



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:57 AM UTC

PDB ID : 8ROF / pdb_00008rof
Title : Human cohesin SMC1A-HD(shortCC-EQ)/RAD21-C complex - ADP-Mg-bound conformation
Authors : Vitoria Gomes, M.; Romier, C.
Deposited on : 2024-01-11
Resolution : 1.65 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)
Xtrriage (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

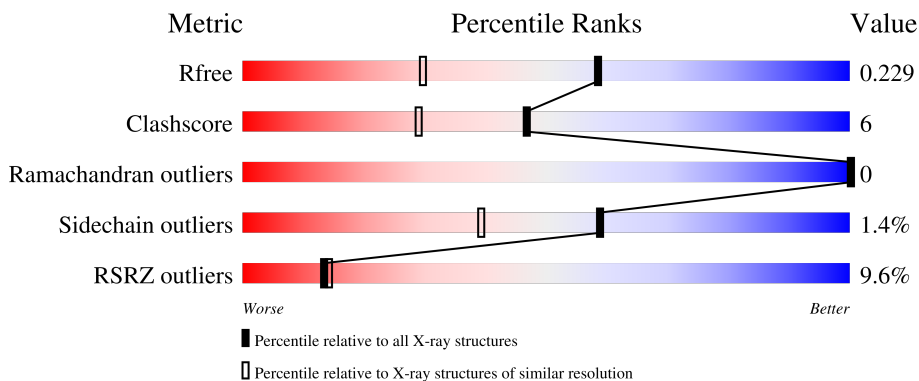
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

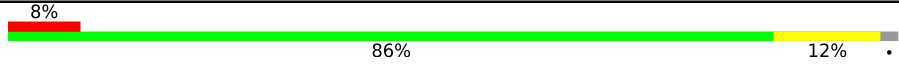
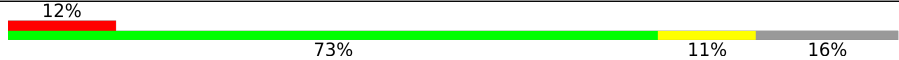
The reported resolution of this entry is 1.65 Å.

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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	366	
2	B	81	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3731 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 Structural maintenance of chromosomes protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2857	1822	483	541	11	0	12	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	GLY	-	linker	UNP Q14683
A	177	SER	-	linker	UNP Q14683
A	178	GLY	-	linker	UNP Q14683
A	179	SER	-	linker	UNP Q14683
A	180	LEU	-	linker	UNP Q14683
A	181	VAL	-	linker	UNP Q14683
A	182	PRO	-	linker	UNP Q14683
A	183	ARG	-	linker	UNP Q14683
A	1051	GLY	-	linker	UNP Q14683
A	1052	SER	-	linker	UNP Q14683
A	1053	GLY	-	linker	UNP Q14683
A	1054	SER	-	linker	UNP Q14683
A	1055	ALA	-	linker	UNP Q14683
A	1056	LYS	-	linker	UNP Q14683
A	1157	GLN	GLU	engineered mutation	UNP Q14683

- Molecule 2 is a protein called 64-kDa C-terminal product.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	68	544	350	93	100	1	0	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	557	MET	-	initiating methionine	UNP O60216

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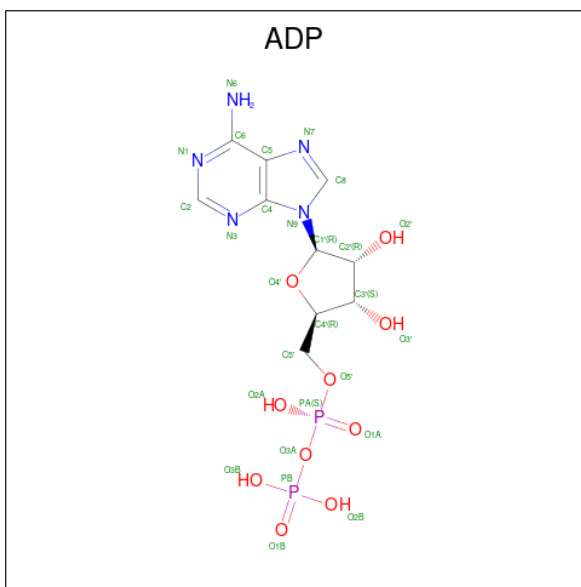
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Chain	Residue	Modelled	Actual	Comment	Reference
B	630	GLY	-	expression tag	UNP O60216
B	631	SER	-	expression tag	UNP O60216
B	632	LEU	-	expression tag	UNP O60216
B	633	GLU	-	expression tag	UNP O60216
B	634	VAL	-	expression tag	UNP O60216
B	635	LEU	-	expression tag	UNP O60216
B	636	PHE	-	expression tag	UNP O60216
B	637	GLN	-	expression tag	UNP O60216

