WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jul 26, 2023 – 01:27 AM EDT

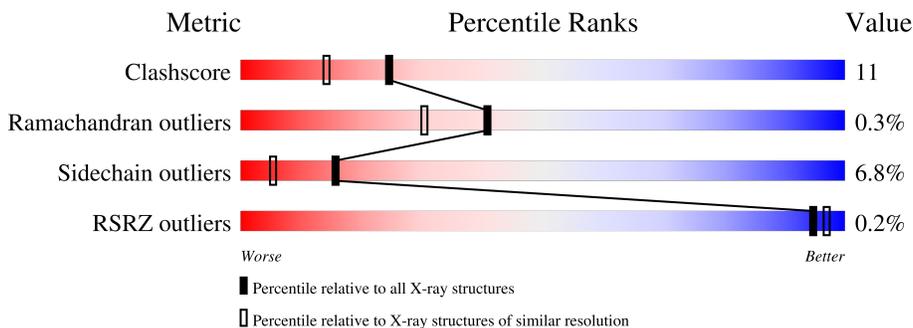|		
PDB ID	:	1A4M
Title	:	ADA STRUCTURE COMPLEXED WITH PURINE RIBOSIDE AT PH 7.0
Authors	:	Wang, Z.; Quiocho, F.A.
Deposited on	:	1998-01-31
Resolution	:	1.95 Å(reported)

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 1.95 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		6.8%
RSRZ outliers		0.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	349	79% 19% •
1	B	349	71% 26% •
1	C	349	% 71% 24% 5%
1	D	349	73% 23% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12313 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.
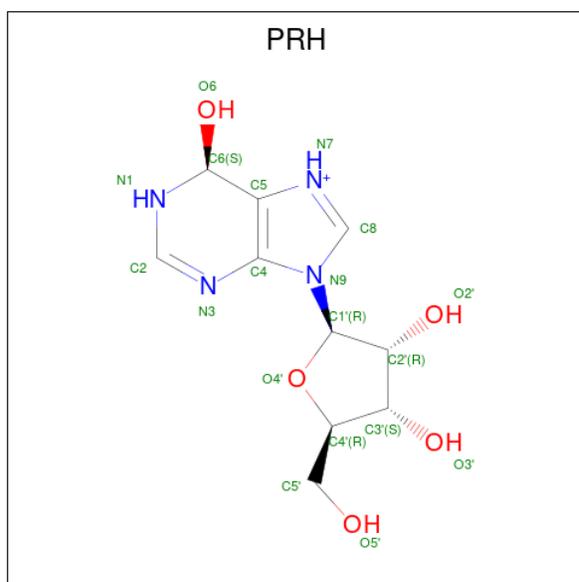
- Molecule 1 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	B	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	C	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	D	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			

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

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

- Molecule 3 is 6-HYDROXY-1,6-DIHYDRO PURINE NUCLEOSIDE (three-letter code: PRH) (formula: $C_{10}H_{15}N_4O_5$).

PRH

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 19	C 10	N 4	O 5	0	0
3	B	1	Total 19	C 10	N 4	O 5	0	0
3	C	1	Total 19	C 10	N 4	O 5	0	0
3	D	1	Total 19	C 10	N 4	O 5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total 287	O 287	0	0
4	B	269	Total 269	O 269	0	0
4	C	242	Total 242	O 242	0	0
4	D	267	Total 267	O 267	0	0

3 Residue-property plots ⓘ

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: ADENOSINE DEAMINASE

Chain A:

- Molecule 1: ADENOSINE DEAMINASE

Chain B:

- Molecule 1: ADENOSINE DEAMINASE

Chain C:

Y1240 H1241 L1252 M1257 H1258 V1261 L1268 W1272 D1273 P1274 N1289 L1292 N1293 T1294 P1297 L1304 D1305 Q1309 K1313 E1321 F1322 L1325 N1326 I1327 N1328 K1331 K1341 E1342 L1343 L1344 E1345 R1346 E1350 Y1351 Q1352

• Molecule 1: ADENOSINE DEAMINASE

Chain D:

