



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 01:09 PM EST

PDB ID : 3THO  
Title : Crystal structure of Mre11:Rad50 in its ATP/ADP bound state  
Authors : Moeckel, C.; Lammens, K.  
Deposited on : 2011-08-19  
Resolution : 2.61 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](mailto:validation@mail.wwpdb.org)

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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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

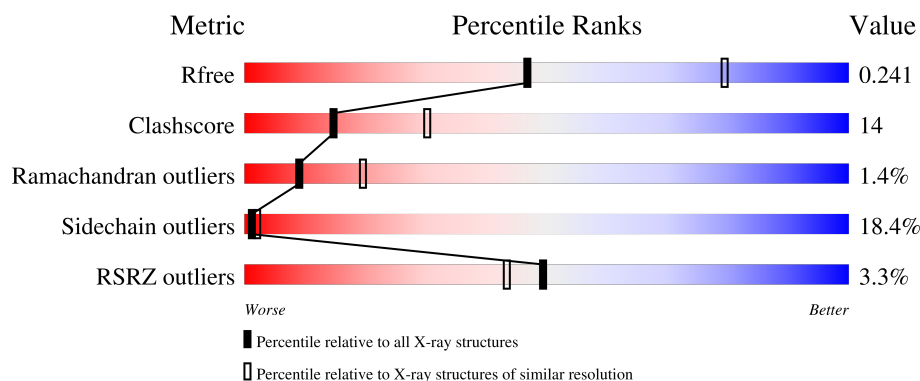
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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	382	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>29%</div> <div>6%</div> <div>7%</div> </div> </div>
2	B	379	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>6%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	854	-	-	X	-
5	SO4	A	855	-	-	X	-
5	SO4	A	857	-	-	X	-
5	SO4	B	387	-	-	X	-
5	SO4	B	5	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5973 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 Probable DNA double-strand break repair Rad50 ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	221	0	0
			2850	1814	494	536	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP Q9X1X1
A	-15	HIS	-	expression tag	UNP Q9X1X1
A	-14	HIS	-	expression tag	UNP Q9X1X1
A	-13	HIS	-	expression tag	UNP Q9X1X1
A	-12	HIS	-	expression tag	UNP Q9X1X1
A	-11	HIS	-	expression tag	UNP Q9X1X1
A	-10	SER	-	expression tag	UNP Q9X1X1
A	-9	SER	-	expression tag	UNP Q9X1X1
A	-8	GLY	-	expression tag	UNP Q9X1X1
A	-7	GLU	-	expression tag	UNP Q9X1X1
A	-6	ASN	-	expression tag	UNP Q9X1X1
A	-5	LEU	-	expression tag	UNP Q9X1X1
A	-4	TYR	-	expression tag	UNP Q9X1X1
A	-3	PHE	-	expression tag	UNP Q9X1X1
A	-2	GLN	-	expression tag	UNP Q9X1X1
A	-1	GLY	-	expression tag	UNP Q9X1X1
A	0	HIS	-	expression tag	UNP Q9X1X1
A	678	GLY	-	linker	UNP Q9X1X1
A	679	GLY	-	linker	UNP Q9X1X1
A	680	ALA	-	linker	UNP Q9X1X1
A	681	GLY	-	linker	UNP Q9X1X1
A	682	GLY	-	linker	UNP Q9X1X1
A	683	ALA	-	linker	UNP Q9X1X1
A	684	GLY	-	linker	UNP Q9X1X1
A	685	GLY	-	linker	UNP Q9X1X1
A	804	CYS	ASP	engineered mutation	UNP Q9X1X1
A	830	CYS	HIS	engineered mutation	UNP Q9X1X1

