WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2023 – 12:34 AM EDT

PDB ID	:	3W2V
Title	:	Crystal structure of the Cmr2dHD-Cmr3 subcomplex bound to 3'-AMP
Authors	:	Numata, T.; Osawa, T.
Deposited on	:	2012-12-06
Resolution	:	2.60 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36
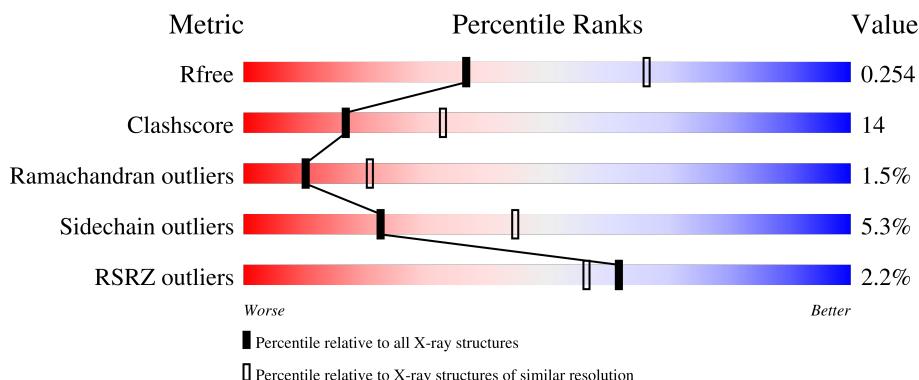
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
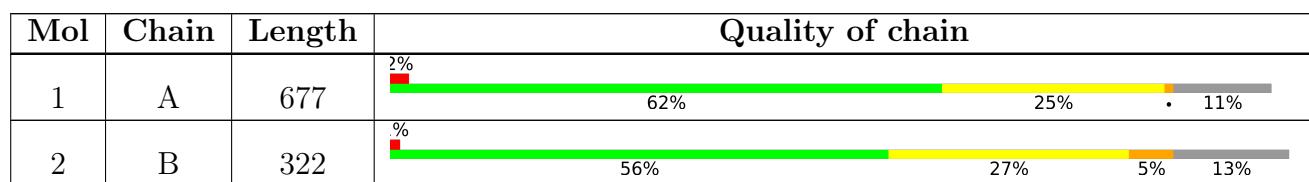
The reported resolution of this entry is 2.60 Å.

