



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2024 – 04:13 pm BST

PDB ID : 8ROA
Title : Human cohesin SMC1A-HD(longCC-EQ)/RAD21-C complex - ADP-bound conformation
Authors : Vitoria Gomes, M.; Romier, C.
Deposited on : 2024-01-11
Resolution : 2.44 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

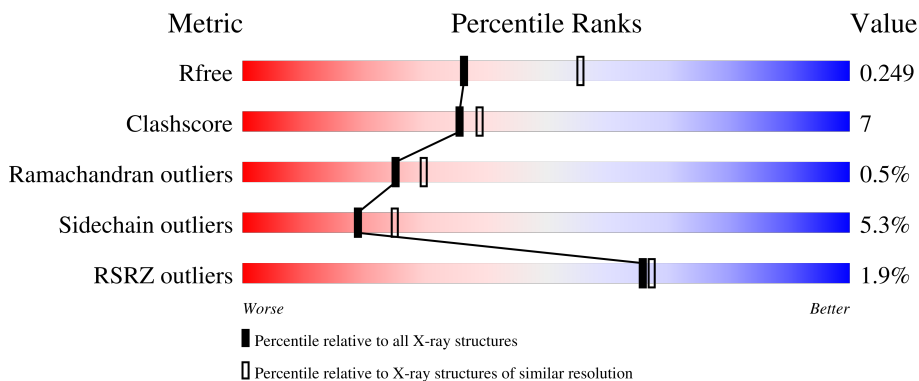
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	456	 2% 56% 16% 26%
1	C	456	 % 62% 16% 20%
2	B	81	 % 64% 11% 25%
2	D	81	 % 67% 11% 22%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6696 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	339	2707	1729	461	509	8	0	6	0
1	C	364	2880	1836	490	544	10	0	1	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	978	GLU	-	linker	UNP Q14683
A	979	SER	-	linker	UNP Q14683
A	980	SER	-	linker	UNP Q14683
A	981	LYS	-	linker	UNP Q14683
A	982	HIS	-	linker	UNP Q14683
A	983	PRO	-	linker	UNP Q14683
A	984	THR	-	linker	UNP Q14683
A	985	SER	-	linker	UNP Q14683
A	986	LEU	-	linker	UNP Q14683
A	987	VAL	-	linker	UNP Q14683
A	988	PRO	-	linker	UNP Q14683
A	989	ARG	-	linker	UNP Q14683
A	990	GLY	-	linker	UNP Q14683
A	991	SER	-	linker	UNP Q14683
A	1157	GLN	GLU	engineered mutation	UNP Q14683
C	978	GLU	-	linker	UNP Q14683
C	979	SER	-	linker	UNP Q14683
C	980	SER	-	linker	UNP Q14683
C	981	LYS	-	linker	UNP Q14683
C	982	HIS	-	linker	UNP Q14683
C	983	PRO	-	linker	UNP Q14683
C	984	THR	-	linker	UNP Q14683
C	985	SER	-	linker	UNP Q14683
C	986	LEU	-	linker	UNP Q14683
C	987	VAL	-	linker	UNP Q14683

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Chain	Residue	Modelled	Actual	Comment	Reference
C	988	PRO	-	linker	UNP Q14683
C	989	ARG	-	linker	UNP Q14683
C	990	GLY	-	linker	UNP Q14683
C	991	SER	-	linker	UNP Q14683
C	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
2	B	61	Total	C	N	O	S	0	0	0
			487	313	82	91	1			
2	D	63	Total	C	N	O	S	0	0	0
			504	321	90	91	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	557	MET	-	initiating methionine	UNP O60216
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
D	557	MET	-	initiating methionine	UNP O60216
D	630	GLY	-	expression tag	UNP O60216
D	631	SER	-	expression tag	UNP O60216
D	632	LEU	-	expression tag	UNP O60216
D	633	GLU	-	expression tag	UNP O60216
D	634	VAL	-	expression tag	UNP O60216
D	635	LEU	-	expression tag	UNP O60216
D	636	PHE	-	expression tag	UNP O60216
D	637	GLN	-	expression tag	UNP O60216