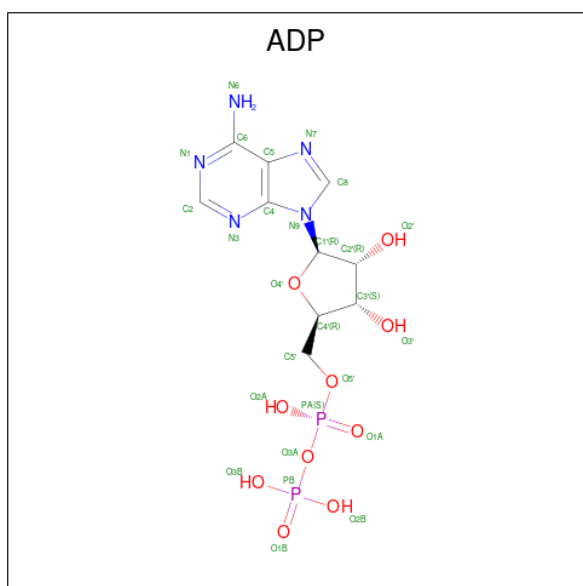
- Molecule 2 is a protein called Exonuclease, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	366	Total	C	N	O	S	270	0	0
			3000	1922	509	562	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	MET	LEU	conflict	UNP Q9X1X0
B	94	GLN	HIS	engineered mutation	UNP Q9X1X0
B	291	SER	PHE	engineered mutation	UNP Q9X1X0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mn	0	0
			2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	18	Total	O	0	0
			18	18		
8	B	25	Total	O	0	0
			25	25		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.77Å 121.77Å 135.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 2.61 49.12 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.12-2.61) 99.6 (49.12-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.204 , 0.242 0.202 , 0.241	Depositor DCC
$R_{free}$ test set	1992 reflections (5.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5973	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, SO4, MN, MG, PO4

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	0.45	0/2891	0.57	0/3874
2	B	0.46	0/3059	0.59	1/4118 (0.0%)
All	All	0.45	0/5950	0.58	1/7992 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	54	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	ILE	Peptide

### 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	2850	0	2922	78	0
2	B	3000	0	3032	72	0
3	A	27	0	10	0	0
4	A	1	0	0	0	0
5	A	25	0	0	8	0
5	B	20	0	0	4	0
6	A	5	0	0	0	0
7	B	2	0	0	0	0
8	A	18	0	0	1	0
8	B	25	0	0	1	0
All	All	5973	0	5964	147	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 14.

The worst 5 of 147 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)
2:B:100:LYS:HB3	2:B:117:MET:HG2	1.49	0.95
2:B:135:LEU:HB3	2:B:164:LEU:HD22	1.54	0.89
1:A:106:ASN:O	1:A:108:LYS:N	2.09	0.85
1:A:22:GLN:HB2	1:A:840:ARG:HH22	1.46	0.79
1:A:71:ARG:NH2	5:A:855:SO4:O4	2.16	0.79

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	353/382 (92%)	323 (92%)	23 (6%)	7 (2%)	<b>6</b> <b>12</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	360/379 (95%)	328 (91%)	29 (8%)	3 (1%)	16	34
All	All	713/761 (94%)	651 (91%)	52 (7%)	10 (1%)	9	19

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
1	A	712	SER
2	B	364	GLU
1	A	107	GLY
1	A	189	SER

### 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	310/326 (95%)	253 (82%)	57 (18%)	1	2
2	B	333/341 (98%)	272 (82%)	61 (18%)	1	2
All	All	643/667 (96%)	525 (82%)	118 (18%)	1	2

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	366	HIS
2	B	111	SER
2	B	363	GLU
2	B	333	GLU

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

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\# Z  > 2$
6	PO4	A	859	-	4,4,4	0.83	0	6,6,6	0.54	0
5	SO4	A	858	-	4,4,4	0.27	0	6,6,6	0.12	0
5	SO4	A	854	-	4,4,4	0.23	0	6,6,6	0.19	0
5	SO4	B	5	-	4,4,4	0.29	0	6,6,6	0.05	0
5	SO4	A	856	-	4,4,4	0.25	0	6,6,6	0.18	0
5	SO4	A	857	-	4,4,4	0.22	0	6,6,6	0.11	0
5	SO4	B	4	-	4,4,4	0.27	0	6,6,6	0.24	0
5	SO4	A	855	-	4,4,4	0.27	0	6,6,6	0.32	0
5	SO4	B	386	-	4,4,4	0.35	0	6,6,6	0.09	0
5	SO4	B	387	-	4,4,4	0.32	0	6,6,6	0.42	0
3	ADP	A	1452	4	24,29,29	1.38	5 (20%)	29,45,45	1.57	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	A	1452	4	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1452	ADP	O2'-C2'	-2.78	1.36	1.43
3	A	1452	ADP	O3'-C3'	-2.60	1.36	1.43
3	A	1452	ADP	C6-N6	2.18	1.41	1.34
3	A	1452	ADP	C5'-C4'	-2.14	1.45	1.51
3	A	1452	ADP	C1'-N9	-2.02	1.44	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1452	ADP	N3-C2-N1	-5.81	120.79	128.67
3	A	1452	ADP	C1'-N9-C4	-2.65	121.98	126.64
3	A	1452	ADP	C4'-O4'-C1'	-2.61	107.53	109.92
3	A	1452	ADP	O5'-C5'-C4'	2.41	117.20	108.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1452	ADP	PA-O3A-PB-O3B
3	A	1452	ADP	O4'-C4'-C5'-O5'
3	A	1452	ADP	C3'-C4'-C5'-O5'