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	Percentile Ranks	Value
Rfree		0.254
Clashscore		14
Ramachandran outliers		1.5%
Sidechain outliers		5.3%
RSRZ outliers		2.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	677	2% / 62% 25% · 11%
2	B	322	% / 56% 27% 5% 13%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7096 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 CRISPR system Cmr subunit Cmr2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	602	4832	3128	806	886	12	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	MET	-	expression tag	UNP Q8U1S6
A	196	GLY	-	expression tag	UNP Q8U1S6
A	197	SER	-	expression tag	UNP Q8U1S6
A	198	SER	-	expression tag	UNP Q8U1S6
A	199	HIS	-	expression tag	UNP Q8U1S6
A	200	HIS	-	expression tag	UNP Q8U1S6
A	201	HIS	-	expression tag	UNP Q8U1S6
A	202	HIS	-	expression tag	UNP Q8U1S6
A	203	HIS	-	expression tag	UNP Q8U1S6
A	204	HIS	-	expression tag	UNP Q8U1S6
A	205	SER	-	expression tag	UNP Q8U1S6
A	206	SER	-	expression tag	UNP Q8U1S6
A	207	GLY	-	expression tag	UNP Q8U1S6
A	208	LEU	-	expression tag	UNP Q8U1S6
A	209	VAL	-	expression tag	UNP Q8U1S6
A	210	PRO	-	expression tag	UNP Q8U1S6
A	211	ARG	-	expression tag	UNP Q8U1S6
A	212	GLY	-	expression tag	UNP Q8U1S6
A	213	SER	-	expression tag	UNP Q8U1S6
A	214	HIS	-	expression tag	UNP Q8U1S6
A	215	MET	-	expression tag	UNP Q8U1S6
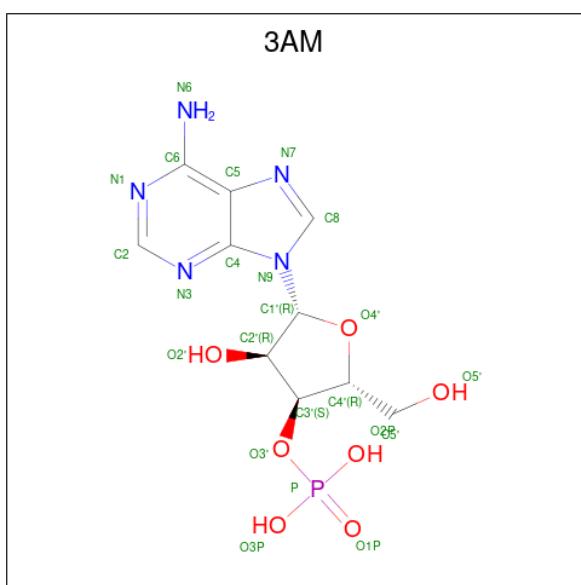
- Molecule 2 is a protein called CRISPR system Cmr subunit Cmr3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	281	Total 2214	C 1454	N 350	O 406	S 4	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl] dihydrogen phosphate (three-letter code: 3AM) (formula: $C_{10}H_{14}N_5O_7P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
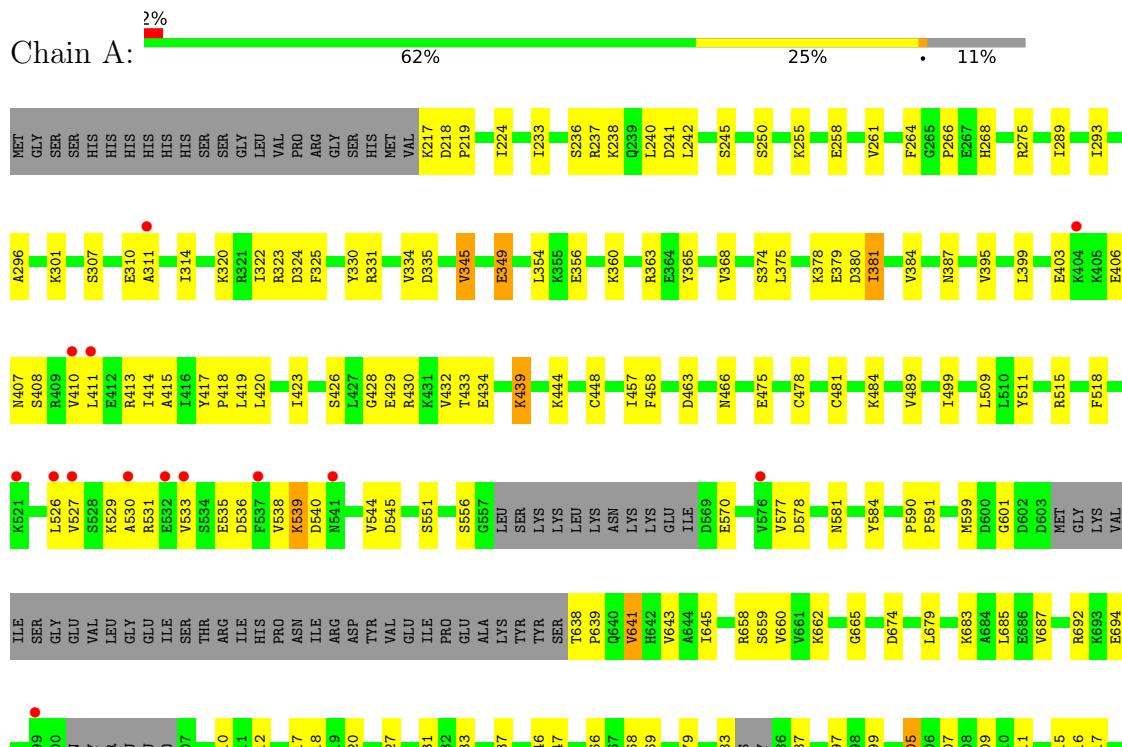
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total 19	O 19	0	0
5	B	7	Total 7	O 7	0	0
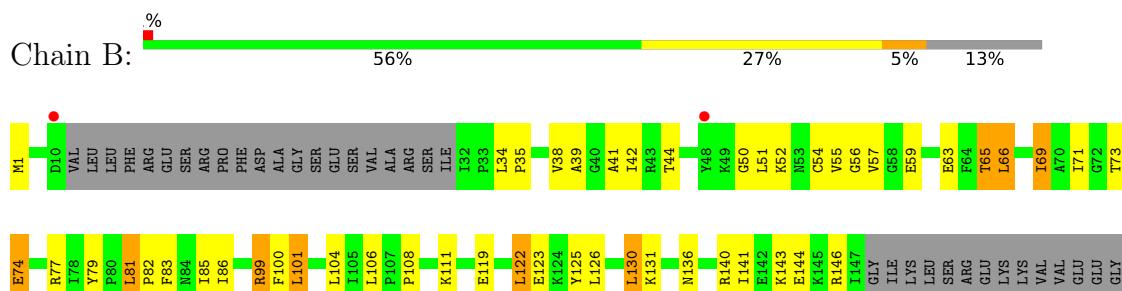
3 Residue-property plots ⓘ
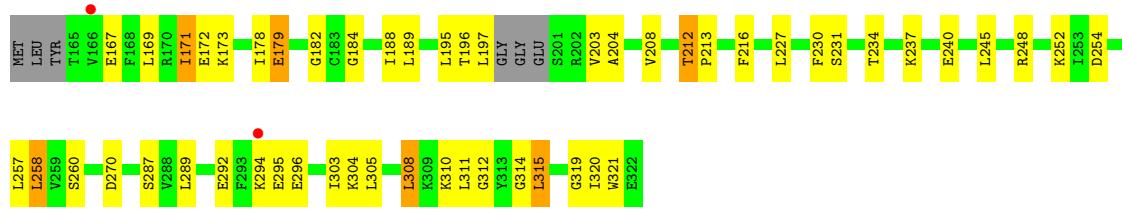
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR system Cmr subunit Cmr2

