Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2023 – 03:49 AM EDT

PDB ID	:	3W2W
Title	:	Crystal structure of the Cmr2dHD-Cmr3 subcomplex bound to ATP
Authors	:	Numata, T.; Osawa, T.
Deposited on	:	2012-12-06
Resolution	:	2.50 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:

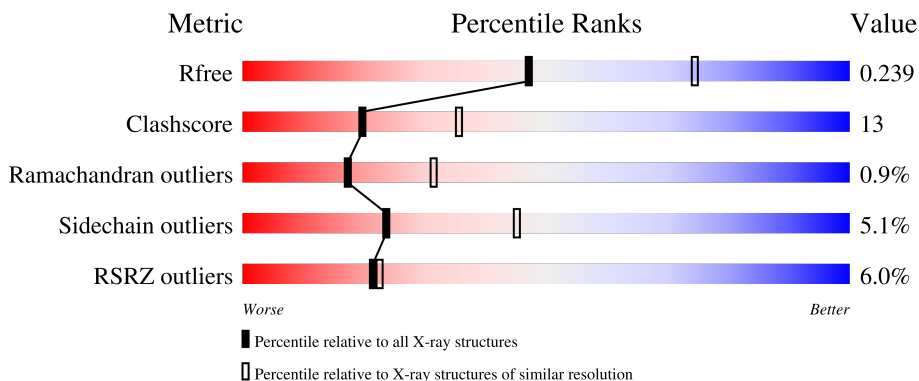|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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		0.239
Clashscore		13
Ramachandran outliers		0.9%
Sidechain outliers		5.1%
RSRZ outliers		6.0%

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	7% / 67% / 23% / · / 9%
2	B	322	3% / 65% / 27% / · / ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7499 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	618	4953	3212	823	905	13	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
			Total	C	N	O	S			
2	B	308	2420	1589	387	439	5	0	0	0

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

ATP
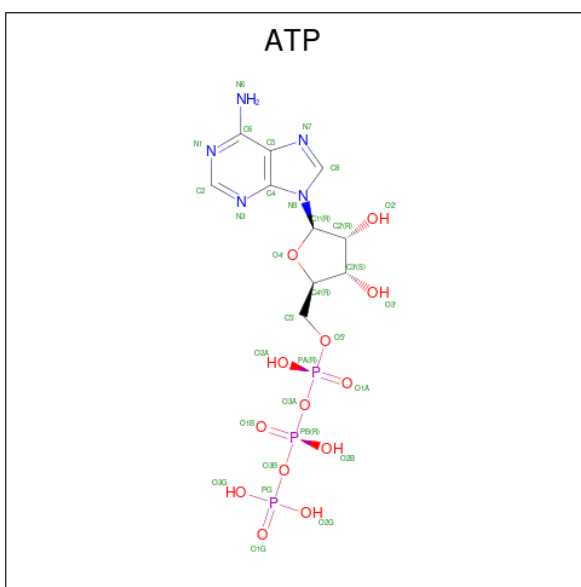
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
			Total	Mg		
5	B	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total O 48 48		0	0
6	B	13	Total O 13 13		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:

G184 I185 Y192 E193 F194 L195 T196 G199 E200 V203 A204 F205 V206 T212 P213 F216 E219 T223 K224 F230 T234 Q243 R248 L249 N250 Y256 L257 L258 V259 S260 S261 R262 P263 D270 M271 H272 E273 K274 K275 K280 P284 P285 L289 F290

K294 E295 L308 L311 G312 Y313 G314 L315 I320 W321 E322

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	103.58Å 135.80Å 191.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 2.50	Depositor
	46.91 – 2.50	EDS
% Data completeness	99.6 (46.91-2.50)	Depositor
(in resolution range)	99.7 (46.91-2.50)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	6.31 (at 2.51Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.211 , 0.246	Depositor
	0.205 , 0.239	DCC
R_{free} test set	2323 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.9	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7499	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 $<|L|>$, $<L^2>$ 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: ATP, ZN, MG

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	0.36	0/5053	0.57	0/6826
2	B	0.37	0/2471	0.65	1/3330 (0.0%)
All	All	0.37	0/7524	0.60	1/10156 (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	5.83	128.71	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	4953	0	4974	129	0
2	B	2420	0	2505	68	0
3	A	1	0	0	0	0
4	A	62	0	24	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	48	0	0	0	0
6	B	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7499	0	7503	189	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 13.

