



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5OFB / pdb_00005ofb
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

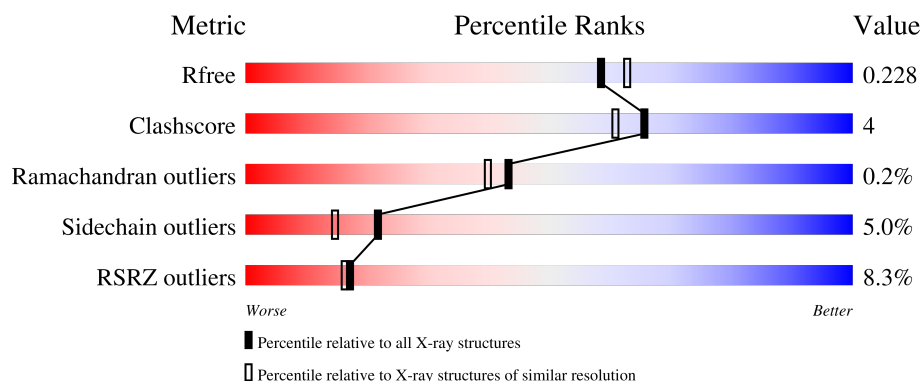
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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	7% 76% 10% • 12%
1	B	606	8% 79% 8% • 11%

2 Entry composition

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
1	B	541	Total	C	N	O	S	0	0	0
			4387	2768	779	812	28			
1	A	534	Total	C	N	O	S	0	0	0
			4326	2728	768	802	28			

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 (CCD ID: 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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	169	Total O 169 169	0	0
5	A	135	Total O 135 135	0	0

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)	Xtriage
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 (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ATP

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	0.94	2/4412 (0.0%)	1.05	20/5940 (0.3%)
1	B	0.97	3/4476 (0.1%)	1.05	19/6028 (0.3%)
All	All	0.95	5/8888 (0.1%)	1.05	39/11968 (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	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	B	83	GLN	N-CA	-6.44	1.38	1.46
1	B	489	ARG	CD-NE	-6.27	1.37	1.46
1	A	86	LYS	CA-C	-6.13	1.45	1.52
1	B	94	SER	C-O	-5.54	1.17	1.24
1	A	431	ALA	C-O	5.42	1.30	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ARG	N-CA-C	10.09	123.32	111.71
1	A	459	ARG	CA-C-N	9.03	139.12	121.41
1	A	459	ARG	C-N-CA	9.03	139.12	121.41
1	A	185	MET	CG-SD-CE	8.11	118.75	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	ILE	CB-CA-C	-7.91	101.46	112.14
1	B	467	GLU	CA-CB-CG	7.51	129.13	114.10
1	B	491	MET	CA-CB-CG	7.40	128.90	114.10
1	B	519	TYR	CA-C-N	7.37	127.37	119.78
1	B	519	TYR	C-N-CA	7.37	127.37	119.78
1	A	85	GLY	O-C-N	-7.26	114.21	122.56
1	B	267	LEU	CB-CG-CD1	7.20	132.30	110.70
1	B	476	ASN	CB-CA-C	6.69	121.26	110.09
1	A	85	GLY	CA-C-N	-6.36	111.13	122.45
1	A	85	GLY	C-N-CA	-6.36	111.13	122.45
1	A	267	LEU	CB-CG-CD1	6.34	129.72	110.70
1	B	489	ARG	CD-NE-CZ	6.34	133.27	124.40
1	A	466	ASP	CB-CA-C	6.31	122.79	110.67
1	B	489	ARG	NE-CZ-NH1	6.22	127.72	121.50
1	B	459	ARG	N-CA-C	6.13	120.97	112.45
1	A	460	GLY	N-CA-C	6.11	127.65	113.18
1	B	459	ARG	CA-C-N	6.10	133.37	121.41
1	B	459	ARG	C-N-CA	6.10	133.37	121.41
1	A	54	ARG	CB-CG-CD	6.04	125.19	111.30
1	B	318	VAL	CB-CA-C	-6.00	104.29	111.97
1	B	83	GLN	CA-C-O	5.97	127.11	120.43
1	A	459	ARG	CA-C-O	-5.87	113.47	120.10
1	B	83	GLN	CB-CA-C	5.71	119.76	110.22
1	A	266	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	B	83	GLN	N-CA-C	-5.45	100.30	108.96
1	A	403	GLY	N-CA-C	-5.43	102.49	110.97
1	A	2	ALA	CA-C-N	5.35	127.77	120.54
1	A	2	ALA	C-N-CA	5.35	127.77	120.54
1	A	328	SER	N-CA-C	5.35	117.11	111.28
1	B	358	ARG	CG-CD-NE	5.33	123.73	112.00
1	B	491	MET	CB-CA-C	-5.33	100.13	110.46
1	A	482	GLU	CA-CB-CG	5.10	124.31	114.10
1	A	463	LYS	CB-CG-CD	5.10	123.03	111.30
1	B	393	MET	CG-SD-CE	5.05	112.02	100.90
1	A	459	ARG	O-C-N	-5.03	116.34	122.22