Chain A:

• Molecule 2: CRISPR system Cmr subunit Cmr3

Chain B:

MET LEU TYR T165 V166 E167 F168 L169 R170 I171 E172 K173 I178 E179 G182 C183 G184 I188 L189 L195 T196 L197 GLY GLY GLU S201 R202 V203 A204 V208 T212 P213 F216 L227 F230 S231 T234 K237 E240 L245 R248 K252 I253 D254

L257 L258 V259 S260 D270 S287 V288 L289 E292 F293 K294 E295 E296 I303 K304 L305 L308 K309 K310 L311 G312 Y313 G314 L315 G319 I320 W321 E322

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	103.94Å 136.67Å 191.97Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	41.73 – 2.60	Depositor
	41.72 – 2.60	EDS
% Data completeness	99.5 (41.73-2.60)	Depositor
(in resolution range)	99.6 (41.72-2.60)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.82 (at 2.61Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.259	Depositor
	0.209 , 0.254	DCC
R_{free} test set	2077 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.1	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7096	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: 3AM, ZN

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	0.38	0/4929	0.59	0/6660
2	B	0.39	0/2262	0.64	1/3054 (0.0%)
All	All	0.38	0/7191	0.61	1/9714 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	81	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4832	0	4825	127	0
2	B	2214	0	2265	77	0
3	A	1	0	0	0	0
4	A	23	0	12	0	0
5	A	19	0	0	1	0
5	B	7	0	0	0	0
All	All	7096	0	7102	200	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 14.