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 27 10 5 10 2	0	0

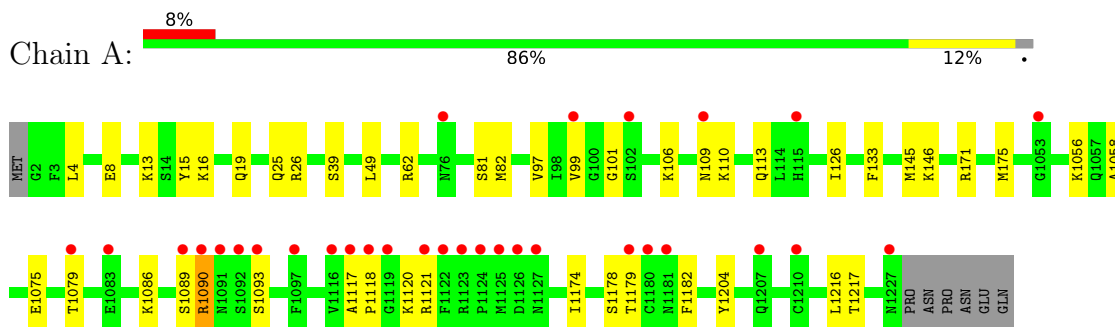
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	245	Total 245	O 245	0	0
5	B	57	Total 57	O 57	0	0

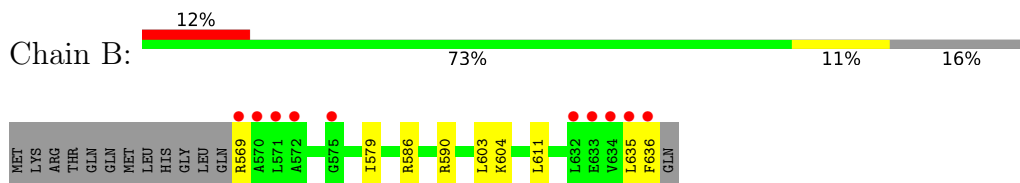
3 Residue-property plots [i](#)

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: Structural maintenance of chromosomes protein 1A



- Molecule 2: 64-kDa C-terminal product



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	66.45Å 113.91Å 133.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.57 – 1.65 43.57 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.57-1.65) 99.7 (43.57-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.65Å)	Xtrriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.196 , 0.228 0.197 , 0.229	Depositor DCC
R_{free} test set	3134 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3731	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: ADP, 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	0.29	0/2945	0.50	0/3964
2	B	0.31	0/559	0.46	0/753
All	All	0.29	0/3504	0.50	0/4717

There are no bond length outliers.

There are no bond angle outliers.

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	2857	0	2898	34	0
2	B	544	0	566	7	0
3	A	1	0	0	0	0
4	A	27	0	12	2	0
5	A	245	0	0	8	1
5	B	57	0	0	2	0
All	All	3731	0	3476	39	1

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 6.