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

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Mol	Chain	Res	Type	Group
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	37	0
1	B	4387	0	4367	31	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	67	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 4.

All (67) 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:390:LEU:HD21	1:A:393:MET:HE2	1.62	0.80
1:A:125:MET:HE3	1:A:185:MET:HE1	1.67	0.77
1:B:154:THR:OG1	1:B:156:GLU:HG2	1.85	0.76
1:A:125:MET:CE	1:A:185:MET:HE1	2.20	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:155:ARG:HG2	1:A:185:MET:HE2	1.82	0.61
1:A:390:LEU:CD2	1:A:393:MET:HE2	2.31	0.59
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
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:B:390:LEU:HD21	1:B:393:MET:HE3	1.91	0.51
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: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: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:133:THR:O	1:A:137:GLU:HG3	2.17	0.45
1:A:155:ARG:CD	1:A:185:MET:HE2	2.47	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:243:TYR:CD1	1:A:393:MET:HE1	2.53	0.43
1:A:292:VAL:O	1:A:296:GLU:HG2	2.18	0.43
1:B:381:GLY:C	1:B:382:MET:HE2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MET:HE1	1:A:185:MET:HE1	1.99	0.43
1:B:390:LEU:HD21	1:B:393:MET:HE2	2.01	0.43
1:B:390:LEU:CD2	1:B:393:MET:HE3	2.48	0.43
1:B:459:ARG:C	1:B:459:ARG:HD3	2.43	0.43
1:A:155:ARG:CG	1:A:185:MET:HE2	2.47	0.43
1:A:125:MET:HE2	1:A:152:ALA:HA	2.02	0.42
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:A:381:GLY:C	1:A:382:MET:HE2	2.46	0.41
1:B:377:ARG:HG3	1:B:475:TRP:CZ2	2.56	0.41
1:B:476:ASN:OD1	1:B:476:ASN:C	2.65	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

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%)	30	22
1	B	535/606 (88%)	521 (97%)	14 (3%)	0	100	100
All	All	1063/1212 (88%)	1034 (97%)	27 (2%)	2 (0%)	43	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ASP
1	A	460	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	465/533 (87%)	440 (95%)	25 (5%)	20	13
1	B	472/533 (89%)	450 (95%)	22 (5%)	23	16
All	All	937/1066 (88%)	890 (95%)	47 (5%)	22	15

All (47) 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
1	B	301	ILE
1	B	324	LEU
1	B	348	VAL
1	B	456	ILE
1	B	459	ARG
1	B	461	ILE
1	B	474	ASN
1	B	476	ASN
1	B	500	ASP
1	B	534	ASP
1	B	544	LYS
1	B	549	THR
1	A	29	LEU
1	A	96	GLN
1	A	99	GLN
1	A	123	ASP
1	A	140	ILE

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Mol	Chain	Res	Type
1	A	141	ASP
1	A	156	GLU
1	A	170	GLU
1	A	266	ARG
1	A	267	LEU
1	A	300	ARG
1	A	305	LYS
1	A	308	GLU
1	A	340	ILE
1	A	348	VAL
1	A	349	LYS
1	A	361	LYS
1	A	461	ILE
1	A	462	ILE
1	A	463	LYS
1	A	483	LEU
1	A	486	LYS
1	A	541	GLN
1	A	543	GLN
1	A	551	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	ASN
1	B	22	ASN
1	B	102	ASN
1	B	376	HIS
1	A	22	ASN
1	A	83	GLN
1	A	96	GLN
1	A	99	GLN
1	A	102	ASN
1	A	376	HIS

5.3.3 RNA ⓘ

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](#)

