



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2024 – 01:02 pm BST

PDB ID : 5OFB
Title : Crystal structure of human MORC2 (residues 1-603) with spinal muscular atrophy mutation S87L
Authors : Douse, C.H.; Liu, Y.; Modis, Y.
Deposited on : 2017-07-10
Resolution : 2.02 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 : 2.36.2
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) : 2.36.2

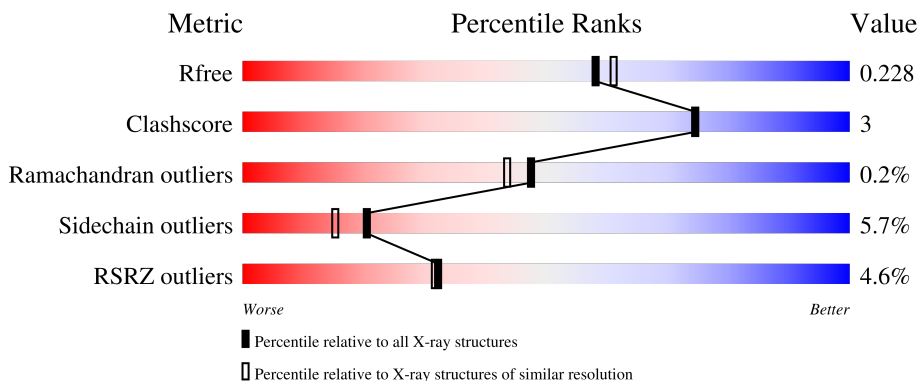
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	606	 5% 75% 11% • 12%
1	B	606	 3% 77% 9% •• 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9084 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 MORC family CW-type zinc finger protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	541	4387	2768	779	812	28	0	0	0
1	A	534	4326	2728	768	802	28	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9Y6X9
B	-1	PRO	-	expression tag	UNP Q9Y6X9
B	0	ARG	-	expression tag	UNP Q9Y6X9
B	87	LEU	SER	engineered mutation	UNP Q9Y6X9
A	-2	GLY	-	expression tag	UNP Q9Y6X9
A	-1	PRO	-	expression tag	UNP Q9Y6X9
A	0	ARG	-	expression tag	UNP Q9Y6X9
A	87	LEU	SER	engineered mutation	UNP Q9Y6X9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

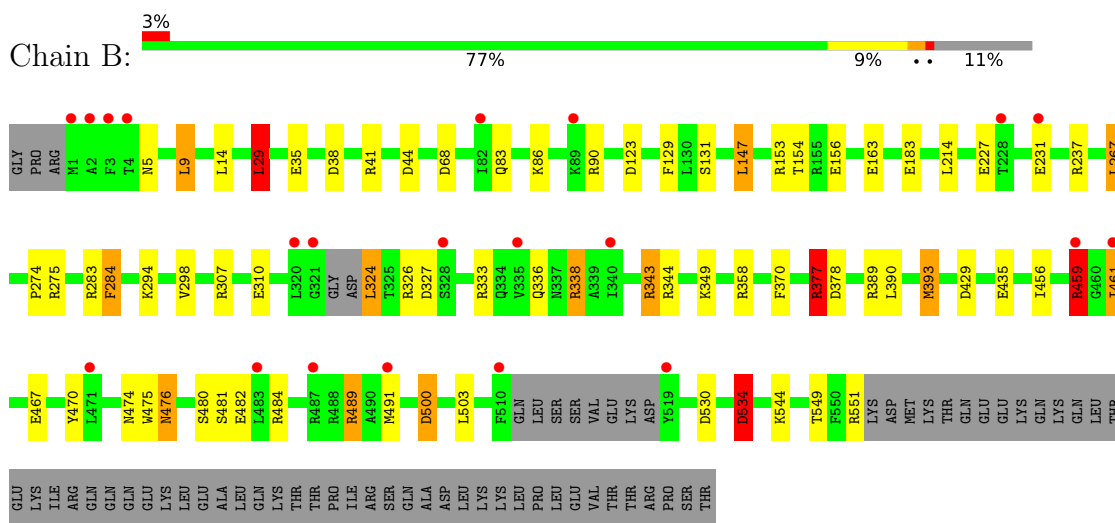
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