73%   23%   •

T1504 K1511 V1512 E1513 L1514 H1517 Y1529 K1532 L1538 P1539 A1540 D1541 T1542 V1543 E1544 E1545 L1546 I1549 P1570 I1579 K1580 F1586 K1590 E1593 G1594 V1595 V1598 E1599 V1600 R1601 L1607 A1608 N1609 V1612 W1617 N1618 Q1619 V1624 T1625 P1626 V1629 V1630 D1631

L1632 V1633 N1634 Q1635 E1641 I1646 R1649 H1657 Q1658 S1662 L1666 E1667 L1668 C1669 K1675 T1676 V1677 M1680 D1681 H1697 H1710 R1711 T1712 V1713 H1714 S1720 P1721 E1722 E1726 L1731 K1732 T1733 E1734 G1737 H1738 H1741 L1752 Y1767 L1768 W1772 T1777

H1778 L1792 N1793 T1794 P1797 T1803 L1804 D1805 D1814 M1815 F1822 L1825 N1826 I1827 K1831 L1835 E1838 E1839 L1843 R1846 L1847 Y1848 Q1852

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.69Å 93.64Å 102.18Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 39.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	70.2 (10.00-1.95) 65.7 (39.56-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.193 , 0.281 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.9	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12313	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0400e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, PRH

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	0.41	0/2856	0.69	1/3864 (0.0%)
1	B	0.42	0/2856	0.70	3/3864 (0.1%)
1	C	0.41	0/2856	0.69	1/3864 (0.0%)
1	D	0.42	0/2856	0.68	1/3864 (0.0%)
All	All	0.42	0/11424	0.69	6/15456 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1825	LEU	CA-CB-CG	8.66	135.22	115.30
1	A	325	LEU	CA-CB-CG	8.64	135.16	115.30
1	C	1325	LEU	CA-CB-CG	7.89	133.44	115.30
1	B	825	LEU	CA-CB-CG	7.54	132.63	115.30
1	B	835	LEU	CA-CB-CG	5.98	129.06	115.30

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	2792	0	2757	50	0
1	B	2792	0	2757	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2792	0	2757	66	0
1	D	2792	0	2757	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	14	2	0
3	B	19	0	14	0	0
3	C	19	0	14	0	0
3	D	19	0	14	1	0
4	A	287	0	0	10	0
4	B	269	0	0	2	0
4	C	242	0	0	10	0
4	D	267	0	0	3	0
All	All	12313	0	11084	244	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 11.

The worst 5 of 244 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:528:LEU:HD13	1:B:546:LEU:HD22	1.55	0.89
1:C:1109:ASN:HD21	1:C:1124:VAL:H	1.22	0.87
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.59	0.83
1:C:1294:THR:HG23	1:C:1297:PRO:HD3	1.62	0.80
1:B:792:LEU:HD22	1:B:825:LEU:HD11	1.66	0.77

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	347/349 (99%)	334 (96%)	12 (4%)	1 (0%)	41	30
1	B	347/349 (99%)	335 (96%)	11 (3%)	1 (0%)	41	30
1	C	347/349 (99%)	333 (96%)	13 (4%)	1 (0%)	41	30
1	D	347/349 (99%)	334 (96%)	12 (4%)	1 (0%)	41	30
All	All	1388/1396 (99%)	1336 (96%)	48 (4%)	4 (0%)	41	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1238	HIS
1	A	238	HIS
1	B	738	HIS
1	D	1738	HIS

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	304/304 (100%)	283 (93%)	21 (7%)	15	5
1	B	304/304 (100%)	286 (94%)	18 (6%)	19	8
1	C	304/304 (100%)	281 (92%)	23 (8%)	13	4
1	D	304/304 (100%)	283 (93%)	21 (7%)	15	5
All	All	1216/1216 (100%)	1133 (93%)	83 (7%)	16	5