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	32,33,33	1.67	5 (15%)	48,52,52	1.74	11 (22%)
3	ATP	B	702	4	32,33,33	1.64	5 (15%)	48,52,52	1.82	12 (25%)

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	-	2/22/38/38	0/3/3/3
3	ATP	B	702	4	-	3/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	ATP	PB-O3B	5.49	1.65	1.59
3	B	702	ATP	PB-O3A	5.17	1.65	1.59
3	A	702	ATP	C5-C4	4.38	1.46	1.39
3	B	702	ATP	C5-C4	3.97	1.46	1.39
3	B	702	ATP	C4-N9	-2.58	1.32	1.37
3	A	702	ATP	C4-N9	-2.56	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ATP	C5-C6	2.53	1.48	1.41
3	A	702	ATP	C8-N7	2.46	1.36	1.31
3	A	702	ATP	C5-C6	2.30	1.47	1.41
3	B	702	ATP	PG-O2G	-2.05	1.47	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	ATP	C5-C4-N3	-4.36	120.71	126.72
3	A	702	ATP	C5-C4-N3	-4.35	120.72	126.72
3	B	702	ATP	N3-C4-N9	4.29	134.47	127.17
3	B	702	ATP	C4-N9-C8	4.09	110.03	105.74
3	A	702	ATP	N3-C2-N1	-3.87	122.72	128.58
3	A	702	ATP	N3-C4-N9	3.71	133.47	127.17
3	B	702	ATP	N3-C2-N1	-3.64	123.07	128.58
3	A	702	ATP	C2-N3-C4	3.27	119.82	111.83
3	B	702	ATP	C2-N3-C4	3.15	119.54	111.83
3	A	702	ATP	C4-N9-C8	3.06	108.95	105.74
3	A	702	ATP	O2B-PB-O1B	2.98	126.33	112.44
3	B	702	ATP	O2'-C2'-C3'	-2.87	102.60	111.82
3	B	702	ATP	N9-C8-N7	-2.63	110.20	113.94
3	A	702	ATP	O2G-PG-O3B	2.47	112.92	104.64
3	B	702	ATP	O3A-PA-O1A	-2.41	103.44	110.70
3	A	702	ATP	C2-N1-C6	2.34	122.57	118.73
3	B	702	ATP	C2-N1-C6	2.25	122.42	118.73
3	A	702	ATP	C4-C5-N7	-2.24	108.02	110.58
3	A	702	ATP	C6-C5-N7	2.21	136.36	132.09
3	B	702	ATP	C4-C5-N7	-2.18	108.09	110.58
3	B	702	ATP	C5-N7-C8	2.16	106.84	103.45
3	A	702	ATP	O2A-PA-O3A	2.10	112.95	107.27
3	B	702	ATP	O2B-PB-O3B	2.08	112.90	107.27

There are no chirality outliers.