All (200) 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:577:VAL:HG12	1:A:581:ASN:HD21	1.33	0.90
1:A:805:VAL:HG13	1:A:809:GLU:HB3	1.58	0.85
1:A:816:ILE:HG23	1:A:831:ARG:NH1	1.94	0.83
2:B:71:ILE:HD12	2:B:171:ILE:HD11	1.63	0.80
1:A:448:CYS:HB2	1:A:478:CYS:HB3	1.64	0.78
1:A:849:ASN:OD1	1:A:851:VAL:HG22	1.82	0.78
2:B:195:LEU:HD23	2:B:196:THR:N	1.99	0.77
2:B:230:PHE:HD1	2:B:234:THR:HG21	1.50	0.76
1:A:638:THR:O	1:A:641:VAL:HG22	1.87	0.75
1:A:769:ARG:HB3	1:A:769:ARG:HH11	1.51	0.74
2:B:140:ARG:HG3	2:B:140:ARG:HH11	1.52	0.74
1:A:380:ASP:O	1:A:384:VAL:HG23	1.89	0.73
2:B:237:LYS:HB2	2:B:240:GLU:HG3	1.70	0.73
1:A:665:GLY:HA3	1:A:679:LEU:HD23	1.71	0.72
1:A:577:VAL:HG12	1:A:581:ASN:ND2	2.04	0.71
2:B:308:LEU:HG	2:B:311:LEU:HD12	1.72	0.71
1:A:381:ILE:HG23	1:A:399:LEU:HD22	1.72	0.70
2:B:230:PHE:CD1	2:B:234:THR:HG21	2.26	0.70
2:B:143:LYS:HD3	2:B:169:LEU:HD23	1.74	0.70
1:A:718:HIS:HD2	1:A:720:LYS:H	1.40	0.69
1:A:531:ARG:HD3	1:A:535:GLU:OE1	1.93	0.68
1:A:779:LYS:O	1:A:783:GLU:HG2	1.93	0.68
2:B:234:THR:HG22	2:B:314:GLY:HA2	1.77	0.67
2:B:65:THR:HG23	2:B:179:GLU:HB3	1.77	0.66
1:A:864:ILE:HD12	1:A:865:THR:HG23	1.78	0.66
2:B:99:ARG:HH12	2:B:292:GLU:CD	1.98	0.66
1:A:322:ILE:HD12	1:A:368:VAL:HG21	1.76	0.65
1:A:578:ASP:HA	1:A:581:ASN:HD22	1.59	0.65
2:B:172:GLU:HG2	2:B:173:LYS:HG2	1.78	0.65
1:A:233:ILE:HG23	1:A:242:LEU:HD12	1.79	0.65
1:A:601:GLY:HA2	1:A:710:LEU:HD12	1.77	0.64
1:A:538:VAL:HG12	1:A:539:LYS:N	2.11	0.64
1:A:331:ARG:O	1:A:334:VAL:HG22	1.98	0.63
1:A:417:TYR:HB3	1:A:418:PRO:HD3	1.79	0.63
1:A:718:HIS:CD2	1:A:720:LYS:H	2.16	0.63
2:B:195:LEU:HD23	2:B:196:THR:H	1.64	0.62
1:A:769:ARG:HB3	1:A:769:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:O	1:A:219:PRO:HD3	2.01	0.60
1:A:766:GLU:OE1	1:A:769:ARG:NH1	2.34	0.59
1:A:236:SER:HB3	1:A:241:ASP:HB2	1.84	0.59
2:B:258:LEU:HD22	2:B:260:SER:HB2	1.84	0.59
1:A:816:ILE:HA	1:A:831:ARG:HD3	1.84	0.58
2:B:208:VAL:HG23	2:B:208:VAL:O	2.03	0.58
2:B:52:LYS:O	2:B:55:VAL:HG12	2.04	0.57
1:A:822:ARG:HG3	1:A:826:GLU:OE2	2.05	0.57
1:A:381:ILE:CG2	1:A:399:LEU:HD22	2.35	0.57
2:B:82:PRO:HD2	2:B:85:ILE:HD12	1.87	0.57
1:A:289:ILE:HD11	1:A:293:ILE:HD13	1.85	0.57
1:A:381:ILE:HD11	1:A:411:LEU:CD1	2.33	0.57
1:A:481:CYS:O	1:A:484:LYS:HB3	2.04	0.57
2:B:184:GLY:O	2:B:188:ILE:HG12	2.05	0.56
1:A:659:SER:O	1:A:662:LYS:HG3	2.05	0.56
1:A:840:ASP:O	1:A:843:GLU:HB2	2.04	0.56
1:A:833:LYS:O	1:A:837:GLU:HG3	2.07	0.55
1:A:428:GLY:O	1:A:432:VAL:HG13	2.07	0.55
2:B:54:CYS:HA	2:B:63:GLU:HB2	1.88	0.55
1:A:399:LEU:HD21	1:A:419:LEU:CD1	2.36	0.55
1:A:381:ILE:HG22	1:A:399:LEU:HD13	1.88	0.55
2:B:38:VAL:HG11	2:B:69:ILE:HD11	1.88	0.55
1:A:387:ASN:O	2:B:99:ARG:N	2.39	0.55
1:A:426:SER:OG	2:B:108:PRO:HD3	2.07	0.54
1:A:821:GLY:H	1:A:827:THR:HB	1.72	0.54
2:B:304:LYS:O	2:B:305:LEU:HD23	2.08	0.54
1:A:811:LEU:O	1:A:815:VAL:HG23	2.07	0.54
1:A:845:VAL:HG21	1:A:857:LEU:HB2	1.90	0.54
2:B:99:ARG:NH1	2:B:292:GLU:OE1	2.40	0.54
2:B:213:PRO:HG2	2:B:216:PHE:CD2	2.42	0.53
1:A:310:GLU:O	1:A:314:ILE:HG13	2.08	0.53
1:A:331:ARG:HG2	1:A:354:LEU:CD2	2.39	0.53