All (189) 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:289:ILE:HD11	1:A:293:ILE:HD13	1.44	0.98
2:B:65:THR:HG23	2:B:179:GLU:HB3	1.46	0.98
1:A:821:GLY:H	1:A:827:THR:HB	1.39	0.86
2:B:234:THR:HG22	2:B:314:GLY:HA2	1.56	0.86
2:B:71:ILE:HD12	2:B:171:ILE:HD11	1.61	0.81
1:A:517:ILE:HG22	1:A:587:ILE:HD13	1.63	0.80
1:A:448:CYS:HB2	1:A:478:CYS:HB3	1.65	0.79
1:A:413:ARG:HG3	1:A:413:ARG:HH11	1.48	0.77
1:A:638:THR:O	1:A:641:VAL:HG22	1.86	0.76
1:A:638:THR:OG1	1:A:639:PRO:HD3	1.86	0.76
2:B:18:ARG:HD2	2:B:21:ASP:OD1	1.86	0.75
2:B:83:PHE:HD1	2:B:260:SER:HA	1.51	0.75
1:A:371:THR:HG22	1:A:431:LYS:HD3	1.69	0.74
2:B:45:LEU:O	2:B:51:LEU:HB2	1.87	0.74
1:A:823:ASN:O	1:A:827:THR:HG22	1.92	0.70
1:A:418:PRO:HG3	1:A:612:VAL:HG12	1.77	0.67
1:A:709:LYS:HE3	1:A:745:ASP:HB2	1.77	0.67
1:A:823:ASN:HD22	1:A:825:GLU:HG2	1.60	0.66
1:A:371:THR:HG22	1:A:431:LYS:CD	2.25	0.66
1:A:371:THR:HG21	1:A:428:GLY:HA2	1.79	0.65
2:B:65:THR:CG2	2:B:179:GLU:HB3	2.23	0.65
1:A:686:GLU:HG3	1:A:690:LYS:HE3	1.79	0.65
2:B:65:THR:HG23	2:B:179:GLU:CB	2.23	0.65
1:A:609:SER:O	1:A:613:LEU:HG	1.97	0.64
1:A:475:GLU:O	1:A:475:GLU:HG3	1.98	0.64
1:A:864:ILE:HD12	1:A:865:THR:HG23	1.79	0.63
1:A:830:LEU:O	1:A:834:ILE:HG12	1.99	0.63
1:A:419:LEU:O	1:A:423:ILE:HG13	1.99	0.63
1:A:531:ARG:HG3	1:A:535:GLU:OE1	1.98	0.63
2:B:136:ASN:HD22	2:B:137:LYS:N	1.97	0.63
2:B:136:ASN:HD22	2:B:136:ASN:C	2.02	0.62
1:A:417:TYR:HB3	1:A:418:PRO:HD3	1.82	0.61
1:A:323:ARG:HG3	1:A:363:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:HD22	2:B:85:ILE:HD12	1.81	0.61
1:A:511:TYR:HB3	1:A:591:PRO:HG2	1.82	0.60
1:A:260:ILE:HD11	1:A:318:ILE:HD11	1.84	0.60
1:A:233:ILE:HG23	1:A:242:LEU:HD12	1.83	0.60
1:A:413:ARG:HG3	1:A:413:ARG:NH1	2.17	0.60
1:A:695:PHE:CD2	1:A:710:LEU:HD13	2.37	0.59
2:B:130:LEU:HD11	2:B:133:VAL:HG22	1.85	0.59
1:A:429:GLU:HA	1:A:432:VAL:HG12	1.85	0.59
2:B:234:THR:HG22	2:B:314:GLY:CA	2.28	0.59
1:A:601:GLY:HA2	1:A:710:LEU:HD12	1.84	0.59
1:A:322:ILE:HD12	1:A:368:VAL:HG11	1.85	0.58
1:A:398:TRP:HH2	1:A:416:ILE:HA	1.68	0.58
2:B:230:PHE:HD1	2:B:234:THR:HG21	1.69	0.58
1:A:346:ASP:CG	1:A:347:ARG:H	2.07	0.58
2:B:40:GLY:O	2:B:195:LEU:HA	2.04	0.57
1:A:236:SER:HB3	1:A:241:ASP:HB2	1.87	0.57
2:B:294:LYS:HG2	2:B:295:GLU:OE2	2.04	0.57
2:B:230:PHE:CD1	2:B:234:THR:HG21	2.40	0.56
1:A:346:ASP:HB3	1:A:349:GLU:HB2	1.88	0.56
1:A:828:LYS:O	1:A:832:GLU:HG3	2.05	0.56
2:B:58:GLY:HA2	2:B:272:HIS:HB2	1.86	0.56
1:A:398:TRP:HZ3	1:A:416:ILE:HG22	1.70	0.56
1:A:538:VAL:HG12	1:A:539:LYS:N	2.21	0.56
1:A:805:VAL:HG12	1:A:809:GLU:CB	2.35	0.55
1:A:429:GLU:O	1:A:433:THR:HG23	2.06	0.55
2:B:95:VAL:HG22	2:B:109:LYS:HD2	1.89	0.55
1:A:441:GLU:HG2	2:B:280:LYS:HG3	1.88	0.55
1:A:533:VAL:HG22	1:A:572:LYS:O	2.07	0.55
1:A:718:HIS:HD2	1:A:720:LYS:H	1.54	0.55
1:A:641:VAL:O	1:A:645:ILE:HG13	2.07	0.54
2:B:74:GLU:H	2:B:74:GLU:CD	2.09	0.54
2:B:308:LEU:HG	2:B:311:LEU:HD12	1.89	0.54
1:A:523:GLY:O	1:A:527:VAL:HG23	2.07	0.54