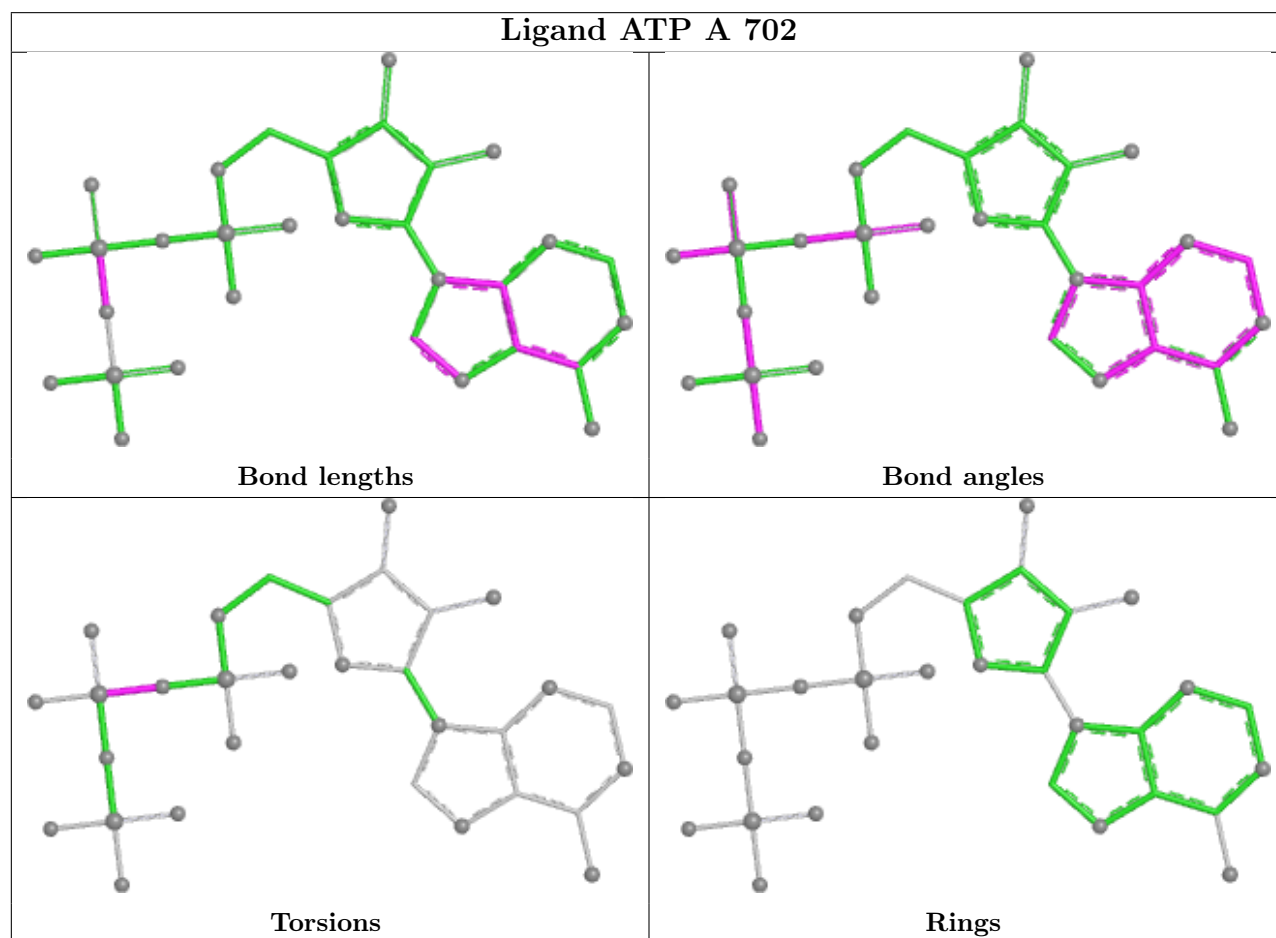
All (5) torsion outliers are listed below:

