



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:01 PM GMT

PDB ID : 4KAJ
Title : X-Ray Structure of the complex of Haloalkane dehalogenase HaloTag7 with HALTS, Northeast Structural Genomics Consortium (NESG) Target OR151
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Deposited on : 2013-04-22
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

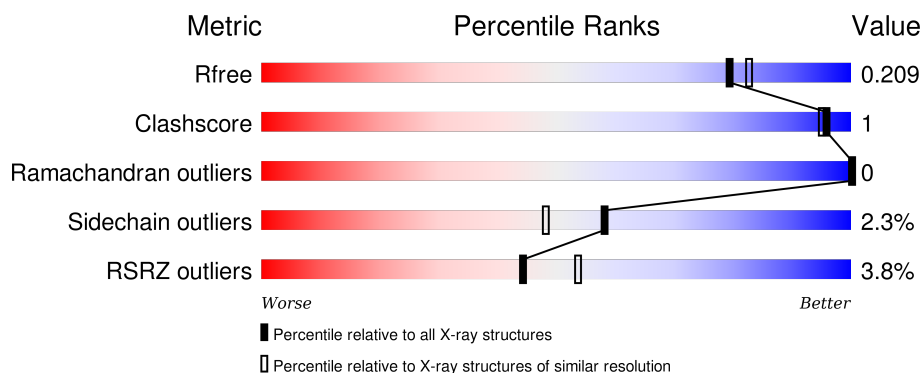
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

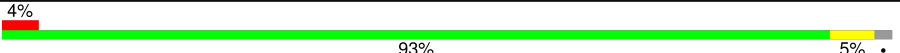
The reported resolution of this entry is 1.95 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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. 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	307	

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
2	1Q9	A	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	306	-	-	-	X
5	EDO	A	307	-	-	-	X
6	GOL	A	308	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2692 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 PENTAETHYLENE GLYCOL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	300	2414	1566	412	427	2	7	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

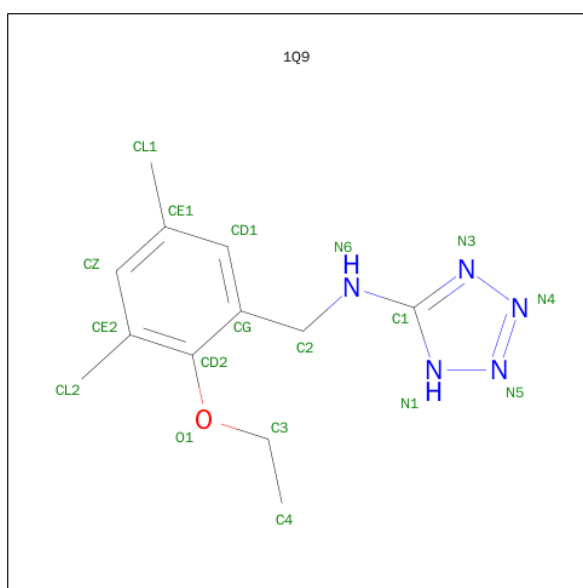
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	EXPRESSION TAG	UNP P0A3G3
A	-9	GLY	-	EXPRESSION TAG	UNP P0A3G3
A	-8	HIS	-	EXPRESSION TAG	UNP P0A3G3
A	-7	HIS	-	EXPRESSION TAG	UNP P0A3G3
A	-6	HIS	-	EXPRESSION TAG	UNP P0A3G3
A	-5	HIS	-	EXPRESSION TAG	UNP P0A3G3
A	-4	HIS	-	EXPRESSION TAG	UNP P0A3G3
A	-3	HIS	-	EXPRESSION TAG	UNP P0A3G3
A	0	HIS	-	EXPRESSION TAG	UNP P0A3G3
A	1	MSE	-	EXPRESSION TAG	UNP P0A3G3
A	2	ALA	-	EXPRESSION TAG	UNP P0A3G3
A	47	VAL	LEU	engineered mutation	UNP P0A3G3
A	58	THR	SER	engineered mutation	UNP P0A3G3
A	78	GLY	ASP	engineered mutation	UNP P0A3G3
A	87	PHE	TYR	engineered mutation	UNP P0A3G3
A	88	MSE	LEU	engineered mutation	UNP P0A3G3
A	128	PHE	CYS	engineered mutation	UNP P0A3G3
A	155	THR	ALA	engineered mutation	UNP P0A3G3
A	160	LYS	GLU	engineered mutation	UNP P0A3G3
A	167	VAL	ALA	engineered mutation	UNP P0A3G3
A	172	THR	ALA	engineered mutation	UNP P0A3G3
A	175	MSE	LYS	engineered mutation	UNP P0A3G3
A	176	GLY	CYS	engineered mutation	UNP P0A3G3
A	195	ASN	LYS	engineered mutation	UNP P0A3G3
A	224	GLU	ALA	engineered mutation	UNP P0A3G3
A	227	ASP	ASN	engineered mutation	UNP P0A3G3
A	257	LYS	GLU	engineered mutation	UNP P0A3G3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	264	ALA	THR	engineered mutation	UNP P0A3G3
A	272	ASN	HIS	engineered mutation	UNP P0A3G3
A	273	LEU	TYR	engineered mutation	UNP P0A3G3
A	291	SER	PRO	engineered mutation	UNP P0A3G3
A	292	THR	ALA	engineered mutation	UNP P0A3G3
A	294	GLU	-	EXPRESSION TAG	UNP P0A3G3
A	295	ILE	-	EXPRESSION TAG	UNP P0A3G3
A	296	SER	-	EXPRESSION TAG	UNP P0A3G3
A	297	GLY	-	EXPRESSION TAG	UNP P0A3G3