1:A:429:GLU:O	1:A:432:VAL:HG12	2.07	0.54
2:B:55:VAL:O	2:B:55:VAL:HG13	2.08	0.54
2:B:196:THR:HA	2:B:203:VAL:HA	1.88	0.54
1:A:531:ARG:HB2	1:A:538:VAL:HG21	1.89	0.54
4:A:902:ATP:O2G	2:B:262:ARG:NH1	2.41	0.54
1:A:511:TYR:HB3	1:A:591:PRO:CG	2.38	0.53
1:A:584:TYR:HB3	1:A:589:ASN:HD22	1.71	0.53
1:A:787:VAL:HA	1:A:790:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:O	1:A:408:SER:N	2.40	0.53
1:A:551:SER:HG	1:A:584:TYR:HE2	1.57	0.53
1:A:823:ASN:HD22	1:A:825:GLU:CG	2.21	0.53
1:A:441:GLU:HG2	2:B:280:LYS:CG	2.39	0.53
1:A:695:PHE:CE2	1:A:710:LEU:HD13	2.44	0.53
2:B:140:ARG:HG3	2:B:140:ARG:HH11	1.74	0.53
1:A:584:TYR:HB3	1:A:589:ASN:ND2	2.25	0.52
1:A:554:TRP:CE2	1:A:576:VAL:HG11	2.45	0.52
2:B:83:PHE:CD1	2:B:260:SER:HA	2.38	0.52
1:A:805:VAL:HG12	1:A:805:VAL:O	2.08	0.52
1:A:797:ARG:NE	1:A:797:ARG:HA	2.25	0.52
2:B:78:ILE:CD1	2:B:141:ILE:HD11	2.41	0.51
1:A:398:TRP:CH2	1:A:416:ILE:HA	2.44	0.51
2:B:87:LYS:HD3	2:B:92:TYR:CZ	2.46	0.51
1:A:603:ASP:O	1:A:607:VAL:HG23	2.09	0.51
1:A:255:LYS:O	1:A:258:GLU:HG2	2.11	0.51
2:B:140:ARG:HH11	2:B:140:ARG:CG	2.24	0.50
1:A:445:GLY:HA2	2:B:275:LYS:HD3	1.92	0.50
1:A:736:ASN:ND2	2:B:113:LYS:HE3	2.25	0.50
2:B:24:SER:HA	2:B:27:VAL:HG12	1.94	0.50
1:A:381:ILE:HG13	1:A:382:TYR:N	2.27	0.50
1:A:492:ARG:HH11	1:A:492:ARG:HG2	1.77	0.50
1:A:343:VAL:HG13	1:A:343:VAL:O	2.12	0.49
2:B:223:THR:HG21	2:B:320:ILE:HG12	1.93	0.49
1:A:379:GLU:HB3	1:A:384:VAL:HG21	1.93	0.49
1:A:390:LEU:HD21	2:B:108:PRO:HD2	1.95	0.49
1:A:821:GLY:N	1:A:827:THR:HB	2.18	0.49
2:B:130:LEU:HD11	2:B:133:VAL:CG2	2.42	0.48
1:A:282:LYS:HB2	1:A:289:ILE:HG12	1.94	0.48
1:A:301:LYS:HD3	4:A:903:ATP:O2'	2.13	0.48
1:A:577:VAL:HG12	1:A:581:ASN:ND2	2.28	0.48
1:A:250:SER:OG	1:A:296:ALA:HB1	2.14	0.48
1:A:264:PHE:HB3	1:A:268:HIS:ND1	2.29	0.47
1:A:345:VAL:HG22	1:A:346:ASP:H	1.78	0.47
2:B:195:LEU:HD12	2:B:206:VAL:HG21	1.96	0.47
1:A:718:HIS:CD2	1:A:720:LYS:H	2.31	0.47
2:B:78:ILE:HD11	2:B:141:ILE:HD11	1.96	0.47
1:A:534:SER:HB3	1:A:537:PHE:CE2	2.50	0.46
1:A:606:LYS:HA	1:A:606:LYS:HE2	1.95	0.46
2:B:73:THR:HB	2:B:74:GLU:OE2	2.15	0.46
2:B:45:LEU:HD21	2:B:192:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:TYR:CE1	1:A:590:PRO:HD3	2.50	0.46
1:A:260:ILE:CD1	1:A:318:ILE:HD11	2.45	0.46
2:B:49:LYS:O	2:B:49:LYS:HG2	2.16	0.45
2:B:199:GLY:O	2:B:200:GLU:HG3	2.17	0.45
2:B:41:ALA:CB	2:B:196:THR:HG23	2.47	0.45
1:A:423:ILE:HG22	2:B:100:PHE:CD1	2.51	0.45
1:A:437:PHE:CE1	2:B:263:PRO:HG3	2.51	0.45
2:B:270:ASP:OD1	2:B:273:GLU:HB2	2.16	0.45
1:A:388:ALA:O	2:B:107:PRO:HB3	2.17	0.45
2:B:136:ASN:C	2:B:136:ASN:ND2	2.68	0.45
1:A:275:ARG:HE	1:A:275:ARG:HB2	1.63	0.45
1:A:690:LYS:O	1:A:694:GLU:HG2	2.16	0.45
1:A:777:ARG:O	1:A:781:LEU:HG	2.16	0.45
2:B:77:ARG:HD2	2:B:119:GLU:OE2	2.17	0.45
1:A:310:GLU:O	1:A:314:ILE:HG13	2.17	0.44
1:A:533:VAL:HG11	1:A:573:VAL:HG22	1.98	0.44
1:A:822:ARG:NH1	1:A:826:GLU:OE1	2.49	0.44
1:A:429:GLU:O	1:A:433:THR:CG2	2.65	0.44