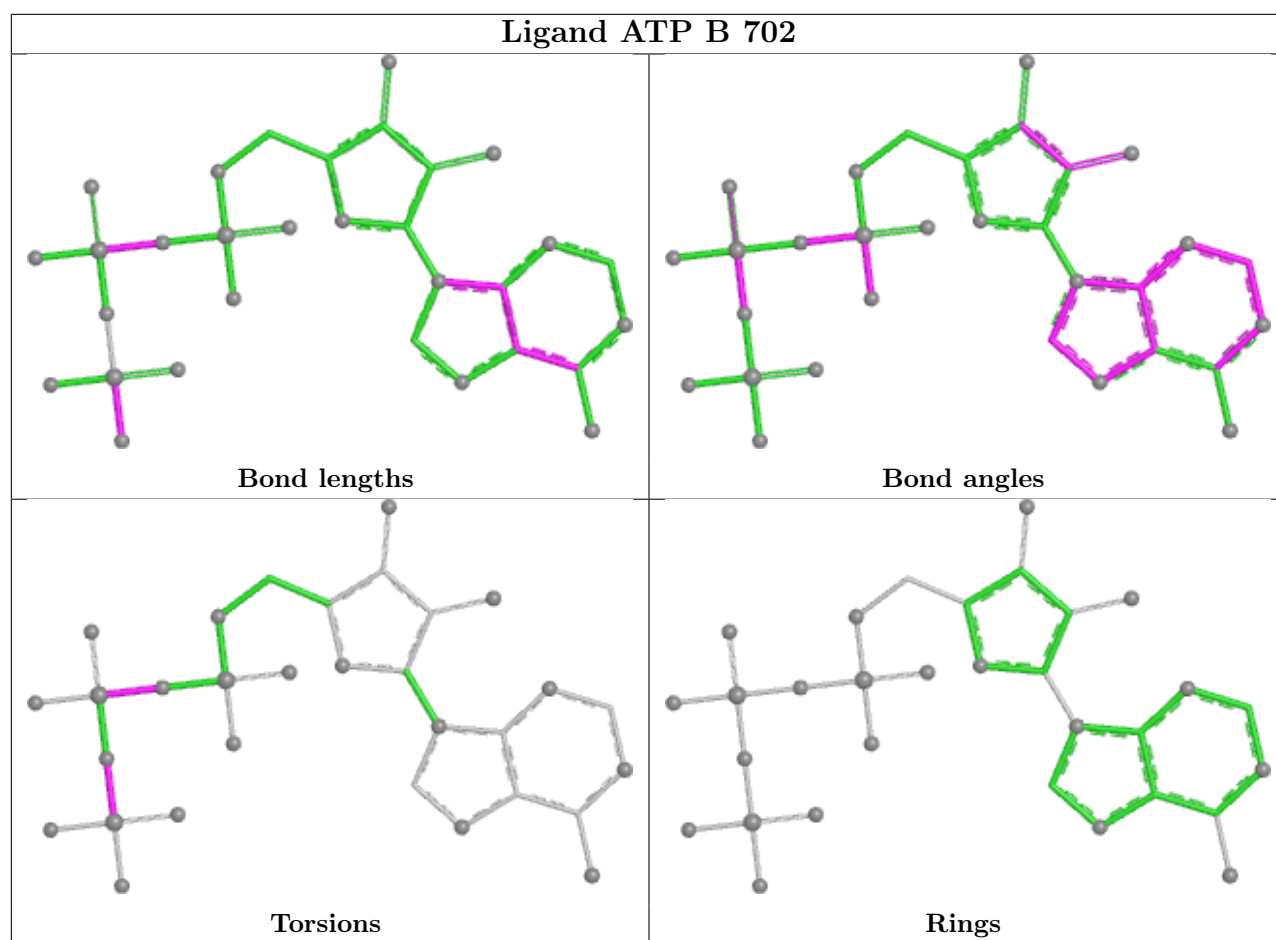
Mol	Chain	Res	Type	Atoms
3	B	702	ATP	PA-O3A-PB-O2B
3	A	702	ATP	PA-O3A-PB-O2B
3	B	702	ATP	PB-O3B-PG-O3G
3	B	702	ATP	PA-O3A-PB-O1B
3	A	702	ATP	PA-O3A-PB-O1B

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%)	0.63	42 (7%) 18 18	31, 50, 90, 136	0
1	B	541/606 (89%)	0.50	47 (8%) 16 15	28, 47, 85, 147	0
All	All	1075/1212 (88%)	0.57	89 (8%) 17 16	28, 49, 88, 147	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	PHE	8.7
1	B	510	PHE	7.5
1	A	510	PHE	7.2
1	B	324	LEU	6.3
1	B	471	LEU	6.0
1	A	2	ALA	5.4
1	A	87	LEU	5.3
1	A	324	LEU	5.1
1	B	3	PHE	4.6
1	A	471	LEU	4.5
1	B	2	ALA	4.4
1	B	82	ILE	4.2
1	B	461	ILE	4.1
1	A	95	THR	3.8
1	B	301	ILE	3.7
1	A	462	ILE	3.6
1	B	4	THR	3.6
1	B	348	VAL	3.5
1	A	509	PRO	3.5
1	A	461	ILE	3.5
1	B	321	GLY	3.4
1	B	335	VAL	3.4
1	A	1	MET	3.4
1	A	4	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	550	PHE	3.3
1	A	466	ASP	3.3
1	B	519	TYR	3.3
1	A	403	GLY	3.3
1	A	456	ILE	3.3
1	A	491	MET	3.3
1	A	549	THR	3.2
1	A	508	LEU	3.2
1	B	341	THR	3.2
1	A	507	THR	3.2
1	B	1	MET	3.1
1	A	521	ASP	3.1
1	A	405	MET	3.1
1	B	320	LEU	2.9
1	B	352	ILE	2.9
1	B	459	ARG	2.9
1	A	463	LYS	2.9
1	A	486	LYS	2.9
1	B	325	THR	2.8
1	A	154	THR	2.8
1	B	309	ALA	2.8
1	A	475	TRP	2.7
1	B	318	VAL	2.7
1	A	483	LEU	2.7
1	B	228	THR	2.6
1	A	318	VAL	2.6
1	B	491	MET	2.6
1	B	305	LYS	2.6
1	B	147	LEU	2.6
1	B	457	ALA	2.6
1	A	189	MET	2.5
1	B	92	PRO	2.4
1	B	520	PRO	2.4
1	A	86	LYS	2.4
1	A	322	GLY	2.3
1	B	490	ALA	2.3
1	B	179	ARG	2.3
1	A	228	THR	2.3
1	A	263	GLN	2.2
1	A	533	GLN	2.2
1	A	493	ILE	2.2
1	B	508	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	509	PRO	2.2
1	B	88	ALA	2.2
1	B	313	ALA	2.2
1	A	270	CYS	2.2
1	B	328	SER	2.2
1	B	337	ASN	2.2
1	A	348	VAL	2.1
1	B	405	MET	2.1
1	B	475	TRP	2.1
1	A	404	GLY	2.1
1	A	473	ALA	2.1
1	B	481	SER	2.1
1	B	483	LEU	2.1
1	A	229	SER	2.1
1	B	458	GLN	2.1
1	B	549	THR	2.1
1	A	297	HIS	2.1
1	B	89	LYS	2.1
1	B	550	PHE	2.1
1	B	14	LEU	2.0
1	A	548	GLY	2.0
1	B	330	VAL	2.0
1	B	522	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