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



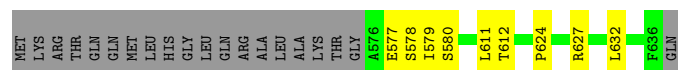
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

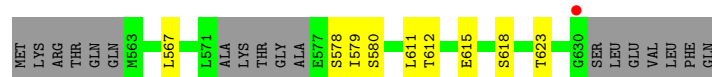
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	5	Total	O	0	0
			5	5		
4	C	25	Total	O	0	0
			25	25		
4	D	2	Total	O	0	0
			2	2		



- Molecule 2: 64-kDa C-terminal product



- Molecule 2: 64-kDa C-terminal product



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.31Å 65.28Å 105.76Å 90.00° 116.66° 90.00°	Depositor
Resolution (Å)	47.81 – 2.44 47.81 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.81-2.44) 99.6 (47.81-2.44)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.42Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.194 , 0.250 0.193 , 0.249	Depositor DCC
R_{free} test set	2126 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6696	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.63% 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: ADP

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	0.42	0/2776	0.58	0/3739
1	C	0.44	0/2935	0.58	0/3946
2	B	0.46	0/496	0.57	0/669
2	D	0.39	0/512	0.53	0/687
All	All	0.43	0/6719	0.58	0/9041

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 [i](#)

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	2707	0	2724	47	0
1	C	2880	0	2893	43	0
2	B	487	0	493	3	0
2	D	504	0	514	5	0
3	A	27	0	12	0	0
3	C	27	0	11	0	0
4	A	32	0	0	1	0
4	B	5	0	0	0	0
4	C	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
All	All	6696	0	6647	96	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 7.

The worst 5 of 96 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:1126:ASP:N	1:A:1126:ASP:OD1	2.19	0.76
1:A:1060:GLU:HA	1:A:1063:LYS:HB3	1.68	0.75
1:A:1062:ILE:HA	1:A:1065:GLU:HG2	1.69	0.74
1:A:1162:LEU:HD13	1:A:1167:ILE:HA	1.69	0.74
1:A:169:ASP:N	1:A:169:ASP:OD1	2.22	0.73

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	341/456 (75%)	322 (94%)	16 (5%)	3 (1%)	14	16
1	C	361/456 (79%)	345 (96%)	15 (4%)	1 (0%)	37	44
2	B	59/81 (73%)	58 (98%)	1 (2%)	0	100	100
2	D	59/81 (73%)	58 (98%)	1 (2%)	0	100	100
All	All	820/1074 (76%)	783 (96%)	33 (4%)	4 (0%)	25	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	GLY

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Mol	Chain	Res	Type
1	A	168	TYR
1	A	1209	ASP
1	C	1166	ASN

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	292/388 (75%)	276 (94%)	16 (6%)	18	23
1	C	307/388 (79%)	291 (95%)	16 (5%)	19	26
2	B	53/69 (77%)	49 (92%)	4 (8%)	11	13
2	D	54/69 (78%)	52 (96%)	2 (4%)	29	40
All	All	706/914 (77%)	668 (95%)	38 (5%)	19	24

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	182	THR
1	C	1225	ASP
1	C	183	GLN
1	C	1126	ASP
2	D	612	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1177	GLN
1	A	1181	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	ADP	C	2000	-	24,29,29	3.44	8 (33%)	29,45,45	1.66	6 (20%)
3	ADP	A	2000	-	24,29,29	3.53	8 (33%)	29,45,45	1.66	4 (13%)

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	ADP	C	2000	-	-	4/12/32/32	0/3/3/3
3	ADP	A	2000	-	-	5/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	ADP	C2'-C3'	-10.46	1.24	1.53
3	C	2000	ADP	C2'-C3'	-10.13	1.25	1.53
3	C	2000	ADP	O4'-C1'	-8.88	1.28	1.41
3	A	2000	ADP	O4'-C1'	-8.21	1.29	1.41
3	A	2000	ADP	C2'-C1'	7.63	1.65	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2000	ADP	N3-C2-N1	-4.86	121.08	128.68
3	A	2000	ADP	N3-C2-N1	-4.57	121.53	128.68
3	A	2000	ADP	C4-C5-N7	-4.31	104.91	109.40
3	C	2000	ADP	O4'-C1'-C2'	-3.37	102.00	106.93
3	C	2000	ADP	C4-C5-N7	-3.25	106.02	109.40

There are no chirality outliers.