1:A:709:LYS:CE	1:A:745:ASP:HB2	2.46	0.44
1:A:346:ASP:CG	1:A:347:ARG:N	2.71	0.44
1:A:277:GLN:O	1:A:278:PRO:C	2.55	0.44
2:B:213:PRO:HG2	2:B:216:PHE:CD2	2.53	0.44
2:B:230:PHE:O	2:B:285:PRO:HA	2.18	0.44
1:A:404:LYS:O	1:A:405:LYS:C	2.57	0.43
1:A:839:LYS:HD2	1:A:839:LYS:HA	1.84	0.43
1:A:433:THR:O	1:A:437:PHE:HD2	2.00	0.43
1:A:525:ASP:O	1:A:528:SER:HB3	2.18	0.43
2:B:144:GLU:HG3	2:B:146:ARG:NH2	2.34	0.43
2:B:223:THR:OG1	2:B:224:LYS:N	2.52	0.43
1:A:218:ASP:HA	1:A:219:PRO:HD2	1.77	0.43
1:A:414:ILE:O	1:A:414:ILE:HG12	2.18	0.43
1:A:284:TYR:HD2	1:A:285:LEU:HD12	1.83	0.43
1:A:378:LYS:HA	1:A:411:LEU:O	2.19	0.43
1:A:779:LYS:HD3	1:A:830:LEU:HD21	2.00	0.43
1:A:374:SER:O	1:A:413:ARG:HG3	2.19	0.43
1:A:529:LYS:O	1:A:533:VAL:HG23	2.19	0.43
2:B:183:CYS:HB2	2:B:185:ILE:HG13	2.01	0.42
1:A:392:ASP:HB2	1:A:394:ASP:OD1	2.19	0.42
2:B:82:PRO:HD2	2:B:85:ILE:HD12	2.01	0.42
2:B:193:GLU:O	2:B:205:PHE:HA	2.19	0.42
2:B:234:THR:CG2	2:B:314:GLY:HA2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HE1	1:A:307:SER:HG	1.66	0.42
1:A:864:ILE:HD12	1:A:864:ILE:C	2.39	0.42
2:B:66:LEU:O	2:B:312:GLY:HA2	2.20	0.42
1:A:533:VAL:CG1	1:A:573:VAL:HG22	2.50	0.42
1:A:783:GLU:HB3	1:A:787:VAL:HB	2.01	0.42
1:A:584:TYR:CD1	1:A:590:PRO:HD3	2.55	0.42
1:A:537:PHE:O	1:A:544:VAL:HG23	2.20	0.42
2:B:140:ARG:CG	2:B:140:ARG:NH1	2.82	0.41
1:A:284:TYR:C	1:A:286:GLY:H	2.24	0.41
2:B:284:PRO:HA	2:B:285:PRO:HD3	1.92	0.41
2:B:256:TYR:HA	2:B:290:PHE:O	2.21	0.41
1:A:457:ILE:O	1:A:458:PHE:HB2	2.20	0.41
1:A:746:THR:HG22	1:A:747:LEU:N	2.36	0.41
1:A:371:THR:HG22	1:A:431:LYS:HD2	2.02	0.41
1:A:514:TRP:CZ2	1:A:590:PRO:HB3	2.56	0.41
1:A:275:ARG:NH1	1:A:647:GLN:HG2	2.36	0.41
1:A:590:PRO:HA	1:A:591:PRO:HD3	1.85	0.41
1:A:492:ARG:HG2	1:A:492:ARG:NH1	2.35	0.41
1:A:511:TYR:CE1	1:A:682:ASP:HB3	2.55	0.41
2:B:41:ALA:HB2	2:B:196:THR:HG23	2.02	0.41
2:B:41:ALA:HB2	2:B:196:THR:CG2	2.50	0.41
1:A:403:GLU:HG3	1:A:408:SER:O	2.21	0.41
1:A:418:PRO:HG3	1:A:612:VAL:CG1	2.48	0.41
1:A:582:ALA:O	1:A:585:LYS:HB2	2.21	0.40
2:B:24:SER:O	2:B:27:VAL:HG12	2.21	0.40
1:A:371:THR:CG2	1:A:431:LYS:HD3	2.43	0.40
1:A:379:GLU:OE1	1:A:413:ARG:NE	2.46	0.40
1:A:506:ASP:OD1	1:A:546:SER:OG	2.28	0.40
1:A:538:VAL:HG12	1:A:539:LYS:H	1.86	0.40
2:B:6:PHE:HB2	2:B:174:ILE:HB	2.04	0.40
2:B:34:LEU:HD12	2:B:34:LEU:HA	1.93	0.40
1:A:395:VAL:HG13	1:A:419:LEU:HD11	2.03	0.40
2:B:29:ARG:HD3	2:B:31:ILE:HG13	2.02	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	608/677 (90%)	571 (94%)	32 (5%)	5 (1%)	19	35
2	B	300/322 (93%)	286 (95%)	11 (4%)	3 (1%)	15	28
All	All	908/999 (91%)	857 (94%)	43 (5%)	8 (1%)	17	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ASP
1	A	275	ARG
1	A	286	GLY
1	A	407	ASN
1	A	570	GLU
2	B	19	PRO
2	B	182	GLY
2	B	50	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	528/604 (87%)	515 (98%)	13 (2%)	47	73
2	B	261/280 (93%)	234 (90%)	27 (10%)	7	14
All	All	789/884 (89%)	749 (95%)	40 (5%)	24	45