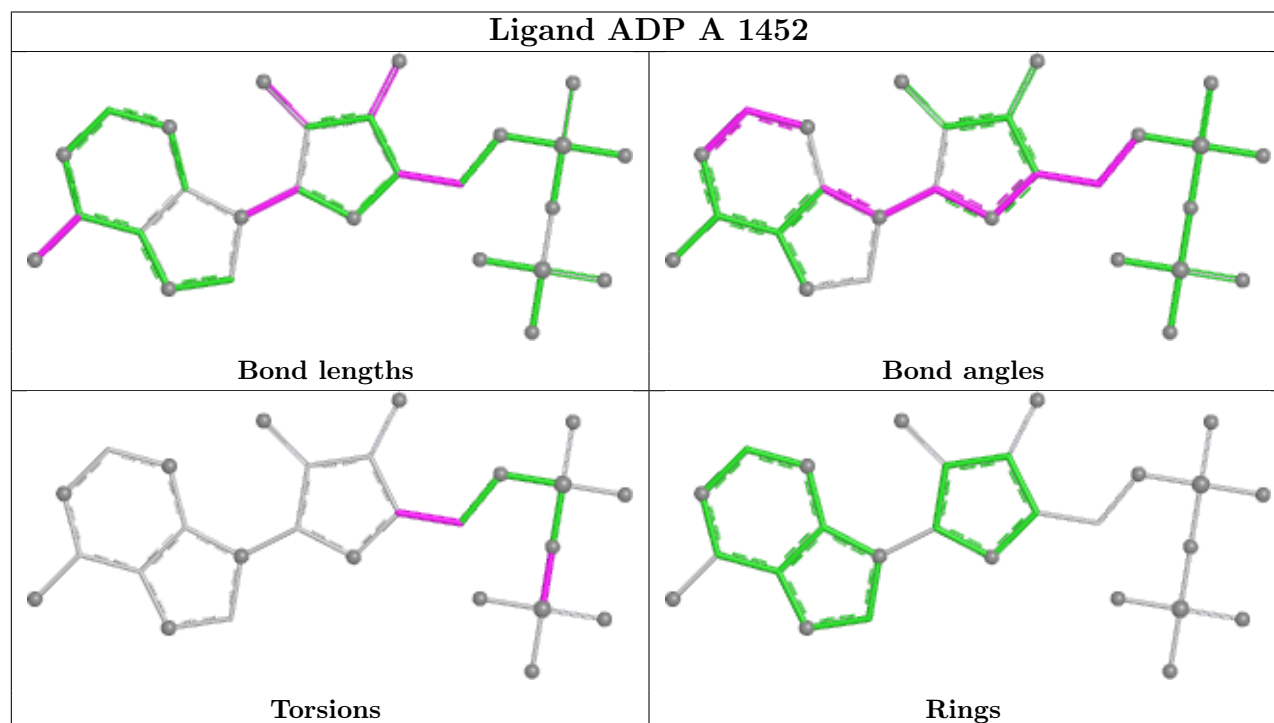
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	858	SO4	1	0
5	A	854	SO4	2	0
5	B	5	SO4	2	0
5	A	857	SO4	3	0
5	A	855	SO4	2	0
5	B	387	SO4	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	356/382 (93%)	0.13	12 (3%)	48	42	31, 58, 91, 118	72 (20%)
2	B	366/379 (96%)	0.07	12 (3%)	49	43	24, 56, 88, 118	75 (20%)
All	All	722/761 (94%)	0.10	24 (3%)	49	43	24, 57, 91, 118	147 (20%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	331	ILE	4.4
2	B	366	HIS	4.1
1	A	707	TYR	3.8
1	A	82	ARG	3.7
1	A	106	ASN	3.4