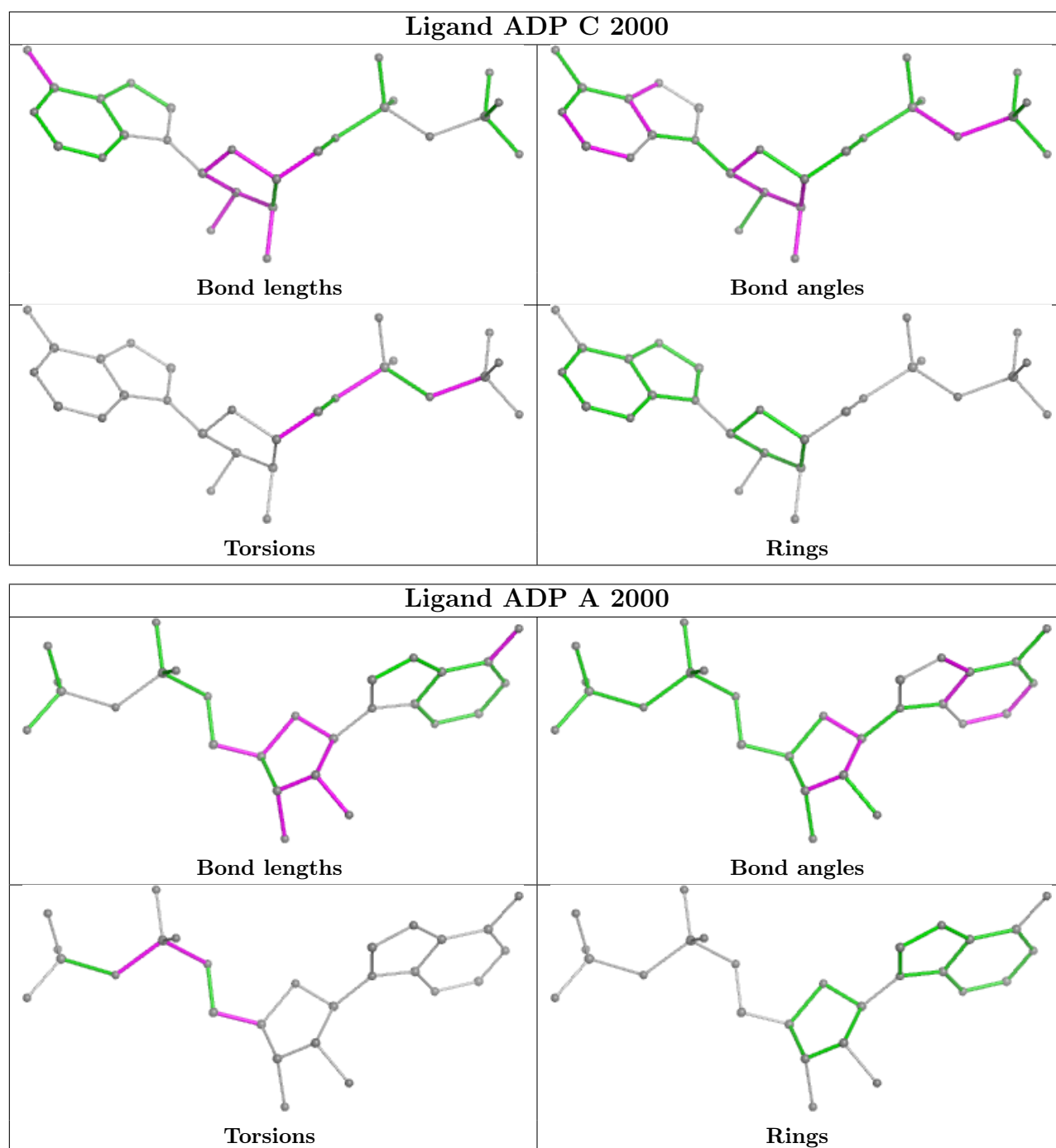
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	ADP	C5'-O5'-PA-O1A
3	A	2000	ADP	O4'-C4'-C5'-O5'
3	A	2000	ADP	C3'-C4'-C5'-O5'
3	C	2000	ADP	O4'-C4'-C5'-O5'
3	C	2000	ADP	C3'-C4'-C5'-O5'