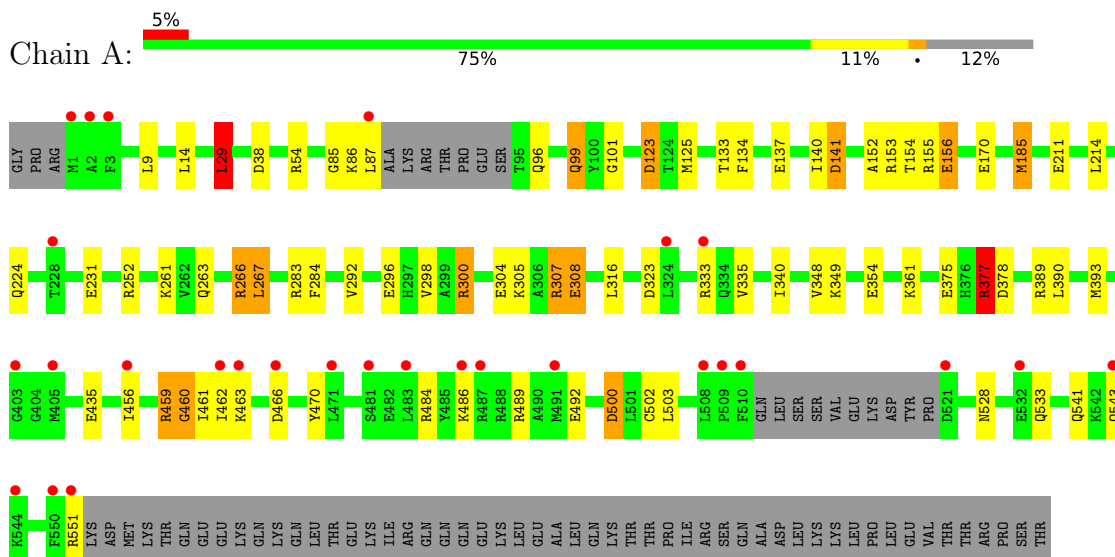
3 Residue-property plots i

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: MORC family CW-type zinc finger protein 2



- Molecule 1: MORC family CW-type zinc finger protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.85Å 124.68Å 80.36Å 90.00° 97.73° 90.00°	Depositor
Resolution (Å)	79.63 – 2.02 79.63 – 2.02	Depositor EDS
% Data completeness (in resolution range)	91.9 (79.63-2.02) 91.9 (79.63-2.02)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.02Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.198 , 0.228 0.202 , 0.228	Depositor DCC
R_{free} test set	4183 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtrriage
Anisotropy	0.290	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9084	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 i

5.1 Standard geometry i

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	0.75	1/4412 (0.0%)	1.03	29/5940 (0.5%)
1	B	0.80	4/4476 (0.1%)	1.08	40/6028 (0.7%)
All	All	0.77	5/8888 (0.1%)	1.06	69/11968 (0.6%)

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	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	GLU	CD-OE1	6.06	1.32	1.25
1	B	35	GLU	CD-OE2	5.46	1.31	1.25
1	B	481	SER	CB-OG	-5.41	1.35	1.42
1	B	489	ARG	CD-NE	-5.28	1.37	1.46
1	B	183	GLU	CD-OE2	-5.16	1.20	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ARG	NE-CZ-NH1	14.84	127.72	120.30
1	A	266	ARG	NE-CZ-NH1	13.51	127.05	120.30
1	B	267	LEU	CB-CG-CD1	12.53	132.30	111.00
1	B	500	ASP	CB-CG-OD2	-12.28	107.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	MET	CG-SD-CE	11.59	118.75	100.20
1	A	267	LEU	CB-CG-CD1	11.01	129.72	111.00
1	B	343	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	B	489	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	B	491	MET	CA-CB-CG	9.18	128.90	113.30
1	A	266	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	147	LEU	CB-CG-CD2	-8.65	96.29	111.00
1	A	500	ASP	CB-CG-OD1	8.65	126.09	118.30
1	B	500	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	459	ARG	C-N-CA	8.01	139.12	122.30
1	B	389	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	534	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	A	38	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	393	MET	CG-SD-CE	7.38	112.02	100.20
1	B	534	ASP	CB-CG-OD2	7.19	124.77	118.30
1	B	467	GLU	CA-CB-CG	7.15	129.13	113.40
1	A	459	ARG	CA-C-N	6.99	130.19	116.20
1	B	389	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	489	ARG	CD-NE-CZ	6.91	133.27	123.60
1	B	183	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	A	500	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	338	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	38	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	307	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	B	343	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	90	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	267	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	466	ASP	CB-CA-C	6.20	122.79	110.40
1	B	503	LEU	CB-CG-CD2	6.19	121.53	111.00
1	B	377	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	141	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	389	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	29	LEU	CB-CG-CD2	6.13	121.42	111.00
1	A	300	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	123	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	237	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	460	GLY	N-CA-C	5.82	127.65	113.10
1	A	9	LEU	CB-CG-CD2	5.79	120.84	111.00
1	A	377	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	358	ARG	CG-CD-NE	5.68	123.73	111.80
1	B	41	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	377	ARG	NE-CZ-NH1	5.57	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	B	44	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	476	ASN	CB-CA-C	5.43	121.26	110.40
1	A	389	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	459	ARG	CA-C-N	5.33	126.85	116.20
1	A	85	GLY	O-C-N	-5.30	114.21	122.70
1	B	9	LEU	CB-CG-CD2	5.28	119.97	111.00
1	A	492	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	B	459	ARG	C-N-CA	5.27	133.37	122.30
1	B	284	PHE	CB-CG-CD1	5.26	124.48	120.80
1	A	54	ARG	CB-CG-CD	5.23	125.19	111.60
1	B	68	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	29	LEU	CB-CG-CD1	5.21	119.86	111.00
1	A	54	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	252	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	491	MET	CB-CA-C	-5.14	100.13	110.40
1	A	377	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	354	GLU	CG-CD-OE1	5.08	128.46	118.30
1	B	307	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	B	456	ILE	CB-CA-C	-5.07	101.46	111.60
1	A	134	PHE	CB-CG-CD1	5.03	124.32	120.80
1	B	344	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	459	ARG	CG-CD-NE	-5.00	101.29	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	GLU	Peptide
1	A	459	ARG	Peptide
1	B	459	ARG	Peptide