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

Mol	Chain	Res	Type
1	A	273	SER
1	A	345	VAL
1	A	425	ASP
1	A	433	THR
1	A	464	HIS
1	A	578	ASP
1	A	660	VAL
1	A	685	LEU
1	A	739	LYS
1	A	797	ARG
1	A	817	ARG
1	A	827	THR
1	A	842	LEU
2	B	18	ARG
2	B	38	VAL
2	B	65	THR
2	B	66	LEU
2	B	74	GLU
2	B	81	LEU
2	B	99	ARG
2	B	104	LEU
2	B	117	VAL
2	B	122	LEU
2	B	130	LEU
2	B	136	ASN
2	B	171	ILE
2	B	196	THR
2	B	212	THR
2	B	219	GLU
2	B	243	GLN
2	B	248	ARG
2	B	250	ASN
2	B	257	LEU
2	B	258	LEU
2	B	262	ARG
2	B	273	GLU
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	383	GLN
1	A	464	HIS
1	A	466	ASN
1	A	581	ASN
1	A	589	ASN
1	A	718	HIS
1	A	735	ASN
1	A	736	ASN
1	A	823	ASN
1	A	848	ASN
2	B	136	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	ATP	A	903	5	26,33,33	1.81	6 (23%)	31,52,52	1.86	5 (16%)
4	ATP	A	902	5	26,33,33	1.81	6 (23%)	31,52,52	1.80	5 (16%)

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	ATP	A	903	5	-	7/18/38/38	0/3/3/3
4	ATP	A	902	5	-	9/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	ATP	C2-N3	5.17	1.40	1.32
4	A	902	ATP	C2-N3	5.13	1.40	1.32
4	A	902	ATP	C2-N1	3.49	1.40	1.33
4	A	903	ATP	C2-N1	3.48	1.40	1.33
4	A	903	ATP	PB-O1B	2.99	1.61	1.50
4	A	902	ATP	PB-O1B	2.95	1.61	1.50
4	A	903	ATP	C5-C4	-2.79	1.33	1.40
4	A	902	ATP	C5-C4	-2.75	1.33	1.40
4	A	902	ATP	C6-C5	-2.61	1.33	1.43
4	A	903	ATP	C6-C5	-2.60	1.33	1.43
4	A	902	ATP	O4'-C1'	2.36	1.44	1.41
4	A	903	ATP	O4'-C1'	2.35	1.44	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	903	ATP	N3-C2-N1	-7.03	117.69	128.68
4	A	902	ATP	N3-C2-N1	-6.91	117.88	128.68
4	A	902	ATP	PB-O3B-PG	-3.28	121.58	132.83
4	A	902	ATP	PA-O3A-PB	-2.92	122.81	132.83
4	A	903	ATP	PA-O3A-PB	-2.89	122.91	132.83
4	A	903	ATP	C2'-C3'-C4'	-2.87	97.07	102.64
4	A	903	ATP	PB-O3B-PG	-2.85	123.04	132.83
4	A	902	ATP	C5-C6-N6	-2.45	116.62	120.35
4	A	903	ATP	C5-C6-N6	-2.45	116.64	120.35
4	A	902	ATP	O2A-PA-O1A	2.01	122.19	112.24

There are no chirality outliers.