All (39) 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:16:LYS:O	1:A:19[B]:GLN:NE2	2.12	0.82
1:A:1093:SER:OG	5:A:2101:HOH:O	2.09	0.69
1:A:1216:LEU:HD11	2:B:611:LEU:HD13	1.73	0.68
1:A:1178:SER:HA	1:A:1182:PHE:O	1.98	0.64
1:A:49:LEU:HD21	1:A:82[A]:MET:HE1	1.80	0.64
1:A:62:ARG:HG3	1:A:101:GLY:HA2	1.82	0.62
1:A:62:ARG:NH2	5:A:2105:HOH:O	2.30	0.61
1:A:15:TYR:C	1:A:19[B]:GLN:HE22	2.10	0.59
2:B:569:ARG:N	5:B:702:HOH:O	2.38	0.56
2:B:586:ARG:O	5:B:701:HOH:O	2.19	0.54
1:A:39[B]:SER:OG	4:A:2001:ADP:O2A	2.26	0.53
1:A:171:ARG:HD2	1:A:1058:ALA:HB1	1.91	0.52
1:A:110:LYS:NZ	5:A:2102:HOH:O	2.23	0.52
1:A:1086:LYS:O	1:A:1090:ARG:N	2.43	0.52
1:A:97:VAL:HG12	1:A:99:VAL:HG23	1.92	0.52
1:A:49:LEU:HD13	1:A:133:PHE:CE2	2.45	0.51
1:A:1090:ARG:HD3	5:A:2176:HOH:O	2.12	0.50
2:B:603:LEU:HD21	2:B:635:LEU:HD13	1.95	0.48
1:A:8:GLU:HB3	1:A:81[A]:SER:OG	2.13	0.48
1:A:106:LYS:HE2	1:A:109:ASN:HA	1.95	0.48
1:A:49:LEU:HD13	1:A:133:PHE:HE2	1.78	0.47
5:A:2152:HOH:O	2:B:590:ARG:HD3	2.15	0.47
1:A:1204:TYR:CD1	2:B:604:LYS:HG2	2.50	0.47
1:A:49:LEU:HD22	1:A:126:ILE:HG21	1.97	0.47
1:A:113:GLN:NE2	5:A:2107:HOH:O	2.33	0.45
1:A:25:GLN:NE2	5:A:2126:HOH:O	2.50	0.45
1:A:1089:SER:HB3	1:A:1118:PRO:HG3	1.98	0.44
1:A:25:GLN:HG3	5:A:2232:HOH:O	2.17	0.44
1:A:175:MET:HE2	1:A:175:MET:HB3	1.75	0.43
1:A:175:MET:HG3	1:A:1056:LYS:HA	2.01	0.43
1:A:1075:GLU:O	1:A:1079:THR:HG23	2.19	0.43
1:A:1117:ALA:HB3	1:A:1120:LYS:HG3	2.01	0.43
1:A:1174:ILE:O	1:A:1178:SER:N	2.50	0.42
1:A:49:LEU:CD2	1:A:82[A]:MET:HE1	2.49	0.41
1:A:26[B]:ARG:NH1	1:A:1179:THR:HG23	2.36	0.41
2:B:579[B]:ILE:HD13	2:B:636:PHE:CG	2.56	0.41
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.95	0.41
1:A:13:LYS:HA	4:A:2001:ADP:N6	2.36	0.40
1:A:146:LYS:HB3	1:A:146:LYS:HE2	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2126:HOH:O	5:A:2301:HOH:O[8_555]	2.16	0.04

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	369/366 (101%)	364 (99%)	5 (1%)	0	100	100
2	B	68/81 (84%)	68 (100%)	0	0	100	100
All	All	437/447 (98%)	432 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	312/307 (102%)	307 (98%)	5 (2%)	55	34
2	B	59/69 (86%)	59 (100%)	0	100	100
All	All	371/376 (99%)	366 (99%)	5 (1%)	59	42

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

Mol	Chain	Res	Type
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	145	MET
1	A	1090	ARG
1	A	1121	ARG
1	A	1217	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1157	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ADP	A	2001	3	28,29,29	3.36	11 (39%)	43,45,45	1.99	10 (23%)

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	ADP	A	2001	3	-	2/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	ADP	C2'-C3'	-10.54	1.24	1.53
4	A	2001	ADP	PA-O3A	8.50	1.68	1.59
4	A	2001	ADP	O4'-C1'	-5.44	1.29	1.42
4	A	2001	ADP	C6-N6	4.81	1.46	1.34
4	A	2001	ADP	C2'-C1'	3.78	1.65	1.53
4	A	2001	ADP	O3'-C3'	3.71	1.52	1.43
4	A	2001	ADP	C5'-C4'	-3.49	1.41	1.51
4	A	2001	ADP	O4'-C4'	3.25	1.52	1.45
4	A	2001	ADP	O2'-C2'	2.66	1.49	1.43
4	A	2001	ADP	C8-N9	-2.52	1.33	1.37
4	A	2001	ADP	C5-N7	-2.06	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	ADP	C5-C4-N3	-6.00	118.45	126.72
4	A	2001	ADP	N3-C2-N1	-4.44	121.86	128.58
4	A	2001	ADP	C4-C5-N7	-4.05	105.95	110.58
4	A	2001	ADP	C2-N3-C4	3.94	121.46	111.83
4	A	2001	ADP	N3-C4-N9	3.81	133.65	127.17
4	A	2001	ADP	C5-N7-C8	3.47	108.90	103.45
4	A	2001	ADP	O4'-C1'-N9	2.92	113.70	108.09
4	A	2001	ADP	N9-C8-N7	-2.90	109.82	113.94
4	A	2001	ADP	O2B-PB-O3A	2.12	111.73	104.64
4	A	2001	ADP	O2A-PA-O3A	2.03	112.75	107.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