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1294	THR
1	D	1632	LEU
1	C	1325	LEU
1	D	1544	GLU
1	D	1733	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1210	HIS
1	D	1609	ASN
1	C	1214	HIS
1	C	1289	ASN
1	D	1634	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PRH	B	854	2	15,21,21	1.93	4 (26%)	14,31,31	2.70	3 (21%)
3	PRH	C	1354	2	15,21,21	1.90	4 (26%)	14,31,31	2.55	3 (21%)
3	PRH	A	354	2	15,21,21	1.96	4 (26%)	14,31,31	2.74	3 (21%)
3	PRH	D	1854	2	15,21,21	1.92	3 (20%)	14,31,31	2.64	3 (21%)

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	PRH	B	854	2	-	0/2/32/32	0/3/3/3
3	PRH	C	1354	2	-	0/2/32/32	0/3/3/3
3	PRH	A	354	2	-	0/2/32/32	0/3/3/3
3	PRH	D	1854	2	-	0/2/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	PRH	O6-C6	5.22	1.61	1.40
3	B	854	PRH	O6-C6	5.19	1.61	1.40
3	D	1854	PRH	O6-C6	5.14	1.60	1.40
3	C	1354	PRH	O6-C6	5.12	1.60	1.40
3	D	1854	PRH	C3'-C4'	3.30	1.61	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	854	PRH	C2'-C3'-C4'	-6.96	89.11	102.64
3	A	354	PRH	C2'-C3'-C4'	-6.93	89.18	102.64
3	D	1854	PRH	C2'-C3'-C4'	-6.84	89.35	102.64
3	C	1354	PRH	C3'-C2'-C1'	6.09	110.15	100.98
3	A	354	PRH	C3'-C2'-C1'	6.08	110.13	100.98

There are no chirality outliers.

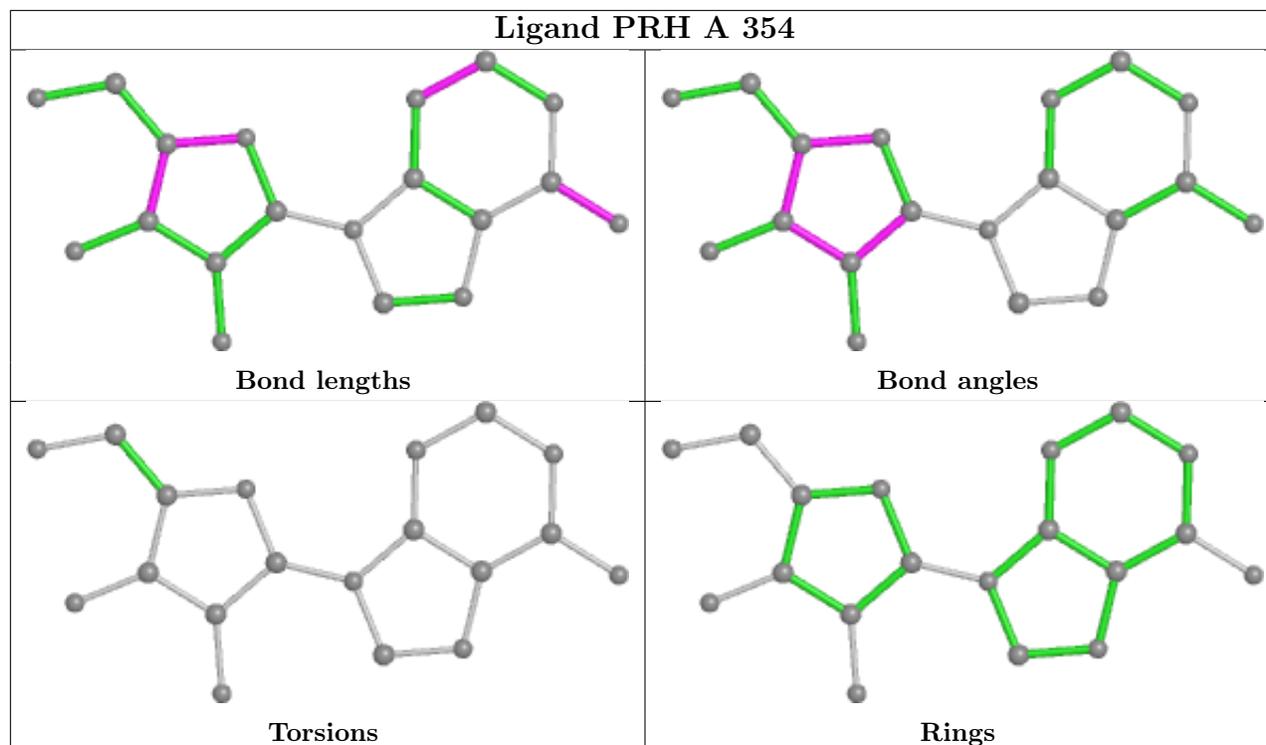There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	354	PRH	2	0
3	D	1854	PRH	1	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 then 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.

