H8N	C44-O9-P1-O10
3	A	901	A1H8N	C18-C19-N3-C20

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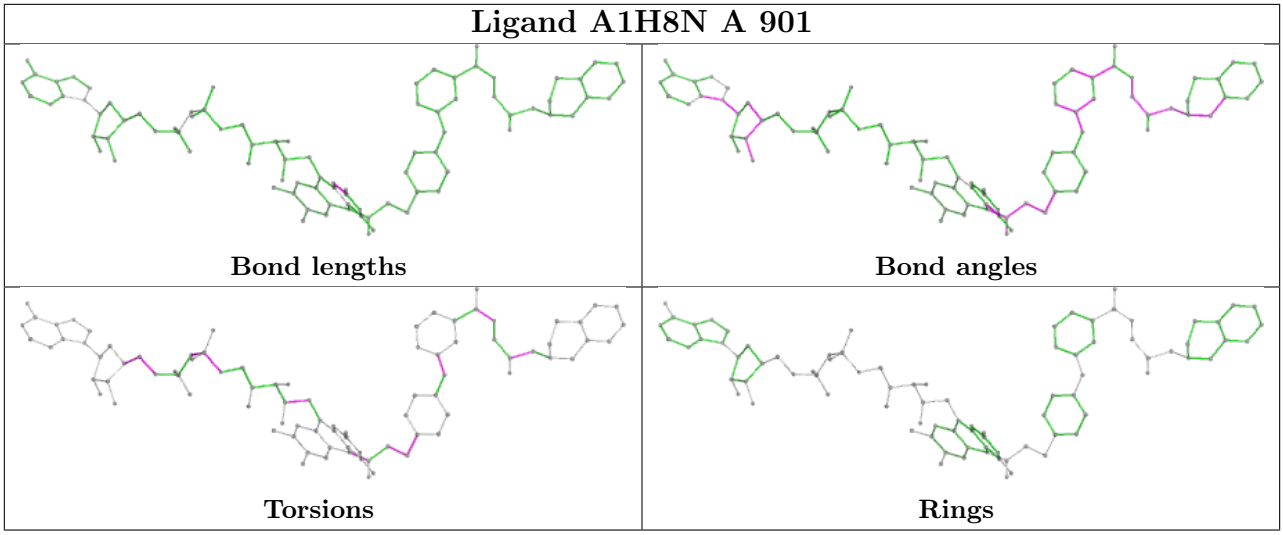
Mol	Chain	Res	Type	Atoms
3	A	901	A1H8N	C9-C10-C11-C12
3	A	901	A1H8N	P2-O12-P1-O9
3	A	901	A1H8N	C46-C45-O15-P2
3	A	901	A1H8N	N8-C40-C41-O6
3	A	901	A1H8N	N5-C16-N2-C15
3	A	901	A1H8N	C17-C16-N2-C15
3	A	901	A1H8N	C10-C11-C12-C13
3	A	901	A1H8N	C44-O9-P1-O12
3	A	901	A1H8N	C10-C11-C12-C35
3	A	901	A1H8N	O15-C45-C46-O16
3	A	901	A1H8N	C44-O9-P1-O11

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	A1H8N	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	666/730 (91%)	-0.22	5 (0%)	82	76	72, 110, 142, 165	0
2	B	133/178 (74%)	-0.01	1 (0%)	82	76	106, 137, 158, 176	0
All	All	799/908 (87%)	-0.19	6 (0%)	82	76	72, 116, 148, 176	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	4.4
1	A	793	ILE	3.5
1	A	171	PRO	3.4
1	A	770	GLY	2.6
2	B	440	GLU	2.2
1	A	667	ASP	2.2

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

There are no monosaccharides in this entry.

6.4 Ligands

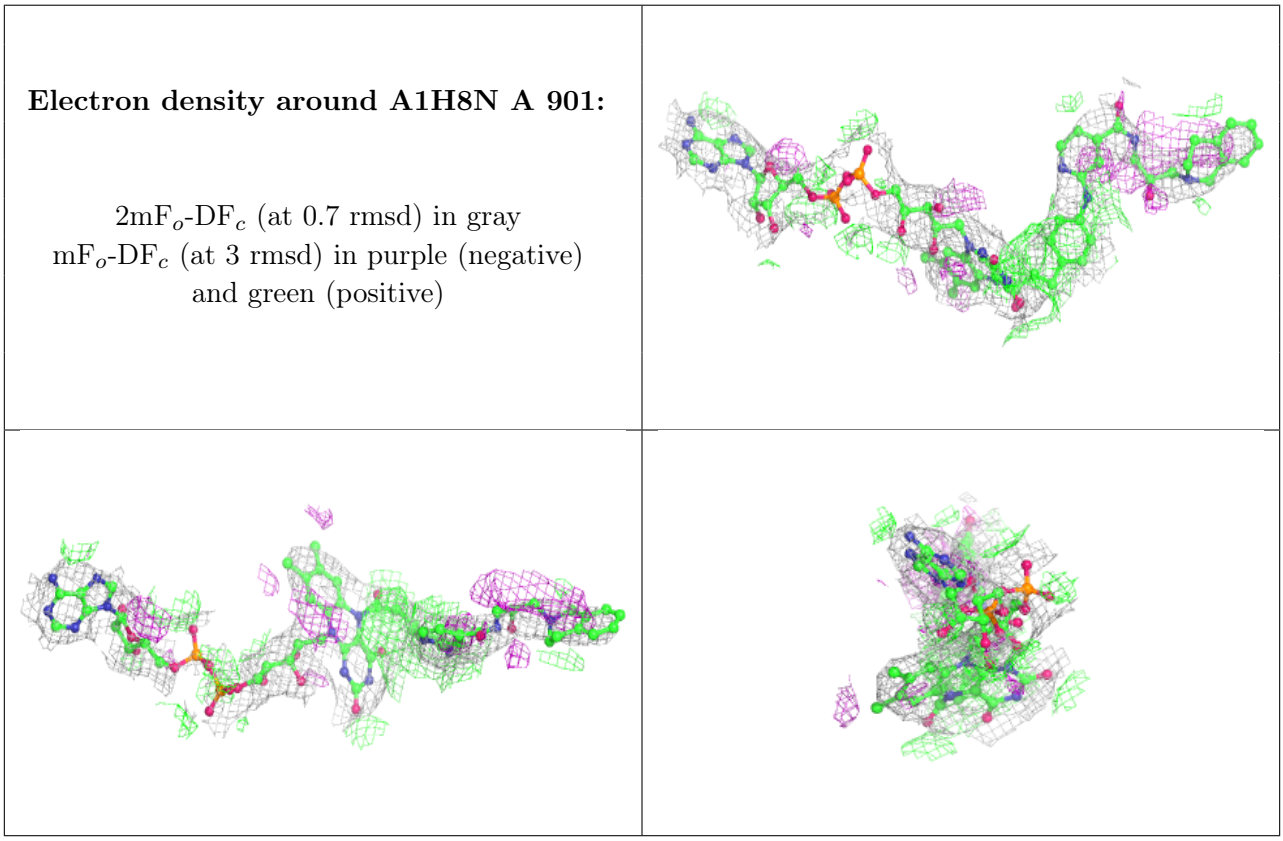
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	A1H8N	A	901	87/87	0.92	0.16	79,98,145,147	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.

Electron density around A1H8N A 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.