2:B:140:ARG:HG3	2:B:140:ARG:NH1	2.22	0.53
2:B:125:TYR:HB2	2:B:130:LEU:HD12	1.91	0.53
1:A:379:GLU:OE2	1:A:384:VAL:HG22	2.09	0.52
1:A:539:LYS:O	1:A:540:ASP:HB2	2.08	0.52
2:B:141:ILE:HG21	2:B:169:LEU:HB3	1.90	0.52
2:B:254:ASP:OD2	2:B:294:LYS:HA	2.09	0.52
1:A:805:VAL:CG1	1:A:809:GLU:HB3	2.36	0.52
1:A:692:ARG:HD3	1:A:710:LEU:HB3	1.92	0.52
1:A:807:ILE:HD11	1:A:851:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLU:O	1:A:475:GLU:HG3	2.09	0.52
2:B:56:GLY:O	2:B:59:GLU:HB2	2.10	0.52
1:A:509:LEU:HB3	1:A:515:ARG:HB2	1.91	0.52
2:B:77:ARG:HD2	2:B:119:GLU:OE2	2.09	0.52
2:B:65:THR:CG2	2:B:179:GLU:HB3	2.39	0.51
1:A:323:ARG:HG3	1:A:363:ARG:HG3	1.93	0.51
1:A:264:PHE:HB3	1:A:268:HIS:CD2	2.46	0.51
2:B:143:LYS:HD2	2:B:167:GLU:HG2	1.91	0.51
1:A:307:SER:HB2	1:A:310:GLU:CG	2.41	0.51
2:B:141:ILE:CG2	2:B:169:LEU:HD22	2.41	0.50
1:A:374:SER:O	1:A:413:ARG:HD2	2.12	0.49
2:B:119:GLU:O	2:B:123:GLU:HG3	2.11	0.49
1:A:255:LYS:O	1:A:258:GLU:HG2	2.11	0.49
1:A:539:LYS:HE3	1:A:540:ASP:OD2	2.12	0.49
1:A:599:MET:HG2	1:A:712:ALA:HB2	1.94	0.49
1:A:658:ARG:HH11	1:A:658:ARG:HG3	1.78	0.49
1:A:783:GLU:HB3	1:A:787:VAL:HB	1.94	0.49
1:A:330:TYR:O	1:A:334:VAL:HG13	2.13	0.49
1:A:429:GLU:O	1:A:432:VAL:HG22	2.13	0.49
2:B:65:THR:HB	2:B:310:LYS:HD3	1.94	0.48
1:A:403:GLU:O	1:A:406:GLU:O	2.31	0.48
1:A:403:GLU:HG3	1:A:408:SER:O	2.13	0.48
1:A:365:TYR:HA	1:A:439:LYS:NZ	2.27	0.48
1:A:538:VAL:HG12	1:A:539:LYS:H	1.74	0.48
1:A:536:ASP:O	1:A:544:VAL:HG21	2.13	0.48
2:B:252:LYS:HG2	2:B:294:LYS:HD2	1.94	0.48
1:A:423:ILE:HG21	2:B:100:PHE:CD2	2.50	0.47
1:A:406:GLU:O	1:A:408:SER:N	2.47	0.47
1:A:410:VAL:C	1:A:411:LEU:HD23	2.34	0.47
2:B:73:THR:HB	2:B:74:GLU:OE2	2.14	0.47
2:B:141:ILE:HG22	2:B:169:LEU:HD22	1.95	0.47
1:A:237:ARG:NH2	1:A:238:LYS:HD2	2.29	0.47
2:B:79:TYR:CD2	2:B:122:LEU:HD12	2.49	0.47
1:A:733:LEU:O	1:A:737:LYS:HB2	2.15	0.47
2:B:39:ALA:HB2	2:B:66:LEU:HD12	1.97	0.47
1:A:766:GLU:HB3	1:A:769:ARG:HH12	1.80	0.47
2:B:122:LEU:O	2:B:126:LEU:HG	2.15	0.47
1:A:665:GLY:HA3	1:A:679:LEU:CD2	2.44	0.47
1:A:320:LYS:HG2	1:A:324:ASP:OD2	2.15	0.47
1:A:538:VAL:CG1	1:A:539:LYS:N	2.77	0.47
1:A:323:ARG:CD	1:A:363:ARG:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:VAL:O	1:A:645:ILE:HG13	2.16	0.46
1:A:395:VAL:O	1:A:399:LEU:HG	2.16	0.46
2:B:74:GLU:H	2:B:74:GLU:CD	2.19	0.46
1:A:381:ILE:HD11	1:A:411:LEU:HD11	1.96	0.46
1:A:240:LEU:HD13	1:A:499:ILE:HD11	1.98	0.45
1:A:432:VAL:HG23	1:A:433:THR:N	2.31	0.45
1:A:518:PHE:CE2	1:A:526:LEU:HD22	2.52	0.45
1:A:551:SER:HG	1:A:584:TYR:HE2	1.64	0.45
1:A:345:VAL:HG21	1:A:458:PHE:CZ	2.51	0.45
1:A:511:TYR:HB3	1:A:591:PRO:HG2	1.96	0.45
2:B:66:LEU:HD21	2:B:69:ILE:CD1	2.46	0.45
1:A:240:LEU:CD1	1:A:499:ILE:HD11	2.46	0.45
2:B:234:THR:CG2	2:B:314:GLY:HA2	2.46	0.45
1:A:307:SER:HB2	1:A:310:GLU:HG2	1.98	0.45
2:B:86:ILE:HG23	2:B:111:LYS:O	2.17	0.45
2:B:227:LEU:C	2:B:227:LEU:HD12	2.36	0.45
1:A:823:ASN:ND2	1:A:826:GLU:H	2.14	0.44
2:B:227:LEU:CD1	2:B:319:GLY:HA3	2.47	0.44
1:A:233:ILE:HG23	1:A:242:LEU:CD1	2.45	0.44
1:A:717:VAL:HG23	5:A:1012:HOH:O	2.16	0.44