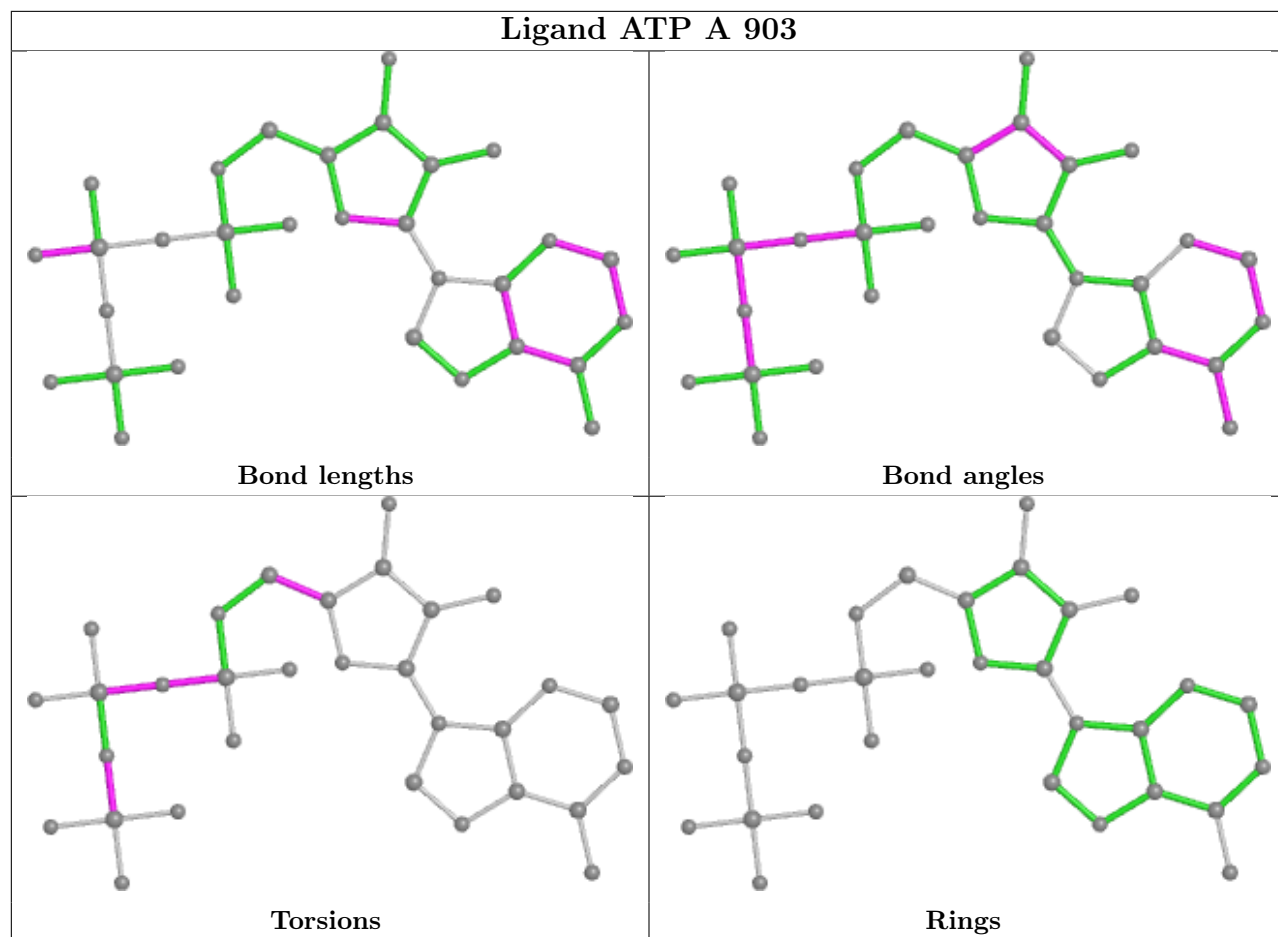All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	ATP	PB-O3B-PG-O2G
4	A	902	ATP	PB-O3B-PG-O3G
4	A	902	ATP	C5'-O5'-PA-O3A
4	A	903	ATP	PB-O3B-PG-O3G
4	A	903	ATP	PA-O3A-PB-O1B
4	A	902	ATP	PB-O3A-PA-O2A
4	A	903	ATP	PB-O3A-PA-O2A
4	A	903	ATP	O4'-C4'-C5'-O5'
4	A	902	ATP	PA-O3A-PB-O1B
4	A	902	ATP	PB-O3A-PA-O1A
4	A	902	ATP	PB-O3B-PG-O1G
4	A	903	ATP	PB-O3B-PG-O2G
4	A	903	ATP	PA-O3A-PB-O2B
4	A	902	ATP	C5'-O5'-PA-O1A
4	A	902	ATP	C5'-O5'-PA-O2A
4	A	903	ATP	PB-O3B-PG-O1G

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	ATP	1	0
4	A	902	ATP	1	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.