- Molecule 2 is N-(2-ETHOXY-3,5-DIMETHYLBENZYL)-1H-TETRAZOL-5-AMINE (three-letter code: 1Q9) (formula: C₁₂H₁₇N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	12	5	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

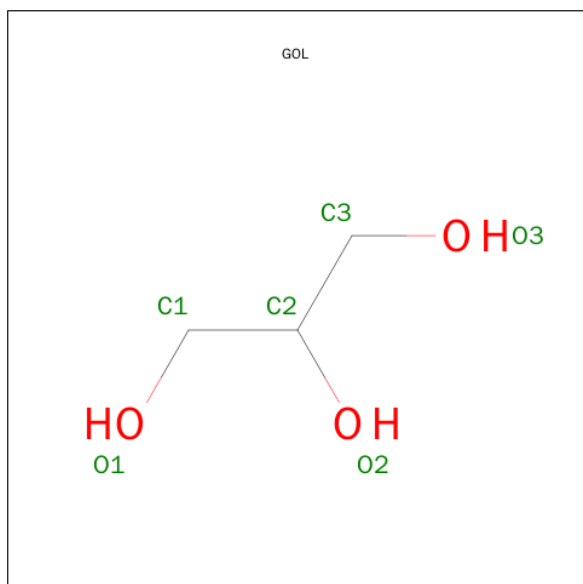
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



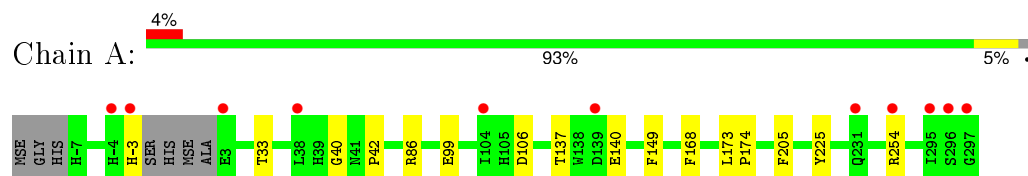
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	242	Total	O	0	8
			242	242		

i

- Molecule 1: PENTAETHYLENE GLYCOL



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.03Å 63.03Å 164.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 1.95 29.42 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.42-1.95) 99.9 (29.42-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1269)	Depositor
R, R_{free}	0.167 , 0.201 0.174 , 0.209	Depositor DCC
R_{free} test set	1254 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25108 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2692	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MN, 1Q9, EDO, 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	0.36	0/2490	0.51	0/3391

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	2414	0	2339	7	0
2	A	18	0	17	3	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	8	0	11	0	0
6	A	6	0	8	0	0
7	A	242	0	0	0	0
All	All	2692	0	2375	7	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 1.

The worst 5 of 7 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:33:THR:HG23	1:A:99:GLU:HG2	1.92	0.51
1:A:149:PHE:CE1	2:A:301:1Q9:H4	2.46	0.49
1:A:40:GLY:HA3	1:A:106:ASP:HB3	1.99	0.44
1:A:149:PHE:CZ	2:A:301:1Q9:H4	2.53	0.44
1:A:42:PRO:HD3	2:A:301:1Q9:H13	2.02	0.41

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	296/307 (96%)	285 (96%)	11 (4%)	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	259/255 (102%)	253 (98%)	6 (2%)	58	48

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	PHE
1	A	254	ARG

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Mol	Chain	Res	Type
1	A	205	PHE
1	A	86	ARG
1	A	225	TYR

Some 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 carbohydrates 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	$\# Z > 2$
2	1Q9	A	301	-	19,19,19	5.40	5 (26%)	23,25,25	1.85	6 (26%)
5	EDO	A	306	4	3,3,3	0.51	0	2,2,2	1.06	0
5	EDO	A	307	-	3,3,3	0.55	0	2,2,2	0.76	0
6	GOL	A	308	-	5,5,5	0.33	0	5,5,5	0.41	0

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
2	1Q9	A	301	-	-	0/6/8/8	0/2/2/2
5	EDO	A	306	4	-	0/1/1/1	0/0/0/0
5	EDO	A	307	-	-	0/1/1/1	0/0/0/0
6	GOL	A	308	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	1Q9	N3-N4	-2.71	1.30	1.34
2	A	301	1Q9	C1-N6	2.71	1.38	1.34
2	A	301	1Q9	C1-N3	7.20	1.42	1.33
2	A	301	1Q9	C1-N1	10.75	1.47	1.33
2	A	301	1Q9	N5-N4	19.08	1.56	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	1Q9	N1-N5-N4	-4.61	106.94	109.59
2	A	301	1Q9	C2-N6-C1	-3.76	118.10	123.35
2	A	301	1Q9	C1-N1-N5	2.01	106.22	104.08
2	A	301	1Q9	C3-O1-CD2	2.21	122.42	115.05
2	A	301	1Q9	O1-CD2-CE2	2.32	122.56	118.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	1Q9	3	0

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	293/307 (95%)	0.04	11 (3%) 44 54	14, 24, 46, 75	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	HIS	5.4
1	A	296	SER	3.9
1	A	3	GLU	3.3
1	A	38	LEU	3.0
1	A	254	ARG	3.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	A	307	4/4	0.92	0.20	3.12	33,36,42,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	A	308	6/6	0.75	0.20	2.92	36,42,45,46	0
5	EDO	A	306	4/4	0.90	0.17	2.66	29,33,33,35	0
2	1Q9	A	301	18/18	0.87	0.18	2.56	16,25,28,28	0
4	NA	A	305	1/1	0.94	0.10	-	50,50,50,50	0
3	MN	A	302	1/1	0.99	0.08	-	33,33,33,33	0
3	MN	A	303	1/1	0.95	0.06	-	59,59,59,59	0
4	NA	A	304	1/1	0.96	0.09	-	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.