



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3TOK
Title : Assaying the energies of biological halogen bonds.
Authors : Carter, M.; Ho, P.S.
Deposited on : 2011-09-05
Resolution : 1.74 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

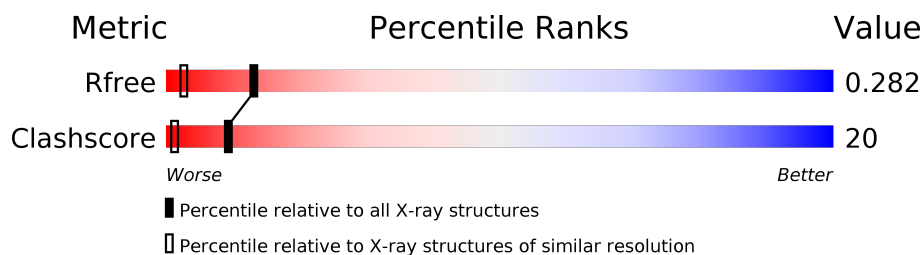
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	10	
2	B	10	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 937 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 DNA chain called DNA (5'-D(*CP*CP*GP*AP*TP*AP*CP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	10	0
			402	192	78	114	18			

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*GP*GP*TP*AP*TP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	10	0
			406	194	76	118	18			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	76	Total	O	0	0
			76	76		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: DNA (5'-D(*CP*CP*GP*AP*TP*AP*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(*CP*CP*GP*GP*TP*AP*TP*CP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	65.36Å 24.60Å 37.41Å 90.00° 110.76° 90.00°	Depositor
Resolution (Å)	40.00 – 1.74 28.57 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.8 (40.00-1.74) 91.1 (28.57-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.291 0.285 , 0.282	Depositor DCC
R_{free} test set	325 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	937	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% 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: NA

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	0.35	0/450	0.65	0/690
2	B	0.40	0/454	0.70	0/698
All	All	0.38	0/904	0.68	0/1388

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	402	0	226	14	2
2	B	406	0	228	13	4
3	B	1	0	0	0	0
4	A	52	0	0	1	2
4	B	76	0	0	2	5
All	All	937	0	454	25	7

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 20.

All (25) 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:13[A]:DG:H2''	2:B:14[A]:DG:N7	1.73	1.02
1:A:9[B]:DG:H1	2:B:12[B]:DC:H42	1.15	0.94
2:B:13[A]:DG:H2''	2:B:14[A]:DG:C8	2.16	0.79
1:A:9[B]:DG:H1	2:B:12[B]:DC:N4	1.89	0.68
1:A:9[A]:DG:H4'	4:A:115:HOH:O	2.00	0.61
1:A:3[B]:DG:H2''	1:A:4[B]:DA:N7	2.16	0.60
2:B:18[A]:DC:H2''	2:B:19[A]:DG:N7	2.16	0.60
2:B:13[A]:DG:H3'	4:B:210:HOH:O	2.02	0.58
1:A:9[B]:DG:H2''	1:A:10[B]:DG:N7	2.19	0.57
1:A:3[A]:DG:H2''	1:A:4[A]:DA:C8	2.40	0.57
2:B:18[A]:DC:H2''	2:B:19[A]:DG:C8	2.41	0.55
1:A:3[A]:DG:H2''	1:A:4[A]:DA:N7	2.21	0.55
2:B:13[B]:DG:H2''	2:B:14[B]:DG:N7	2.23	0.53
2:B:18[B]:DC:H2''	2:B:19[B]:DG:N7	2.23	0.53
1:A:5[B]:DT:H2''	1:A:6[B]:DA:C8	2.48	0.48
2:B:19[B]:DG:H2''	2:B:20[B]:DG:N7	2.29	0.48
2:B:13[B]:DG:H2''	2:B:14[B]:DG:C8	2.48	0.47
1:A:9[A]:DG:H2''	1:A:10[A]:DG:N7	2.31	0.46
1:A:9[B]:DG:H2''	1:A:10[B]:DG:C8	2.51	0.45
2:B:12[B]:DC:H1'	2:B:13[B]:DG:C4	2.51	0.45
1:A:3[B]:DG:H2''	1:A:4[B]:DA:C8	2.51	0.45
2:B:16[B]:DA:H4'	4:B:214:HOH:O	2.17	0.44
1:A:7[A]:DC:H2'	1:A:8[A]:DC:C5	2.55	0.41
1:A:6[B]:DA:H2''	1:A:7[B]:DC:O5'	2.20	0.41
1:A:7[B]:DC:H2''	1:A:8[B]:DC:C5	2.56	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12[B]:DC:O2	4:A:117:HOH:O[2_657]	1.64	0.56
2:B:12[A]:DC:OP1	4:A:102:HOH:O[2_657]	1.65	0.55
2:B:13[B]:DG:O6	4:B:220:HOH:O[1_556]	1.81	0.39
1:A:4[A]:DA:OP2	4:B:273:HOH:O[1_545]	2.01	0.19
1:A:4[B]:DA:OP2	4:B:261:HOH:O[2_658]	2.05	0.15
4:B:244:HOH:O	4:B:267:HOH:O[1_565]	2.07	0.13
2:B:14[B]:DG:OP2	4:B:233:HOH:O[2_647]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.