Ligand ATP A 903

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 902

Bond lengths

Bond angles

Torsions

Rings
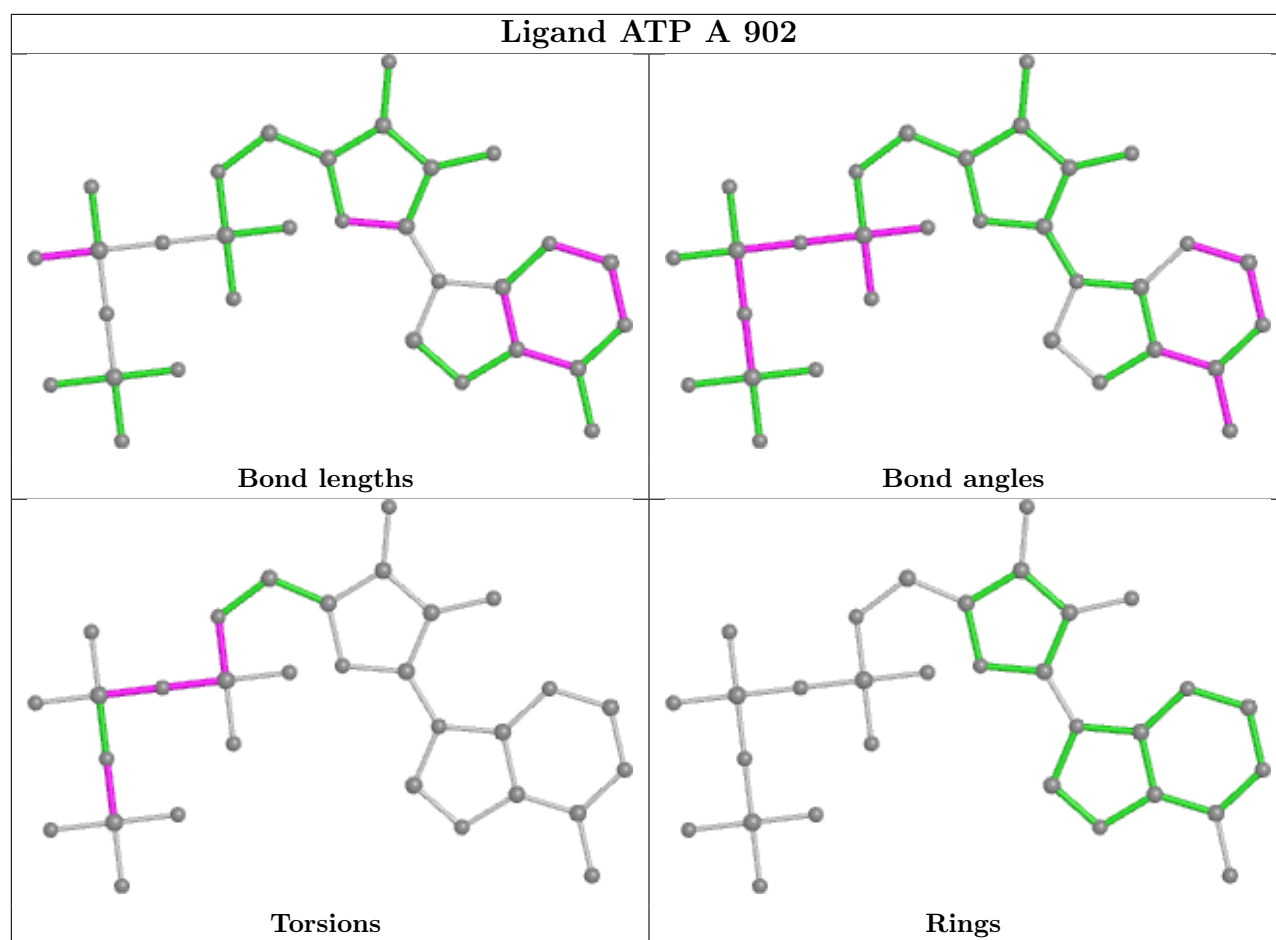
5.7 Other polymers ⓘ

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	618/677 (91%)	0.47	45 (7%)	15	15	29, 50, 88, 104	0
2	B	308/322 (95%)	0.33	11 (3%)	42	46	31, 53, 87, 100	0
All	All	926/999 (92%)	0.42	56 (6%)	21	22	29, 51, 88, 104	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	LEU	5.9
2	B	51	LEU	4.1
1	A	401	PHE	4.1
1	A	587	ILE	4.1
2	B	199	GLY	4.0
1	A	407	ASN	3.8
1	A	532	GLU	3.7
1	A	525	ASP	3.7
1	A	530	ALA	3.6
1	A	537	PHE	3.6
1	A	822	ARG	3.5
1	A	528	SER	3.5
2	B	57	VAL	3.4
1	A	576	VAL	3.4
1	A	535	GLU	3.1
1	A	541	ASN	3.1
1	A	579	PHE	3.1
2	B	43	ARG	3.1
1	A	538	VAL	3.1
1	A	406	GLU	3.0
1	A	518	PHE	3.0
1	A	772	TYR	3.0
1	A	529	LYS	3.0
1	A	311	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	554	TRP	2.9
2	B	44	THR	2.8
1	A	540	ASP	2.7
1	A	285	LEU	2.6
1	A	381	ILE	2.6
2	B	38	VAL	2.5
1	A	462	TYR	2.4