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	4326	0	4302	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4387	0	4367	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	135	0	0	2	0
5	B	169	0	0	3	0
All	All	9084	0	8693	56	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 3.

All (56) 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:B:154:THR:OG1	1:B:156:GLU:HG2	1.85	0.76
1:B:377:ARG:HD2	1:B:470:TYR:CE1	2.28	0.69
1:B:298:VAL:HG12	1:B:349:LYS:HD2	1.73	0.69
1:A:298:VAL:HG12	1:A:349:LYS:HD2	1.74	0.68
1:A:377:ARG:HD2	1:A:470:TYR:CE1	2.28	0.67
1:B:310:GLU:OE1	1:B:343:ARG:HD3	1.94	0.67
1:B:14:LEU:HG	1:A:14:LEU:HG	1.77	0.67
1:B:29:LEU:CD1	1:B:214:LEU:HD21	2.25	0.67
1:B:480:SER:O	1:B:489:ARG:NH2	2.28	0.66
1:A:375:GLU:OE2	1:A:489:ARG:HB3	1.98	0.64
1:A:29:LEU:CD1	1:A:214:LEU:HD21	2.29	0.63
1:A:29:LEU:HD13	1:A:214:LEU:HD21	1.81	0.62
1:A:456:ILE:HG22	1:A:456:ILE:O	1.99	0.62
1:B:310:GLU:OE1	1:B:343:ARG:CD	2.48	0.61
1:B:283:ARG:NH1	1:B:435:GLU:HG3	2.18	0.59
1:A:123:ASP:OD2	1:A:153:ARG:NE	2.36	0.59
1:B:461:ILE:HD11	5:B:880:HOH:O	2.02	0.58
1:B:29:LEU:HD13	1:B:214:LEU:HD21	1.86	0.57
1:A:86:LYS:HB2	1:A:101:GLY:HA3	1.86	0.57
1:B:480:SER:OG	1:B:482:GLU:HG2	2.04	0.57
1:B:390:LEU:HD21	1:B:393:MET:CE	2.35	0.56
1:A:263:GLN:NE2	5:A:801:HOH:O	1.82	0.55
1:A:283:ARG:NH1	1:A:435:GLU:HG3	2.22	0.54
1:B:275:ARG:NH1	5:B:803:HOH:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLN:NE2	5:A:802:HOH:O	2.32	0.52
1:A:316:LEU:HD23	1:A:335:VAL:HG21	1.91	0.52
1:A:528:ASN:HD22	1:A:533:GLN:HB2	1.75	0.51
1:B:227:GLU:N	5:B:807:HOH:O	2.44	0.50
1:B:377:ARG:HG2	1:B:378:ASP:N	2.25	0.50
1:B:298:VAL:CG1	1:B:349:LYS:HD2	2.39	0.50
1:A:29:LEU:HD22	1:A:29:LEU:O	2.12	0.50
1:B:390:LEU:HD21	1:B:393:MET:HE2	1.94	0.48
1:A:154:THR:HG23	1:A:156:GLU:H	1.78	0.48
1:A:377:ARG:HG2	1:A:378:ASP:N	2.27	0.48
1:A:155:ARG:HG2	1:A:185:MET:HE1	1.95	0.47
1:A:456:ILE:O	1:A:456:ILE:CG2	2.62	0.47
1:B:326:ARG:NH2	1:B:327:ASP:OD1	2.48	0.47
1:A:502:CYS:O	1:A:503:LEU:HB2	2.14	0.47