Ligand PRH B 854

Bond lengths

Bond angles

Torsions

Rings

Ligand PRH C 1354

Bond lengths

Bond angles

Torsions

Rings

Ligand PRH A 354

Bond lengths

Bond angles

Torsions

Rings

Ligand PRH D 1854

Bond lengths

Bond angles

Torsions

Rings
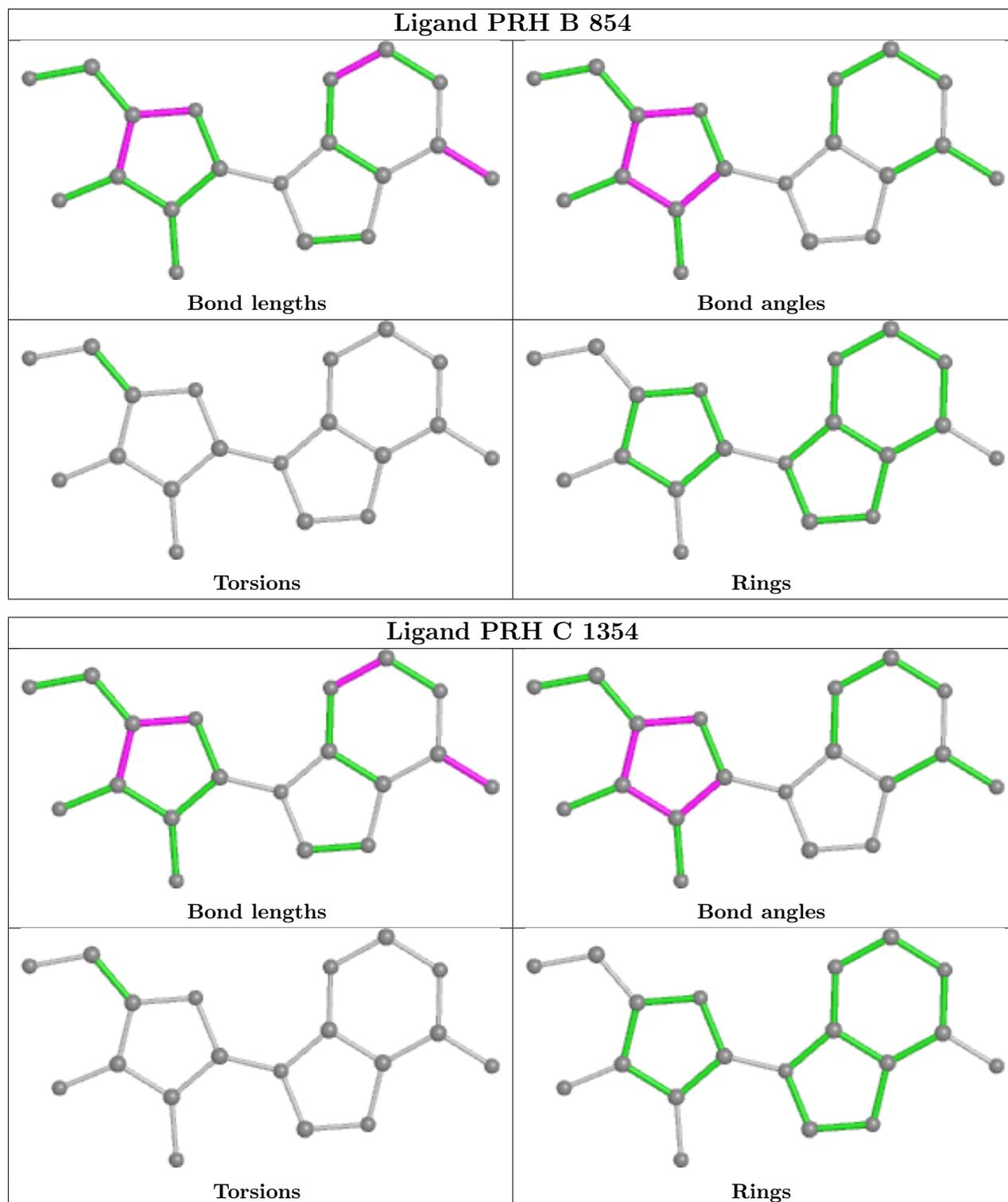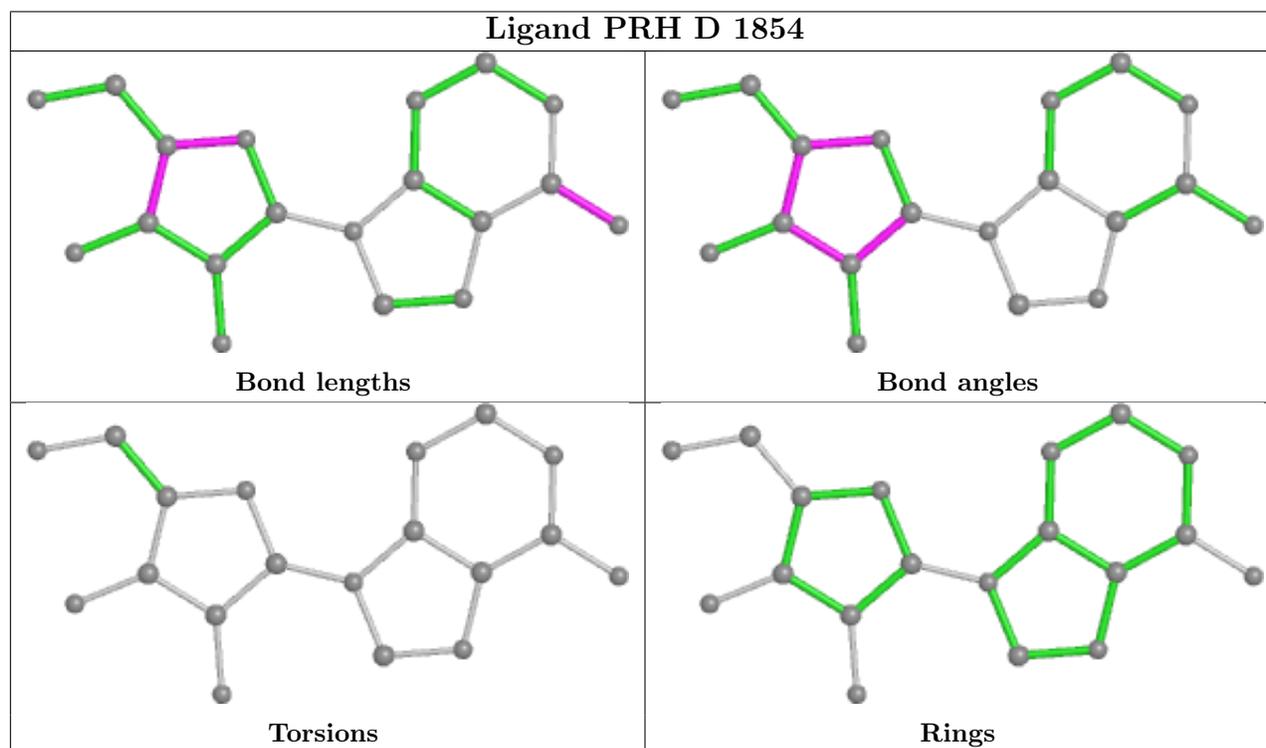
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	349/349 (100%)	-0.42	0	100	100	8, 16, 29, 44	0
1	B	349/349 (100%)	-0.42	0	100	100	7, 15, 29, 44	0
1	C	349/349 (100%)	-0.38	2 (0%)	89	93	7, 16, 28, 44	0
1	D	349/349 (100%)	-0.35	1 (0%)	94	96	8, 16, 29, 43	0
All	All	1396/1396 (100%)	-0.39	3 (0%)	95	97	7, 16, 29, 44	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1504	THR	2.3
1	C	1206	LYS	2.2
1	C	1004	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