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	339/456 (74%)	-0.06	9 (2%) 56 57	28, 55, 106, 133	6 (1%)
1	C	364/456 (79%)	-0.19	6 (1%) 70 72	33, 55, 94, 124	1 (0%)
2	B	61/81 (75%)	-0.44	0 100 100	39, 52, 81, 89	0
2	D	63/81 (77%)	-0.13	1 (1%) 70 72	40, 53, 99, 121	0
All	All	827/1074 (77%)	-0.15	16 (1%) 66 67	28, 55, 102, 133	7 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1058	ALA	4.9
2	D	630	GLY	4.5
1	C	1045	PHE	4.1
1	A	3	PHE	2.9
1	A	1169	LYS	2.7

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](#)

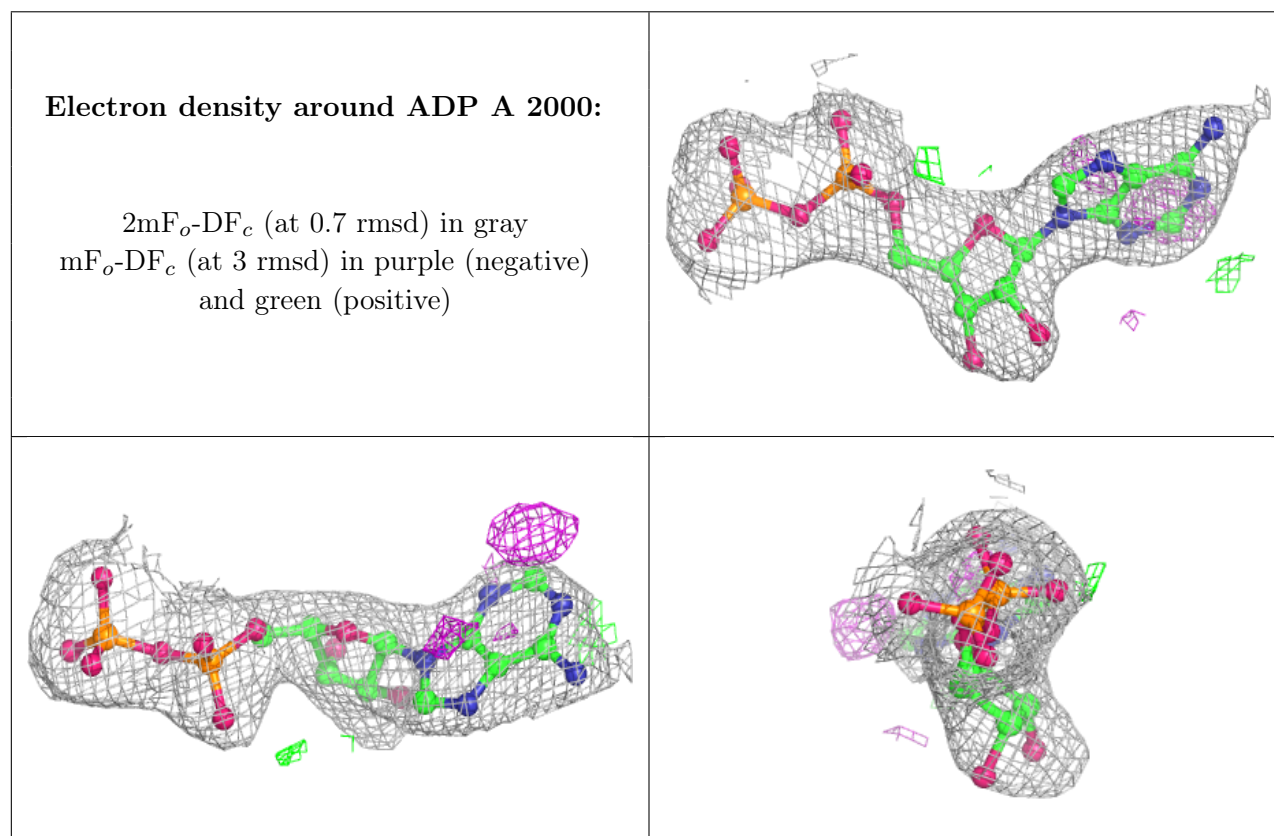
There are no monosaccharides in this entry.