1	A	548	LEU	2.4
1	A	580	LEU	2.4
2	B	52	LYS	2.3
1	A	414	ILE	2.3
1	A	233	ILE	2.3
2	B	295	GLU	2.3
1	A	286	GLY	2.3
1	A	288	ASN	2.3
1	A	536	ASP	2.2
1	A	531	ARG	2.2
1	A	527	VAL	2.2
2	B	42	ILE	2.2
1	A	409	ARG	2.2
2	B	14	PHE	2.2
1	A	516	LYS	2.2
1	A	571	GLU	2.1
2	B	271	MET	2.1
1	A	636	TYR	2.1
1	A	582	ALA	2.1
1	A	412	GLU	2.0
1	A	461	MET	2.0
1	A	825	GLU	2.0
1	A	396	LYS	2.0
1	A	533	VAL	2.0
1	A	542	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.
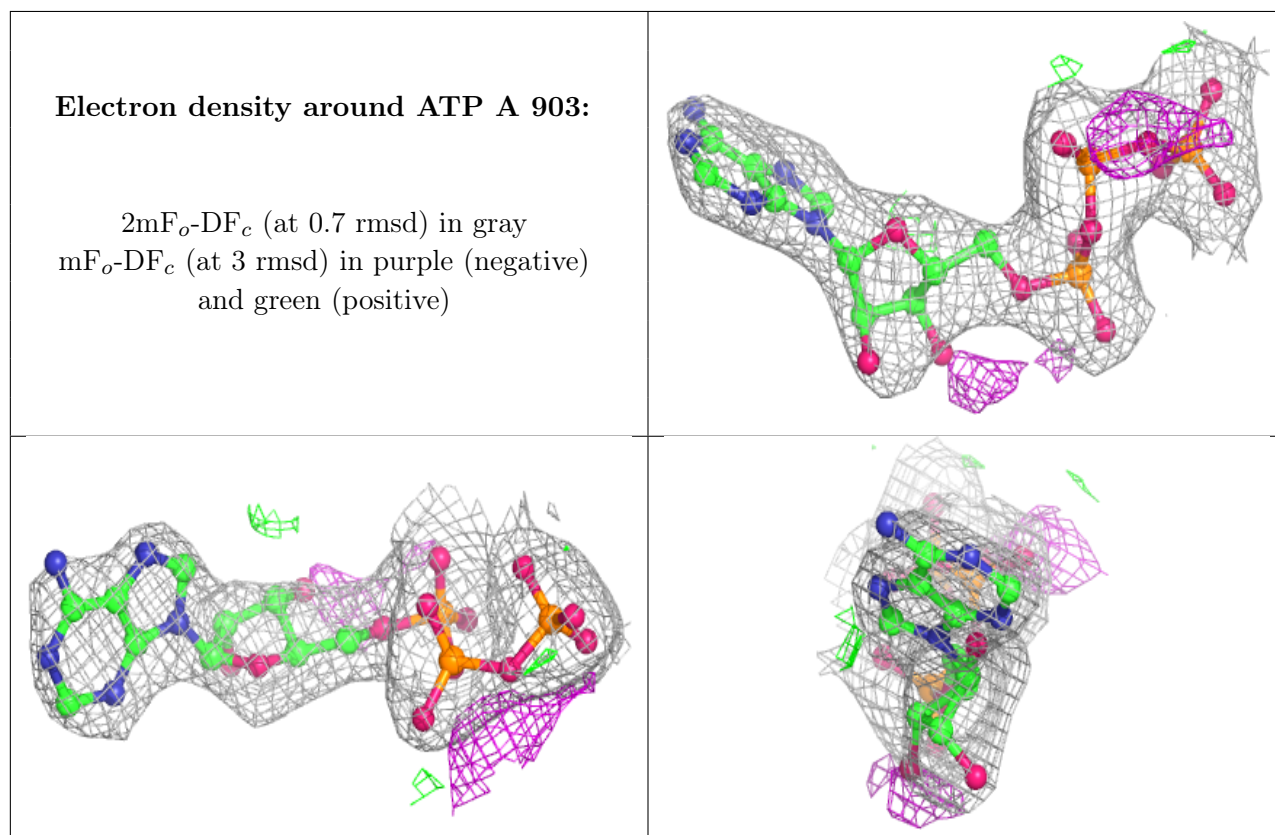
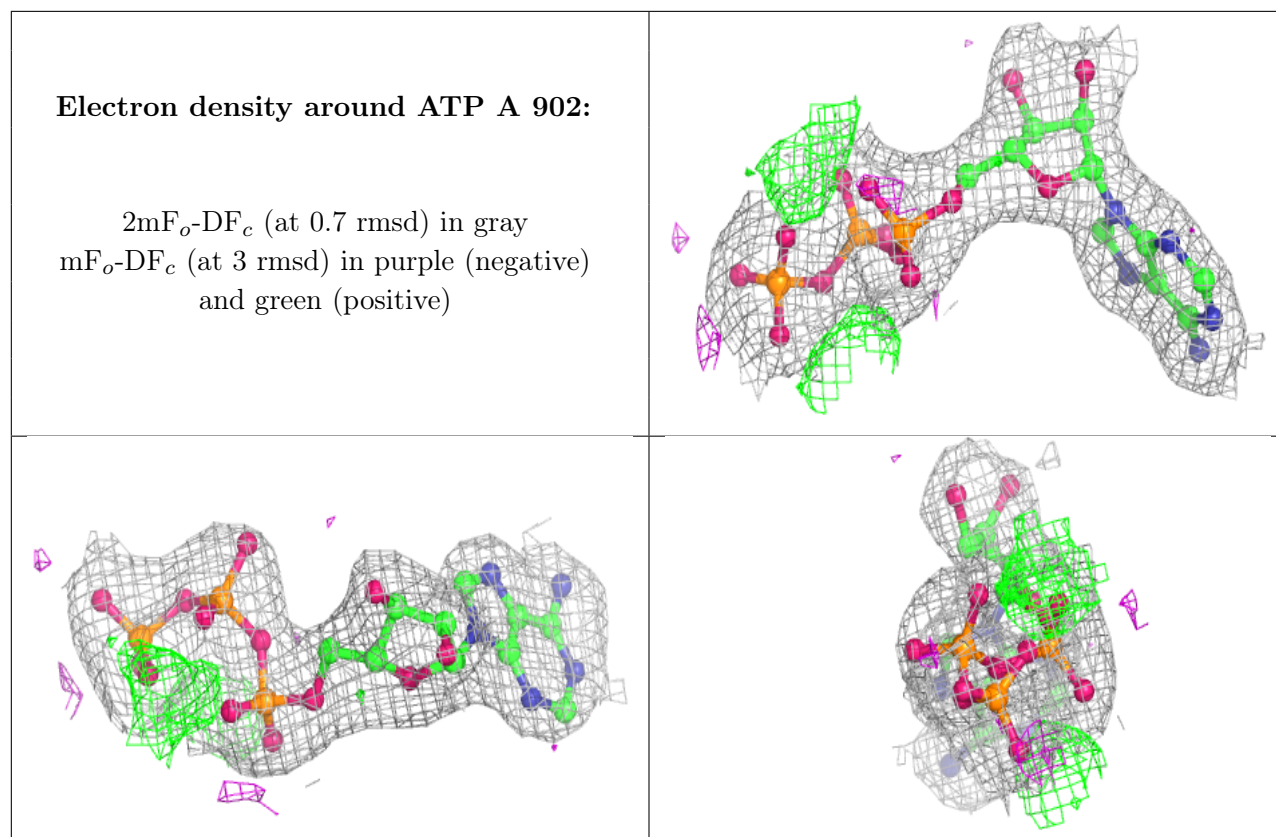## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	B	401	1/1	0.91	0.40	41,41,41,41	0
5	MG	A	904	1/1	0.96	0.18	44,44,44,44	0
4	ATP	A	903	31/31	0.97	0.14	38,65,70,72	0
4	ATP	A	902	31/31	0.98	0.21	33,40,42,43	0
3	ZN	A	901	1/1	0.99	0.16	46,46,46,46	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 ATP A 903:

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

Electron density around ATP A 902:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.