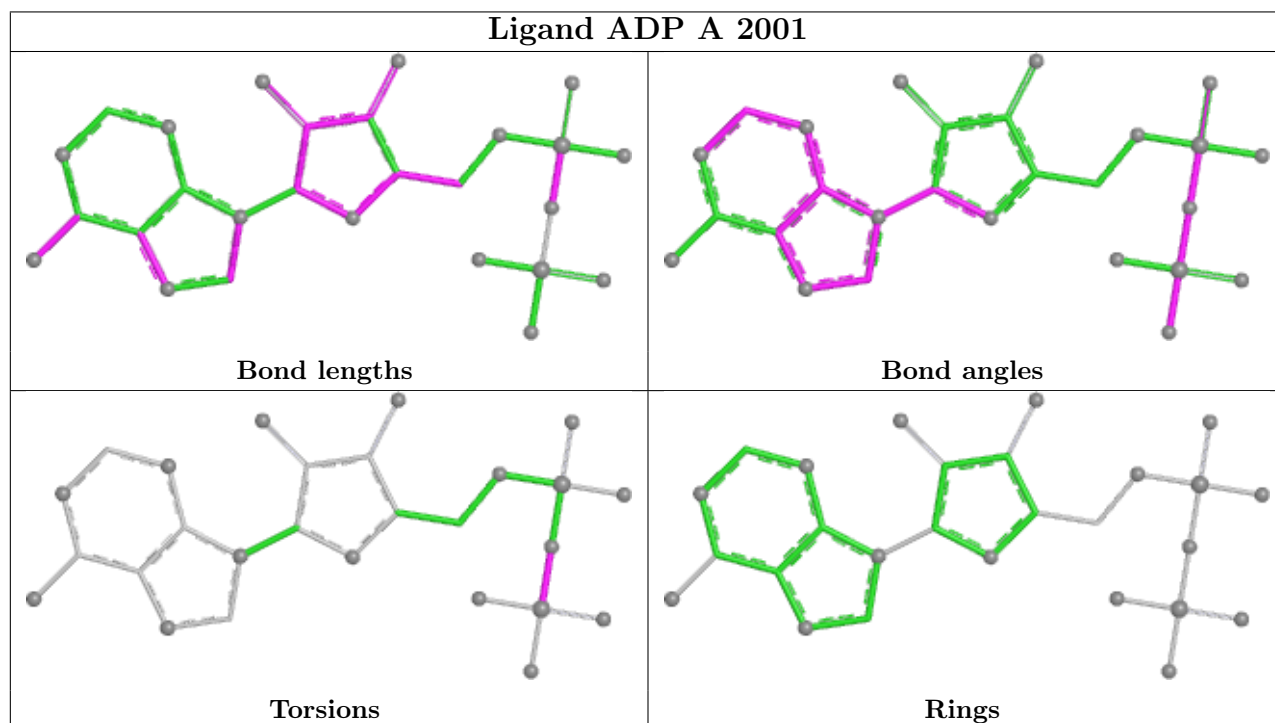
Mol	Chain	Res	Type	Atoms
4	A	2001	ADP	PA-O3A-PB-O3B
4	A	2001	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	359/366 (98%)	0.47	31 (8%) 16 18	12, 29, 59, 112	12 (3%)
2	B	68/81 (83%)	0.40	10 (14%) 6 6	13, 26, 62, 115	2 (2%)
All	All	427/447 (95%)	0.46	41 (9%) 13 14	12, 28, 61, 115	14 (3%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1123	ARG	7.2
1	A	1118	PRO	6.8
1	A	1090	ARG	5.3
1	A	1122	PHE	5.3
1	A	1124	PRO	5.2
1	A	1097	PHE	5.2
1	A	1121	ARG	4.7
2	B	570	ALA	4.4
1	A	1091	ASN	4.3
1	A	1180	CYS	4.3
2	B	636	PHE	4.3
1	A	1179	THR	4.3
2	B	634	VAL	4.3
1	A	1117	ALA	3.8
1	A	1092	SER	3.5
1	A	1119	GLY	3.3
2	B	572	ALA	3.3
2	B	635	LEU	3.2
2	B	569	ARG	3.2
2	B	632	LEU	3.0
1	A	1181	ASN	3.0
1	A	1125	MET	2.8
2	B	571	LEU	2.7
1	A	102	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1093	SER	2.6
1	A	1210	CYS	2.6
1	A	1127	ASN	2.6
1	A	99	VAL	2.5
1	A	1053	GLY	2.5
1	A	1089	SER	2.4
1	A	109	ASN	2.4
1	A	1227	ASN	2.4
1	A	1126	ASP	2.4
1	A	115	HIS	2.4
2	B	633	GLU	2.4
1	A	1207	GLN	2.3
1	A	76[A]	ASN	2.2
1	A	1079	THR	2.1
1	A	1116	VAL	2.1
2	B	575	GLY	2.1
1	A	1083	GLU	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](#)