1:A:747:LEU:CD2	1:A:768:ILE:HD11	2.47	0.44
2:B:237:LYS:HB2	2:B:240:GLU:CG	2.42	0.44
2:B:34:LEU:N	2:B:35:PRO:CD	2.81	0.43
2:B:41:ALA:HB2	2:B:197:LEU:HD23	2.00	0.43
1:A:799:VAL:HG11	1:A:854:VAL:HG11	2.00	0.43
2:B:65:THR:HG23	2:B:179:GLU:CB	2.47	0.43
2:B:140:ARG:NH1	2:B:140:ARG:CG	2.81	0.43
1:A:261:VAL:HG13	1:A:266:PRO:HD3	2.00	0.43
1:A:746:THR:HG22	1:A:747:LEU:N	2.33	0.43
1:A:307:SER:O	1:A:310:GLU:N	2.45	0.43
1:A:805:VAL:HG13	1:A:805:VAL:O	2.19	0.43
2:B:65:THR:HB	2:B:310:LYS:CD	2.48	0.43
1:A:250:SER:OG	1:A:296:ALA:HB1	2.19	0.43
1:A:375:LEU:HD13	1:A:414:ILE:HD12	2.00	0.43
2:B:143:LYS:HD3	2:B:169:LEU:CD2	2.47	0.43
1:A:527:VAL:O	1:A:530:ALA:HB3	2.19	0.43
1:A:334:VAL:HG23	1:A:335:ASP:N	2.33	0.43
2:B:55:VAL:HG13	2:B:57:VAL:HG23	1.99	0.43
1:A:255:LYS:HE3	1:A:325:PHE:CD1	2.54	0.43
1:A:264:PHE:HB3	1:A:268:HIS:HD2	1.84	0.43
1:A:345:VAL:HG22	1:A:349:GLU:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:HD21	1:A:419:LEU:HD12	2.00	0.43
1:A:457:ILE:O	1:A:458:PHE:HB2	2.18	0.43
1:A:590:PRO:HA	1:A:591:PRO:HD3	1.86	0.43
2:B:101:LEU:HD22	2:B:101:LEU:HA	1.91	0.42
1:A:356:GLU:HA	1:A:356:GLU:OE1	2.19	0.42
1:A:674:ASP:OD2	1:A:674:ASP:N	2.47	0.42
2:B:50:GLY:O	2:B:52:LYS:N	2.46	0.42
2:B:234:THR:HG22	2:B:314:GLY:CA	2.48	0.42
1:A:463:ASP:OD1	1:A:466:ASN:ND2	2.53	0.42
1:A:529:LYS:O	1:A:533:VAL:HG23	2.20	0.42
2:B:99:ARG:NH1	2:B:292:GLU:OE2	2.48	0.42
1:A:658:ARG:HG3	1:A:658:ARG:NH1	2.34	0.42
2:B:42:ILE:CD1	2:B:178:ILE:HD11	2.50	0.42
2:B:189:LEU:CB	2:B:208:VAL:HG11	2.49	0.42
1:A:224:ILE:O	1:A:301:LYS:HA	2.20	0.42
1:A:683:LYS:O	1:A:687:VAL:HG23	2.19	0.42
2:B:66:LEU:O	2:B:312:GLY:HA2	2.20	0.42
2:B:83:PHE:HD1	2:B:287:SER:HA	1.85	0.42
2:B:248:ARG:HG2	2:B:303:ILE:HD11	2.02	0.42
1:A:378:LYS:HA	1:A:411:LEU:O	2.20	0.42
2:B:320:ILE:HG22	2:B:321:TRP:N	2.35	0.41
1:A:444:LYS:HE2	2:B:270:ASP:OD1	2.20	0.41
1:A:430:ARG:O	1:A:434:GLU:HG3	2.20	0.41
2:B:203:VAL:HG22	2:B:204:ALA:N	2.36	0.41
1:A:694:GLU:OE2	1:A:694:GLU:HA	2.21	0.41
1:A:864:ILE:HD12	1:A:865:THR:CG2	2.48	0.41
1:A:245:SER:OG	1:A:484:LYS:HD2	2.19	0.41
2:B:100:PHE:CE1	2:B:101:LEU:HB2	2.55	0.41
2:B:248:ARG:HH11	2:B:248:ARG:HG3	1.85	0.41
2:B:1:MET:HB3	2:B:212:THR:HG22	2.02	0.41
1:A:538:VAL:CG1	1:A:539:LYS:H	2.34	0.41
1:A:639:PRO:O	1:A:643:VAL:HG23	2.21	0.41
1:A:413:ARG:C	1:A:415:ALA:H	2.24	0.40
2:B:79:TYR:CG	2:B:122:LEU:HD12	2.56	0.40
1:A:420:LEU:HD12	1:A:420:LEU:HA	1.99	0.40
1:A:535:GLU:OE1	1:A:535:GLU:HA	2.22	0.40
2:B:99:ARG:HE	2:B:99:ARG:HB2	1.70	0.40
2:B:131:LYS:HD3	2:B:131:LYS:HA	1.93	0.40
2:B:231:SER:OG	2:B:315:LEU:HD13	2.21	0.40
2:B:144:GLU:OE1	2:B:146:ARG:NH2	2.55	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	592/677 (87%)	548 (93%)	34 (6%)	10 (2%)	9	18
2	B	273/322 (85%)	254 (93%)	16 (6%)	3 (1%)	14	30
All	All	865/999 (87%)	802 (93%)	50 (6%)	13 (2%)	10	21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	ILE
2	B	296	GLU
1	A	311	ALA
1	A	570	GLU
2	B	51	LEU
1	A	275	ARG
1	A	349	GLU
1	A	407	ASN
1	A	824	LYS
1	A	439	LYS
1	A	539	LYS
1	A	556	SER
2	B	182	GLY