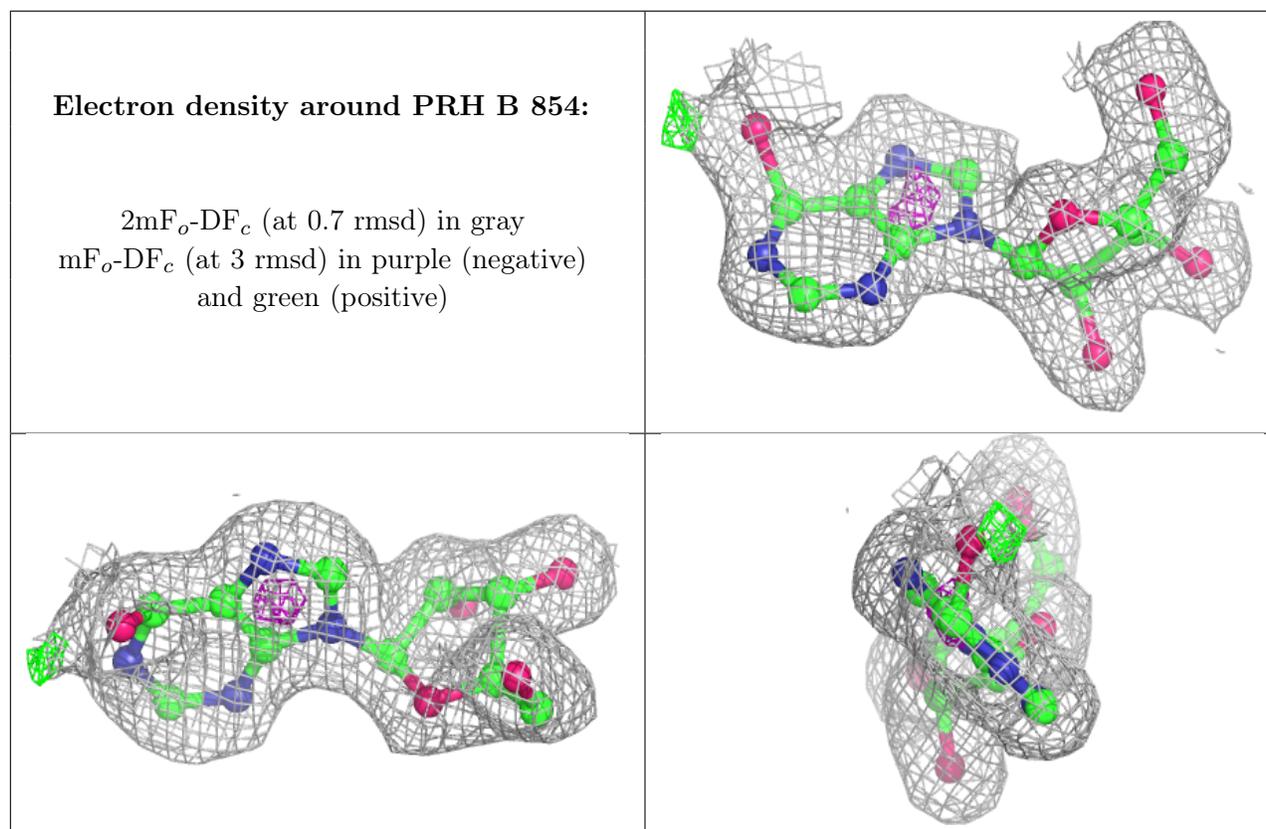There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