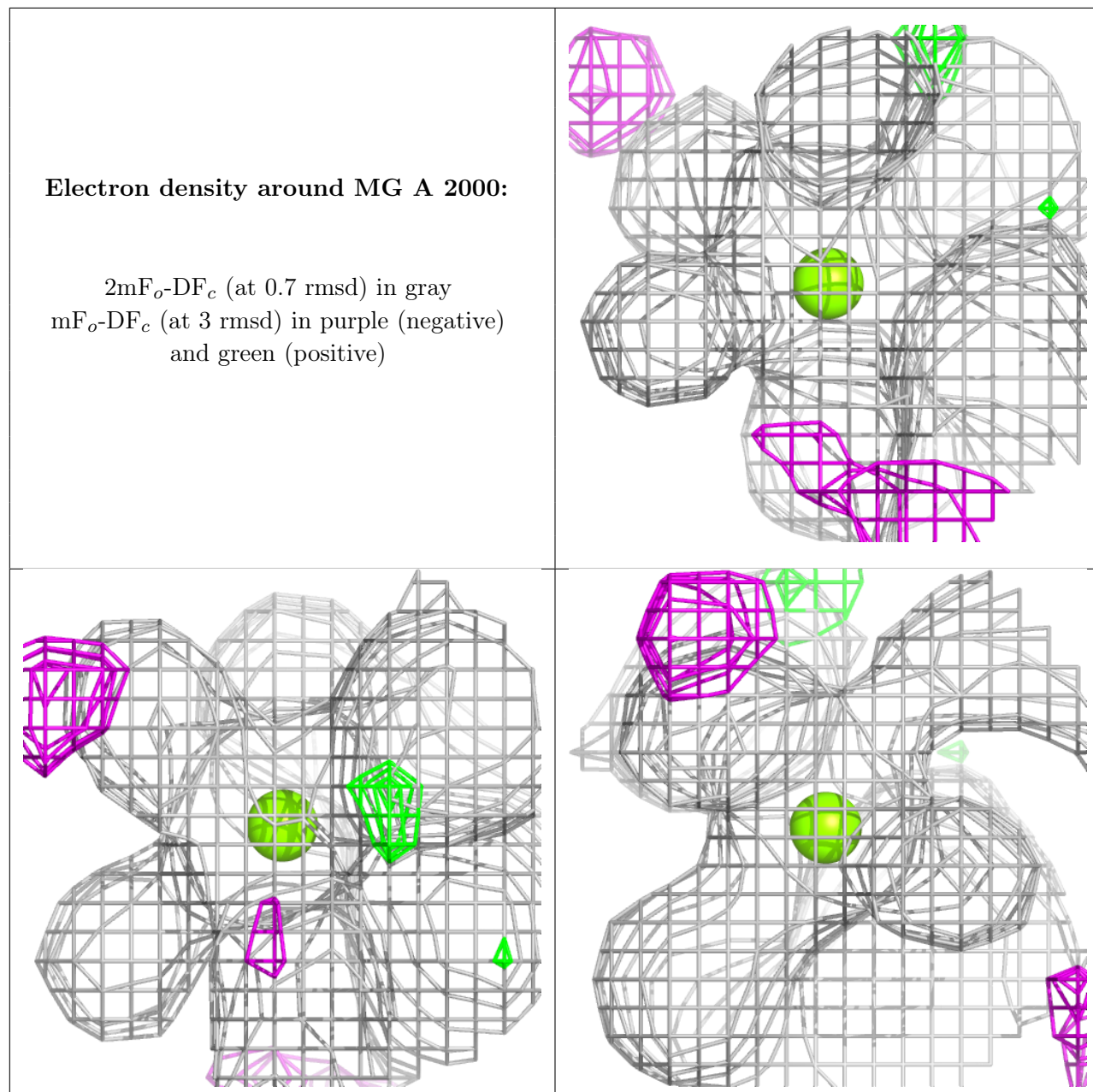
There are no oligosaccharides in this entry.