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	512/604 (85%)	495 (97%)	17 (3%)	38	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	238/280 (85%)	215 (90%)	23 (10%)	8	15
All	All	750/884 (85%)	710 (95%)	40 (5%)	22	45

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASP
1	A	345	VAL
1	A	360	LYS
1	A	489	VAL
1	A	545	ASP
1	A	641	VAL
1	A	660	VAL
1	A	685	LEU
1	A	727	LEU
1	A	731	ARG
1	A	797	ARG
1	A	805	VAL
1	A	817	ARG
1	A	823	ASN
1	A	827	THR
1	A	829	GLU
1	A	842	LEU
2	B	44	THR
2	B	65	THR
2	B	66	LEU
2	B	69	ILE
2	B	74	GLU
2	B	81	LEU
2	B	99	ARG
2	B	101	LEU
2	B	104	LEU
2	B	106	LEU
2	B	122	LEU
2	B	130	LEU
2	B	136	ASN
2	B	171	ILE
2	B	179	GLU
2	B	212	THR
2	B	245	LEU
2	B	257	LEU
2	B	258	LEU

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Mol	Chain	Res	Type
2	B	289	LEU
2	B	295	GLU
2	B	308	LEU
2	B	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
1	A	268	HIS
1	A	383	GLN
1	A	581	ASN
1	A	718	HIS
1	A	735	ASN
1	A	794	HIS
1	A	823	ASN
1	A	848	ASN
2	B	136	ASN
2	B	217	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	3AM	A	902	-	22,25,25	1.80	5 (22%)	24,38,38	1.85	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3AM	A	902	-	-	0/7/27/27	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	3AM	C2-N3	5.09	1.40	1.32
4	A	902	3AM	C2-N1	3.51	1.40	1.33
4	A	902	3AM	C5-C4	-2.75	1.33	1.40
4	A	902	3AM	C6-C5	-2.62	1.33	1.43
4	A	902	3AM	O4'-C1'	2.24	1.44	1.41

All (3) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	902	3AM	N3-C2-N1	-6.89	117.92	128.68
4	A	902	3AM	O4'-C4'-C3'	-2.61	99.27	104.87
4	A	902	3AM	C5-C6-N6	-2.58	116.43	120.35

There are no chirality outliers.
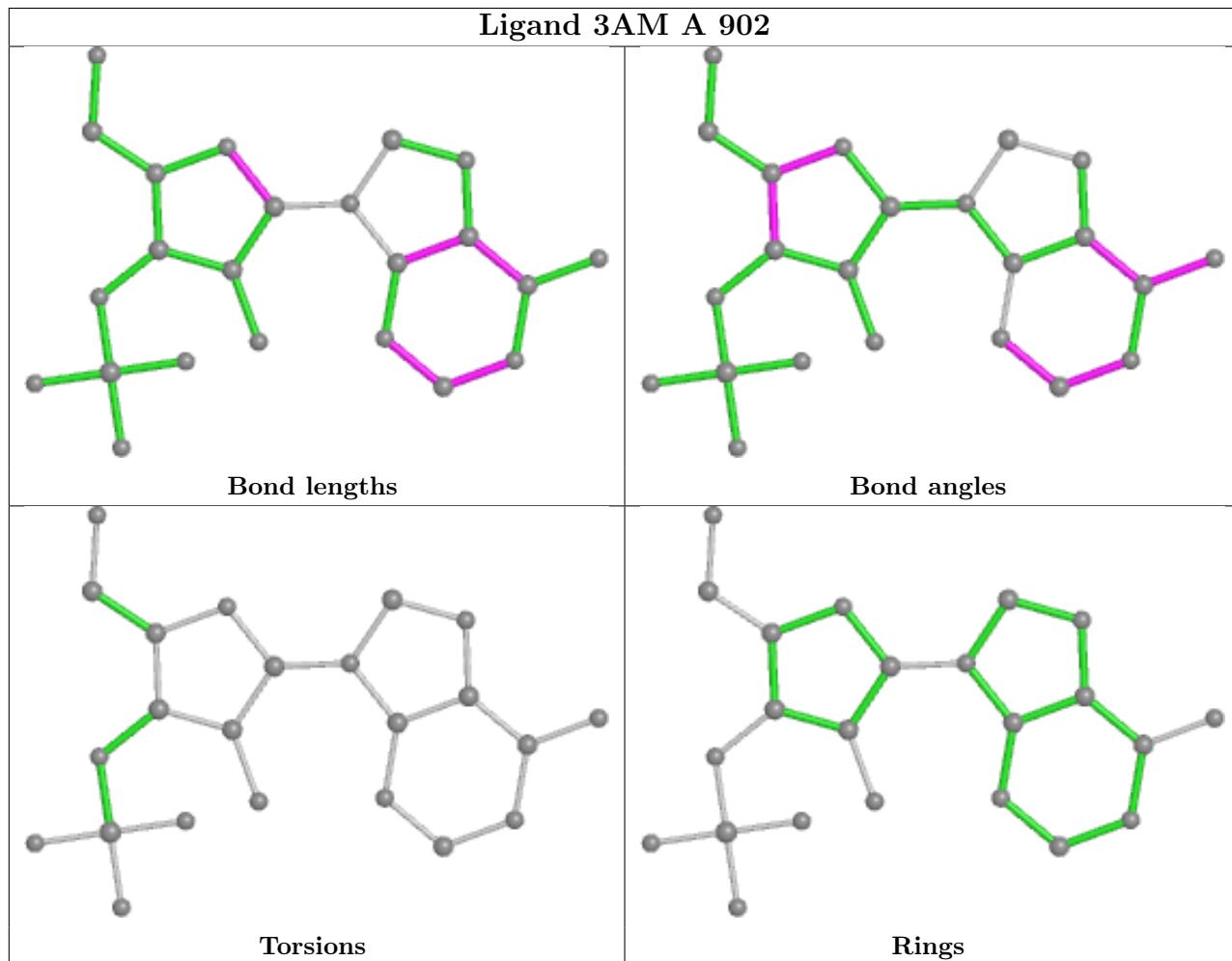
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