W O R L D W I D E
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	PRH	B	854	19/19	0.96	0.08	5,9,13,14	0
3	PRH	A	354	19/19	0.97	0.08	5,10,15,19	0
3	PRH	C	1354	19/19	0.97	0.08	2,10,14,17	0
3	PRH	D	1854	19/19	0.97	0.08	3,8,11,12	0
2	ZN	D	1900	1/1	0.99	0.07	16,16,16,16	0
2	ZN	C	1400	1/1	1.00	0.07	15,15,15,15	0
2	ZN	A	400	1/1	1.00	0.07	13,13,13,13	0
2	ZN	B	900	1/1	1.00	0.09	16,16,16,16	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.
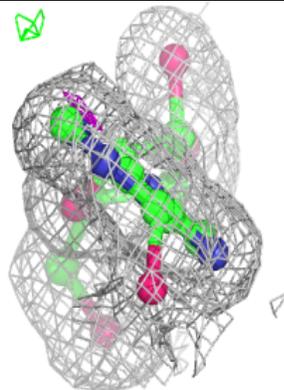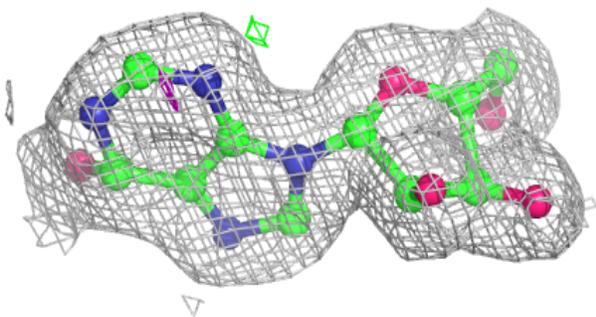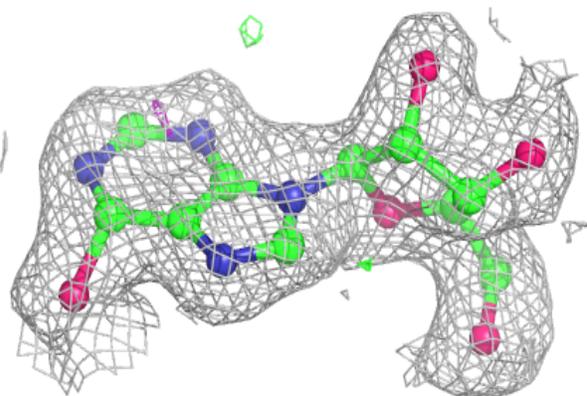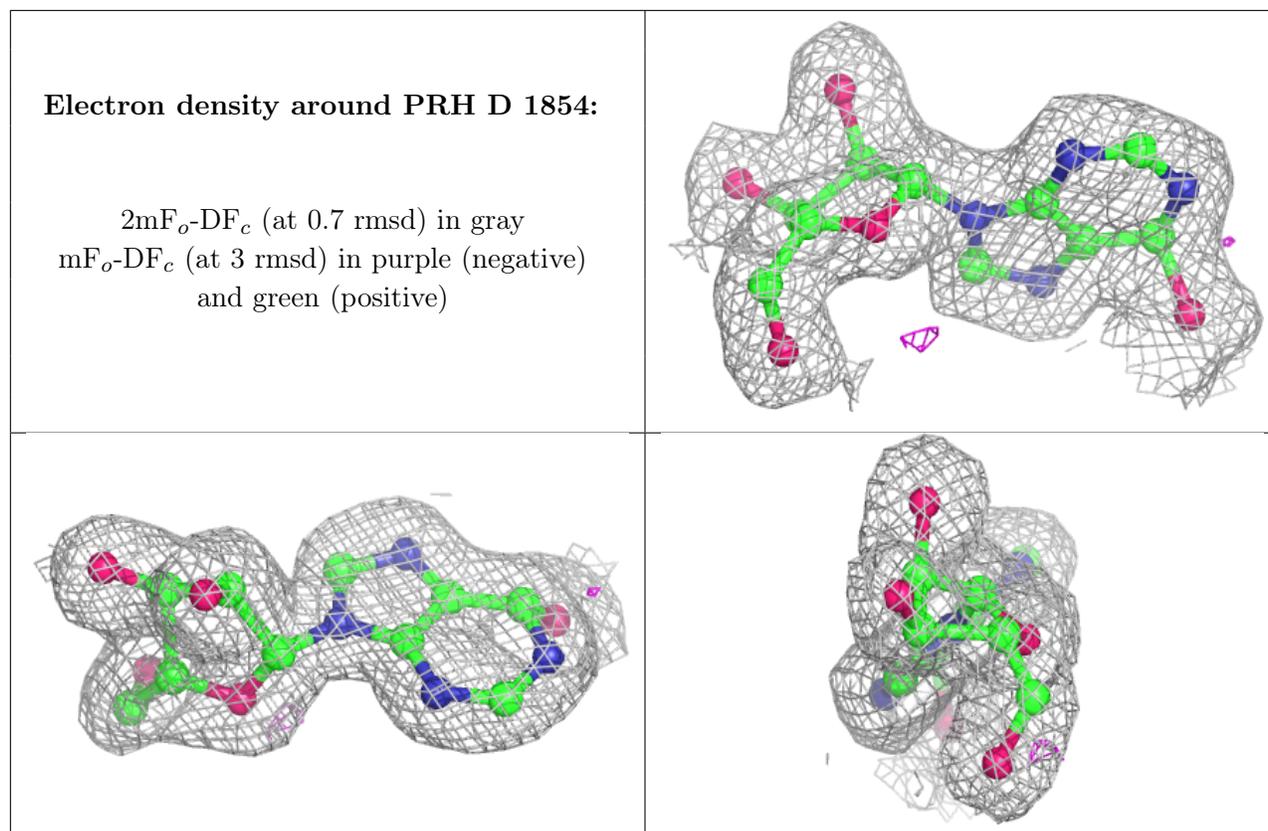