1:A:298:VAL:CG1	1:A:349:LYS:HD2	2.43	0.47
1:B:530:ASP:O	1:B:534:ASP:HB3	2.16	0.46
1:A:87:LEU:HD11	1:A:99:GLN:HA	1.98	0.46
1:A:261:LYS:HZ2	1:A:500:ASP:CG	2.19	0.45
1:A:133:THR:O	1:A:137:GLU:HG3	2.17	0.45
1:B:390:LEU:HD21	1:B:393:MET:HE3	1.98	0.45
1:A:300:ARG:O	1:A:304:GLU:HG3	2.17	0.45
1:B:274:PRO:HA	1:B:370:PHE:O	2.17	0.44
1:A:211:GLU:HA	1:A:211:GLU:OE1	2.18	0.43
1:A:292:VAL:O	1:A:296:GLU:HG2	2.18	0.43
1:B:324:LEU:HD23	1:B:324:LEU:N	2.35	0.41
1:B:333:ARG:NH1	1:B:336:GLN:OE1	2.54	0.41
1:A:86:LYS:HB2	1:A:101:GLY:CA	2.50	0.41
1:B:377:ARG:HG3	1:B:475:TRP:CZ2	2.56	0.41
1:A:390:LEU:HD21	1:A:393:MET:HE2	2.03	0.40
1:B:129:PHE:CZ	1:B:131:SER:HB2	2.55	0.40
1:B:310:GLU:OE1	1:B:343:ARG:HD2	2.18	0.40
1:A:125:MET:HE2	1:A:152:ALA:HA	2.04	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	528/606 (87%)	513 (97%)	13 (2%)	2 (0%)	34	28
1	B	535/606 (88%)	521 (97%)	14 (3%)	0	100	100
All	All	1063/1212 (88%)	1034 (97%)	27 (2%)	2 (0%)	47	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ASP
1	A	460	GLY

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	465/533 (87%)	438 (94%)	27 (6%)	20	15
1	B	472/533 (89%)	446 (94%)	26 (6%)	21	16
All	All	937/1066 (88%)	884 (94%)	53 (6%)	20	15

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	ASN
1	B	9	LEU
1	B	29	LEU
1	B	83	GLN
1	B	86	LYS
1	B	147	LEU
1	B	153	ARG
1	B	163	GLU
1	B	231	GLU
1	B	267	LEU

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Mol	Chain	Res	Type
1	B	284	PHE
1	B	294	LYS
1	B	324	LEU
1	B	338	ARG
1	B	377	ARG
1	B	429	ASP
1	B	459	ARG
1	B	461	ILE
1	B	474	ASN
1	B	476	ASN
1	B	484	ARG
1	B	500	ASP
1	B	534	ASP
1	B	544	LYS
1	B	549	THR
1	B	551	ARG
1	A	29	LEU
1	A	96	GLN
1	A	99	GLN
1	A	123	ASP
1	A	140	ILE
1	A	141	ASP
1	A	156	GLU
1	A	170	GLU
1	A	266	ARG
1	A	267	LEU
1	A	284	PHE
1	A	305	LYS
1	A	307	ARG
1	A	308	GLU
1	A	333	ARG
1	A	340	ILE
1	A	348	VAL
1	A	361	LYS
1	A	377	ARG
1	A	461	ILE
1	A	462	ILE
1	A	463	LYS
1	A	484	ARG
1	A	486	LYS
1	A	541	GLN
1	A	543	GLN