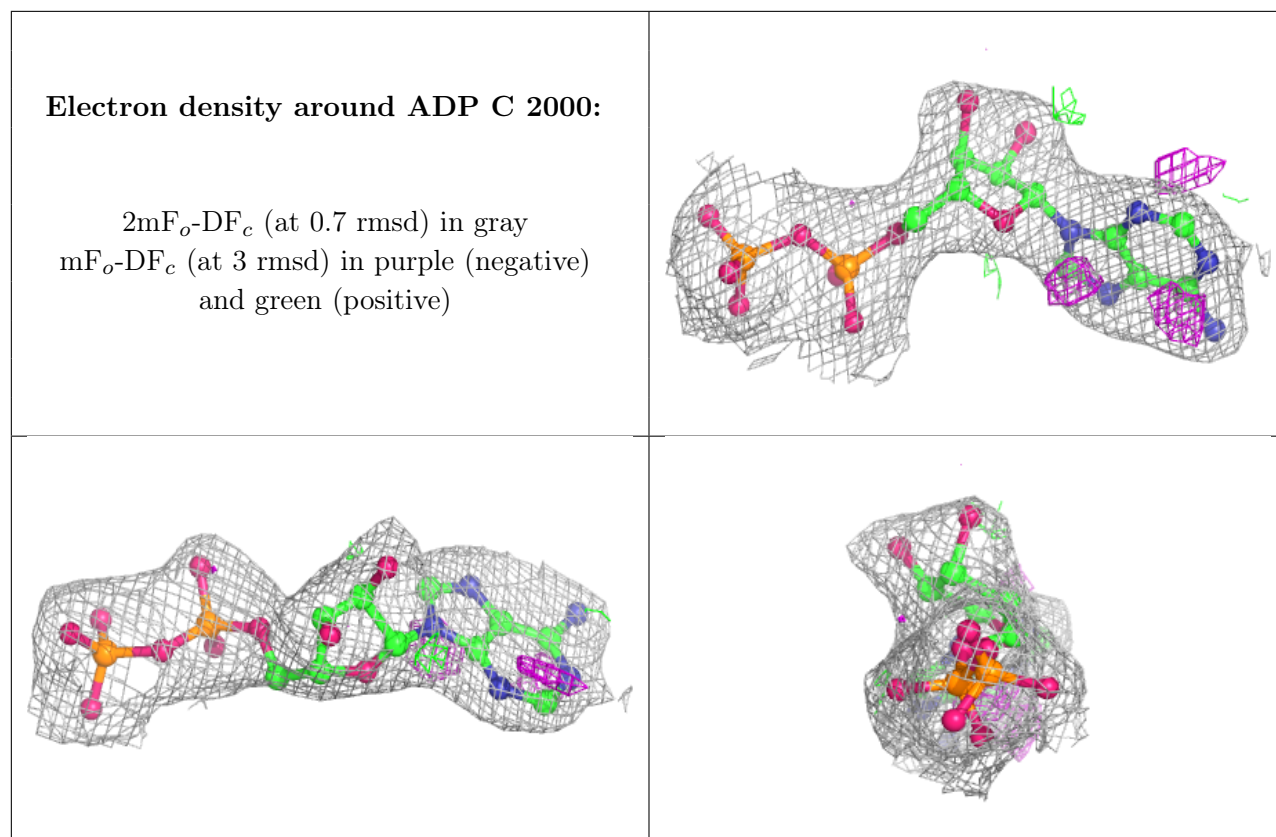
6.4 Ligands [i](#)

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
3	ADP	A	2000	27/27	0.93	0.09	51,61,79,82	0
3	ADP	C	2000	27/27	0.93	0.09	44,61,74,81	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.