Electron density around PRH B 854:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around PRH A 354:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
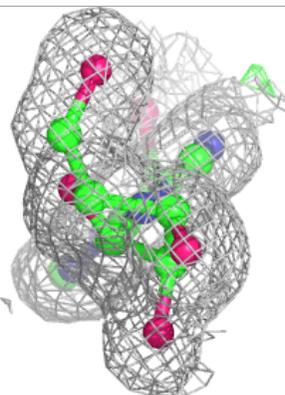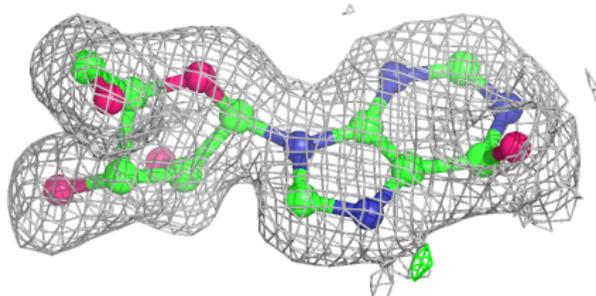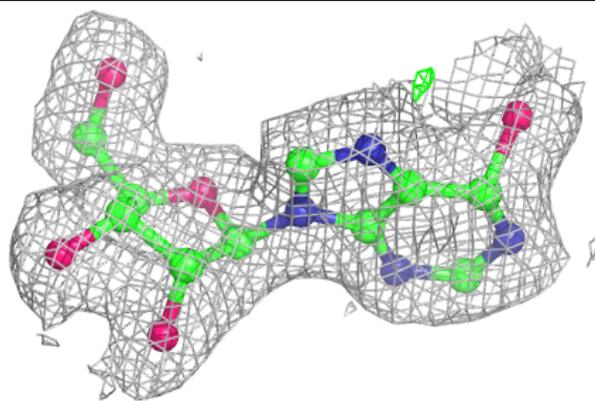
Electron density around PRH C 1354:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PRH D 1854:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.