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Mol	Chain	Res	Type
1	A	551	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 7 ligands modelled in this entry, 5 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
3	ATP	A	702	4	26,33,33	1.00	1 (3%)	31,52,52	1.54	7 (22%)
3	ATP	B	702	4	26,33,33	1.04	0	31,52,52	1.49	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
3	ATP	A	702	4	-	2/18/38/38	0/3/3/3
3	ATP	B	702	4	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	ATP	C5-C4	2.26	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ATP	N3-C2-N1	-3.81	122.72	128.68
3	B	702	ATP	N3-C2-N1	-3.59	123.07	128.68
3	A	702	ATP	O2B-PB-O1B	2.85	126.33	112.24
3	B	702	ATP	O2'-C2'-C3'	-2.85	102.60	111.82
3	B	702	ATP	PA-O3A-PB	-2.73	123.46	132.83
3	A	702	ATP	C3'-C2'-C1'	2.59	104.87	100.98
3	A	702	ATP	O2G-PG-O3B	2.47	112.92	104.64
3	A	702	ATP	C1'-N9-C4	-2.34	122.52	126.64
3	A	702	ATP	C2-N1-C6	2.23	122.57	118.75
3	B	702	ATP	C1'-N9-C4	-2.20	122.77	126.64
3	A	702	ATP	PA-O3A-PB	-2.16	125.43	132.83
3	B	702	ATP	C2-N1-C6	2.15	122.42	118.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

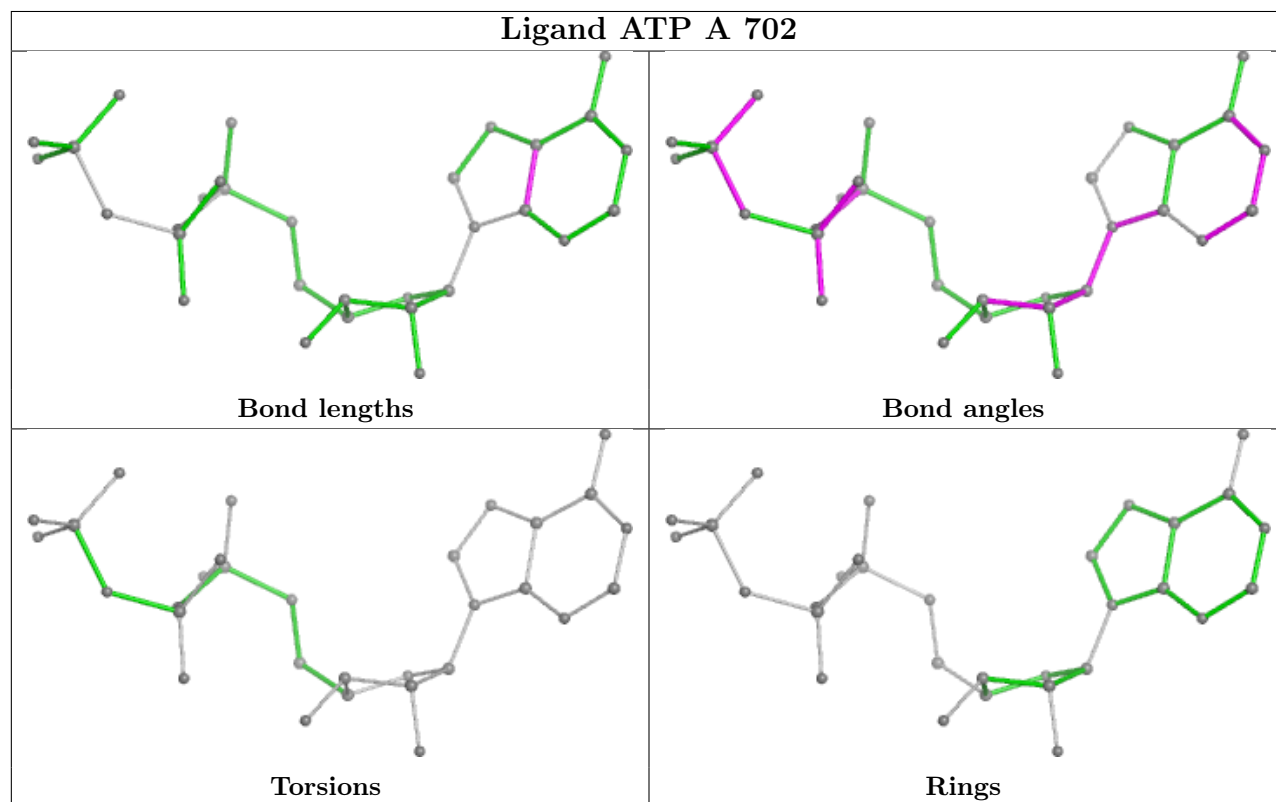
Mol	Chain	Res	Type	Atoms
3	B	702	ATP	PA-O3A-PB-O2B
3	A	702	ATP	PA-O3A-PB-O2B
3	B	702	ATP	PB-O3B-PG-O3G
3	B	702	ATP	PA-O3A-PB-O1B
3	A	702	ATP	PA-O3A-PB-O1B