Ligand 3AM A 902

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	602/677 (88%)	0.10	15 (2%)	57	51	33, 61, 97, 119	0
2	B	281/322 (87%)	-0.12	4 (1%)	75	71	36, 60, 89, 104	0
All	All	883/999 (88%)	0.03	19 (2%)	62	56	33, 61, 96, 119	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	VAL	3.5
1	A	526	LEU	3.1
1	A	537	PHE	2.9
2	B	166	VAL	2.8
1	A	576	VAL	2.8
1	A	699	PHE	2.8
2	B	10	ASP	2.6
1	A	822	ARG	2.6
1	A	521	LYS	2.5
1	A	311	ALA	2.3
1	A	404	LYS	2.2
1	A	530	ALA	2.1
1	A	532	GLU	2.1
2	B	48	TYR	2.1
1	A	411	LEU	2.1
1	A	533	VAL	2.1
1	A	541	ASN	2.1
2	B	294	LYS	2.0
1	A	527	VAL	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 ⓘ
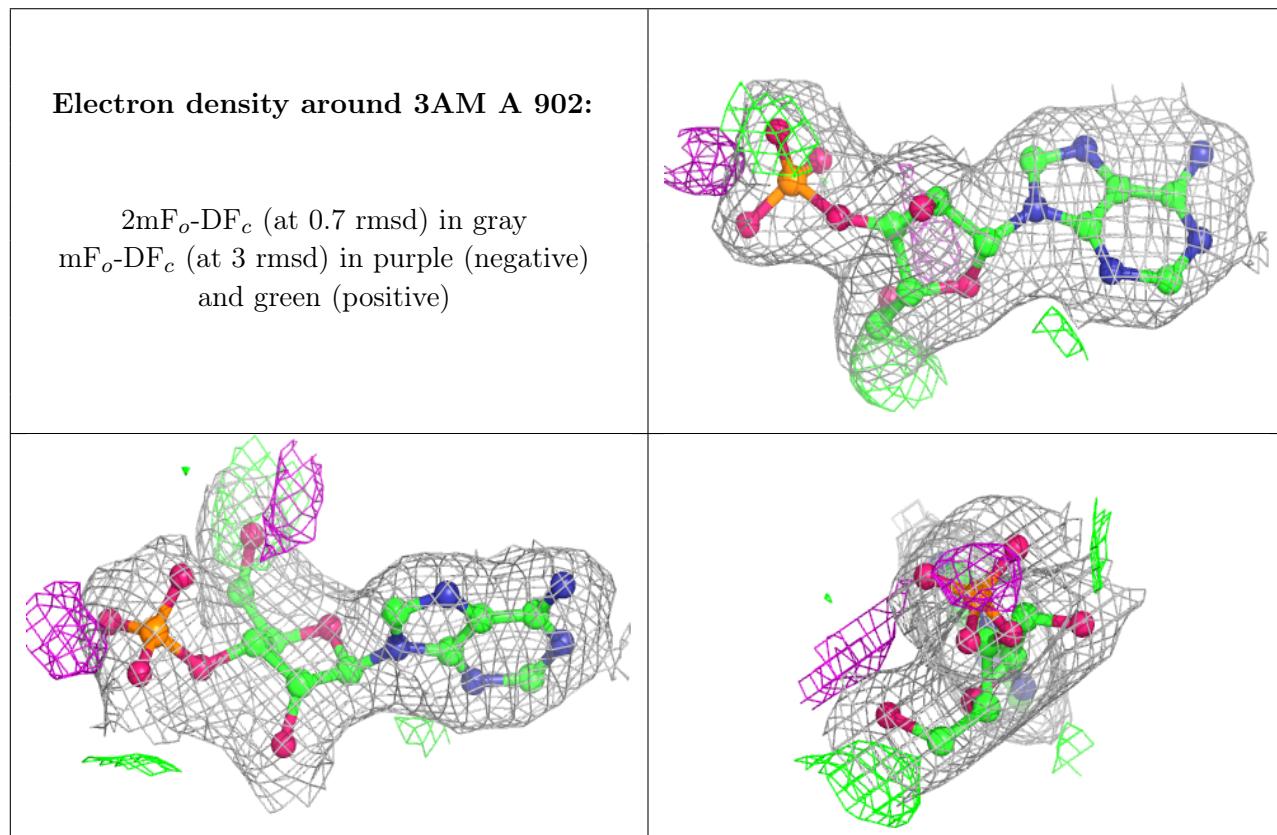
There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	3AM	A	902	23/23	0.95	0.19	43,53,70,71	0
3	ZN	A	901	1/1	0.99	0.16	53,53,53,53	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 3AM A 902:

$2mF_o$-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 (i)

There are no such residues in this entry.