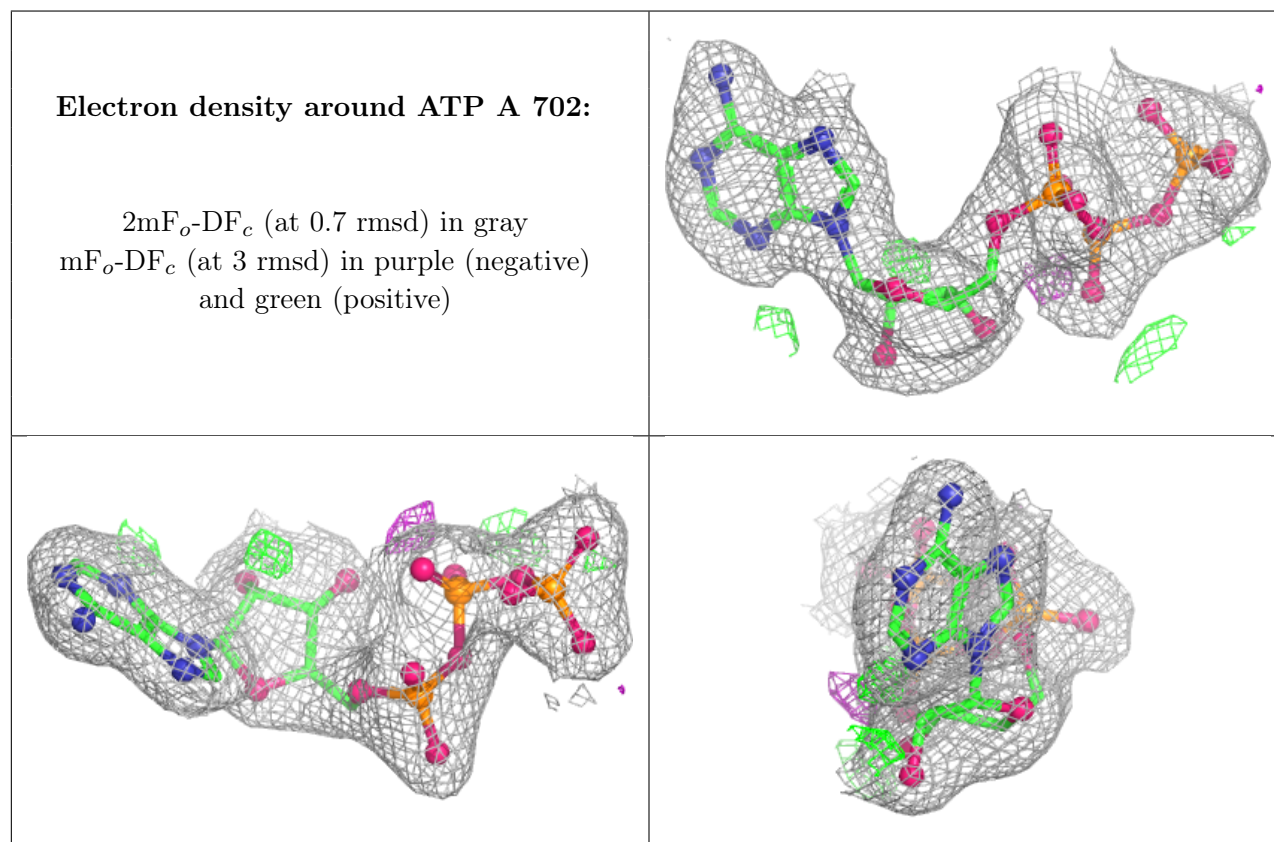
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