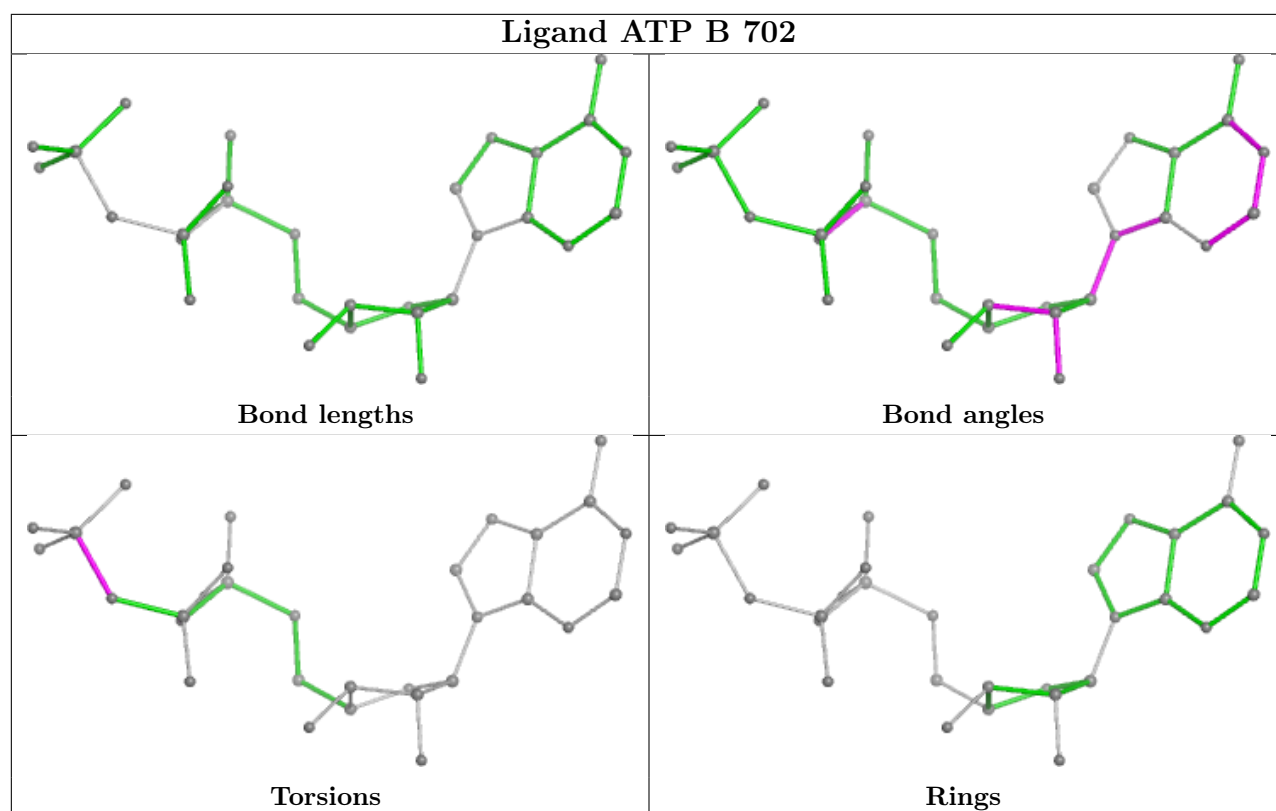
There are no ring outliers.