### 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.

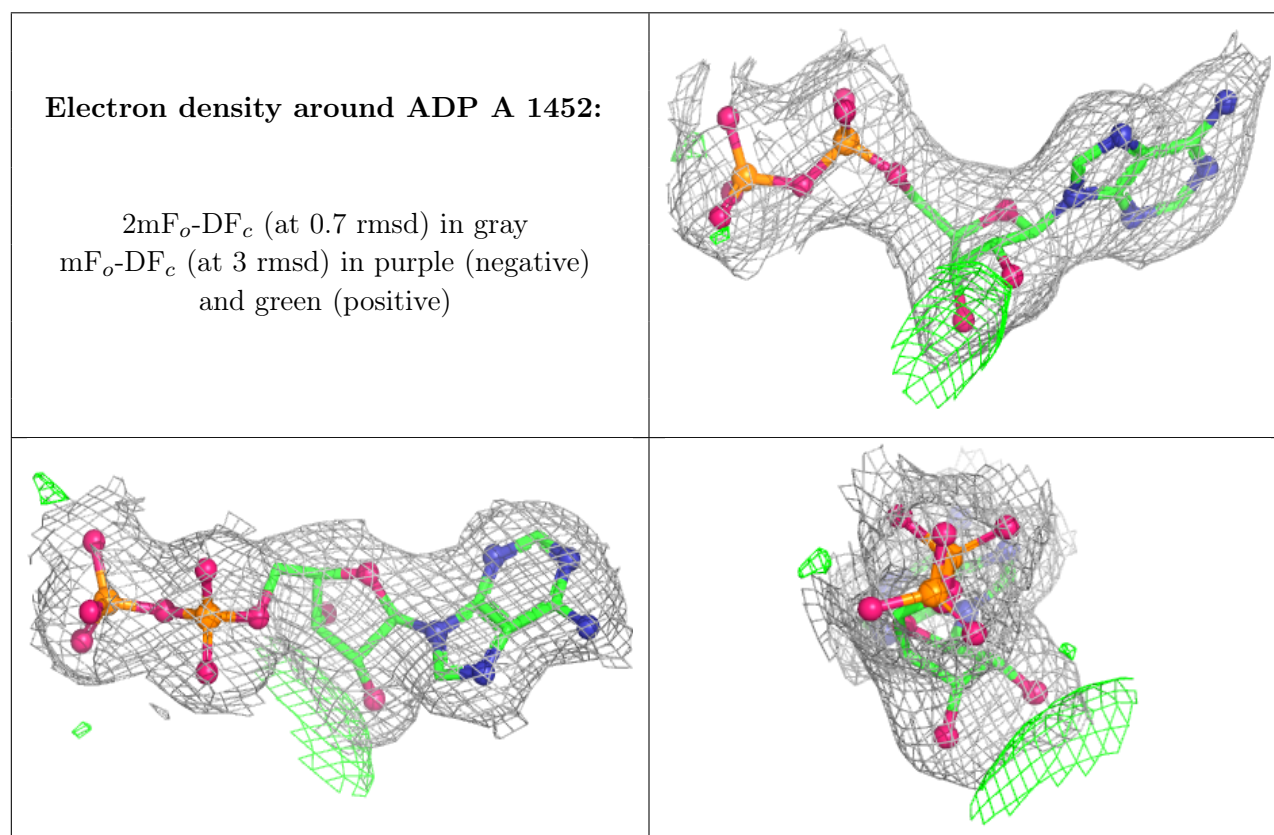
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	858	5/5	0.70	0.14	81,82,89,92	5
5	SO4	B	4	5/5	0.82	0.09	97,97,114,118	0
5	SO4	B	387	5/5	0.84	0.26	50,50,52,56	5
5	SO4	B	5	5/5	0.85	0.14	77,79,83,95	5
5	SO4	A	857	5/5	0.85	0.22	61,62,65,65	5
5	SO4	A	856	5/5	0.86	0.11	62,75,81,83	5
5	SO4	A	854	5/5	0.87	0.11	67,68,71,75	5
5	SO4	A	855	5/5	0.89	0.09	64,66,74,77	5
6	PO4	A	859	5/5	0.90	0.14	66,69,76,78	5
5	SO4	B	386	5/5	0.94	0.10	75,76,90,91	0
4	MG	A	853	1/1	0.97	0.07	56,56,56,56	0
7	MN	B	1	1/1	0.97	0.08	49,49,49,49	1
3	ADP	A	1452	27/27	0.98	0.06	38,44,48,49	0
7	MN	B	2	1/1	1.00	0.04	38,38,38,38	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 ⓘ

There are no such residues in this entry.