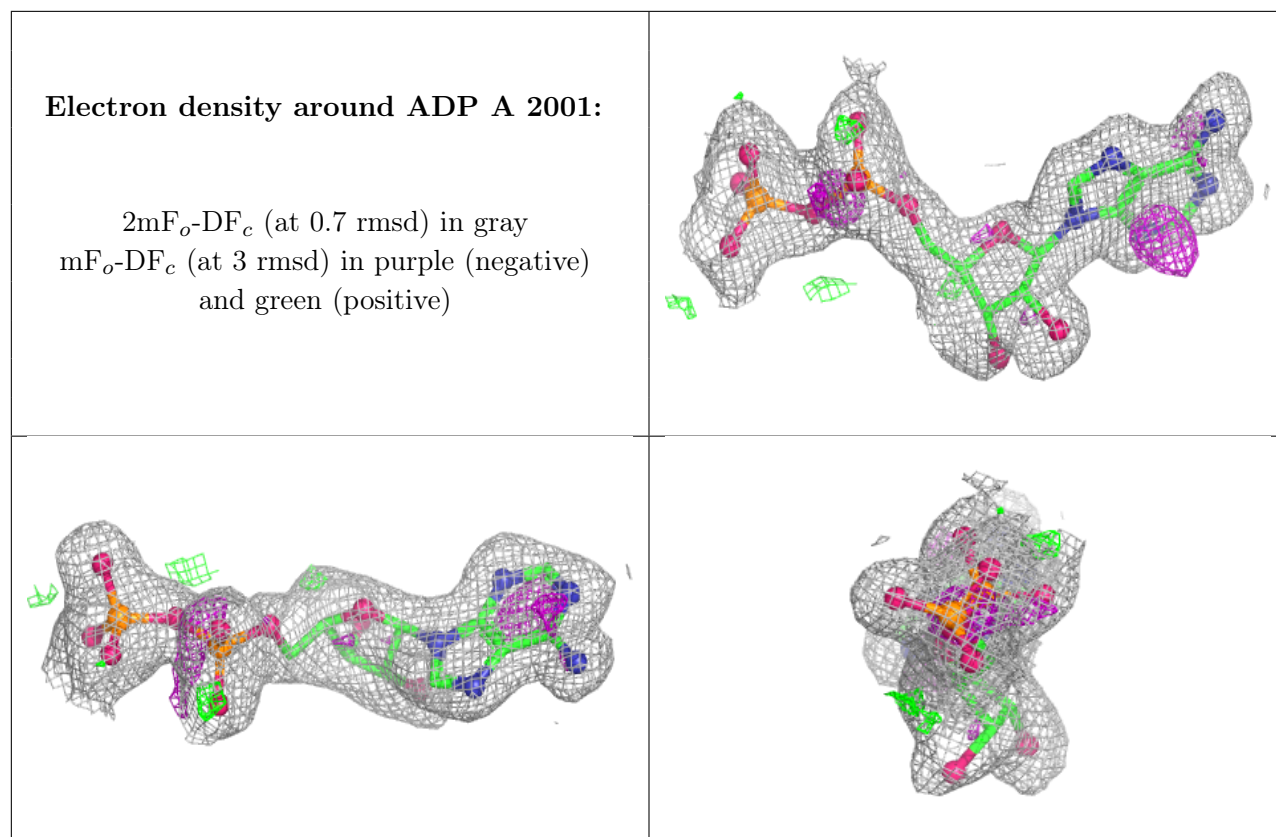
6.4 Ligands [i](#)

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	2000	1/1	0.92	0.14	45,45,45,45	0
4	ADP	A	2001	27/27	0.93	0.11	21,44,65,73	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.