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 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	534/606 (88%)	0.32	28 (5%) 27 26	31, 50, 90, 136	0
1	B	541/606 (89%)	0.30	21 (3%) 39 39	28, 47, 85, 147	0
All	All	1075/1212 (88%)	0.31	49 (4%) 32 32	28, 49, 88, 147	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	19.1
1	A	3	PHE	16.9
1	A	2	ALA	16.1
1	B	3	PHE	11.7
1	A	1	MET	8.0
1	B	231	GLU	6.5
1	A	471	LEU	6.2
1	A	510	PHE	5.4
1	B	4	THR	5.0
1	B	1	MET	4.9
1	B	471	LEU	4.7
1	B	321	GLY	4.6
1	B	510	PHE	4.4
1	A	551	ARG	3.9
1	B	459	ARG	3.8
1	A	462	ILE	3.5
1	A	403	GLY	3.5
1	B	519	TYR	3.4
1	A	228	THR	3.2
1	A	466	ASP	3.2
1	A	87	LEU	3.1
1	A	324	LEU	3.0
1	A	456	ILE	2.9
1	B	89	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	509	PRO	2.8
1	A	487	ARG	2.8
1	A	486	LYS	2.7
1	A	544	LYS	2.6
1	B	228	THR	2.6
1	A	550	PHE	2.6
1	A	532	GLU	2.5
1	A	491	MET	2.4
1	B	82	ILE	2.4
1	A	543	GLN	2.4
1	B	491	MET	2.4
1	A	483	LEU	2.4
1	B	335	VAL	2.4
1	A	463	LYS	2.4
1	B	461	ILE	2.3
1	B	320	LEU	2.2
1	A	481	SER	2.2
1	A	333	ARG	2.2
1	A	508	LEU	2.1
1	B	340	ILE	2.1
1	A	521	ASP	2.1
1	B	328	SER	2.0
1	B	483	LEU	2.0
1	A	405	MET	2.0
1	B	487	ARG	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](#)

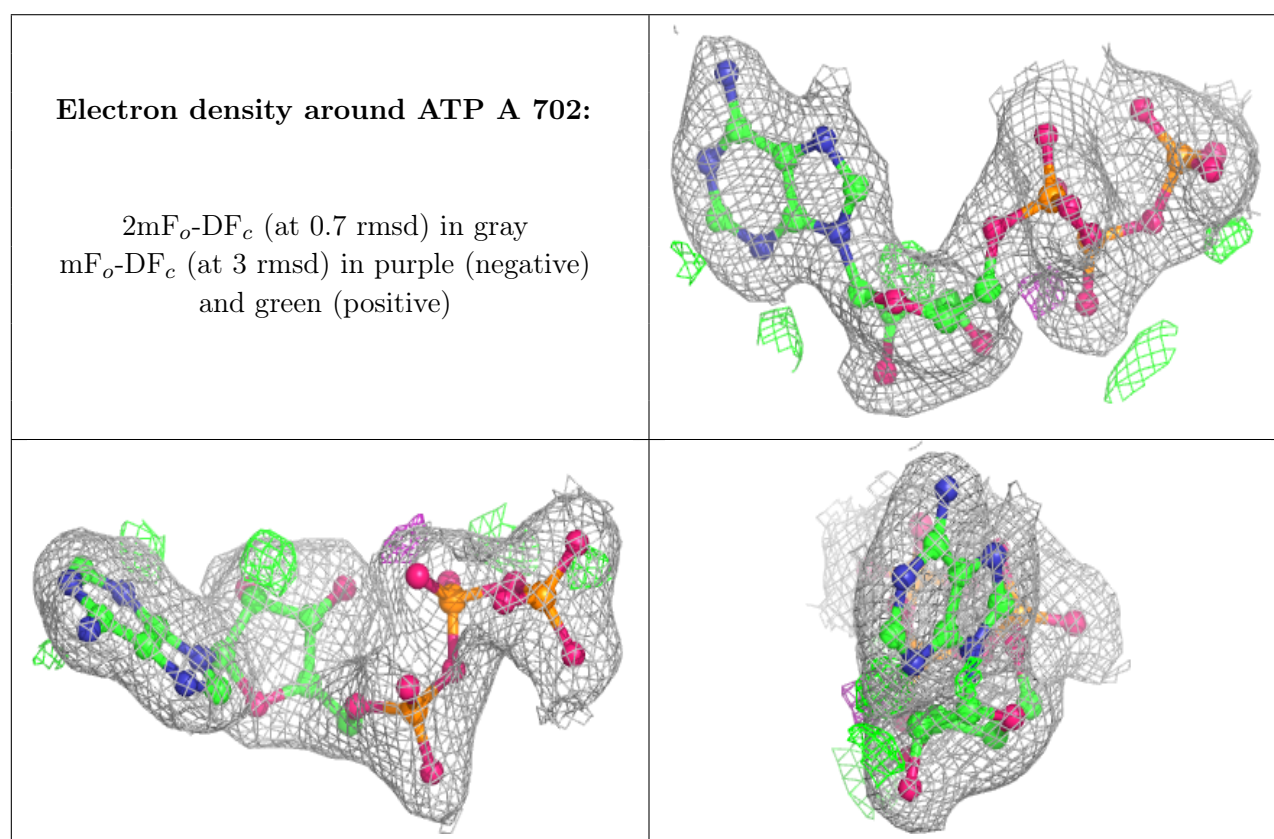
There are no monosaccharides in this entry.