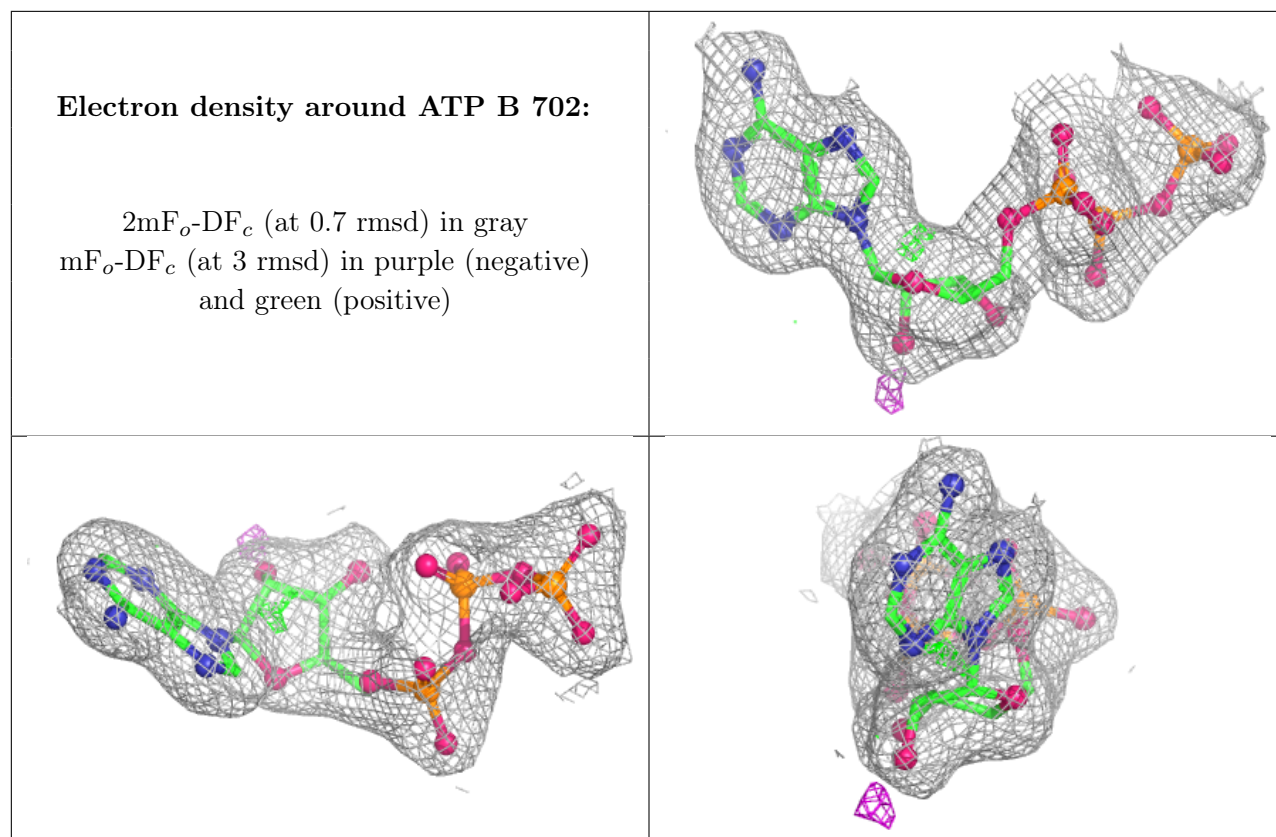
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	704	1/1	0.91	0.07	39,39,39,39	1
3	ATP	A	702	31/31	0.98	0.05	30,37,45,51	0
3	ATP	B	702	31/31	0.98	0.05	26,31,38,40	0
4	MG	B	703	1/1	0.99	0.03	30,30,30,30	0
4	MG	A	703	1/1	0.99	0.04	36,36,36,36	0
2	ZN	A	701	1/1	1.00	0.05	48,48,48,48	0
2	ZN	B	701	1/1	1.00	0.02	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.