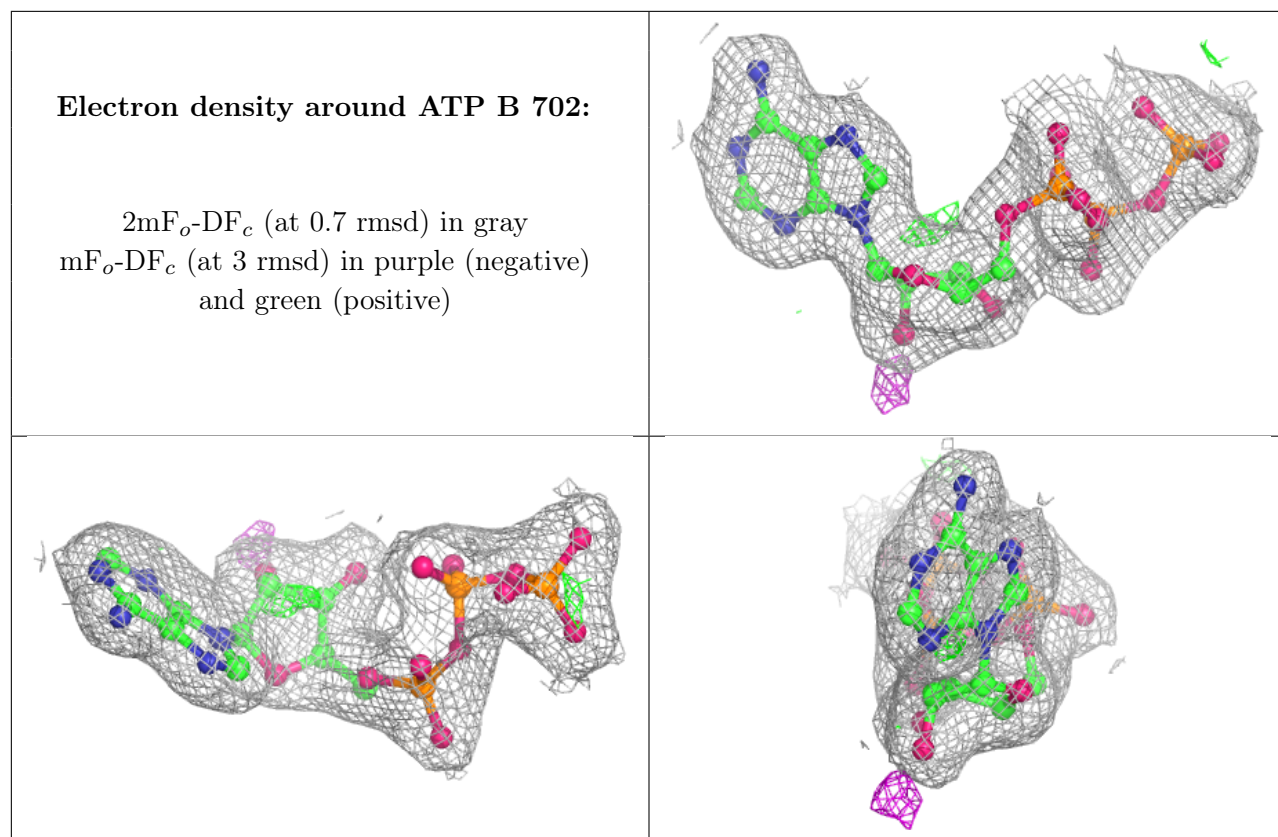
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	MG	B	704	1/1	0.79	0.12	39,39,39,39	1
4	MG	B	703	1/1	0.94	0.11	30,30,30,30	0
3	ATP	A	702	31/31	0.99	0.13	30,37,45,51	0
2	ZN	A	701	1/1	0.99	0.10	48,48,48,48	0
3	ATP	B	702	31/31	0.99	0.13	26,31,38,40	0
4	MG	A	703	1/1	0.99	0.15	36,36,36,36	0
2	ZN	B	701	1/1	1.00	0.14	37,37,37,37	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.