



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 PM UTC

PDB ID : 1EDD / pdb_00001edd
Title : CRYSTALLOGRAPHIC AND FLUORESCENCE STUDIES OF THE INTERACTION OF HALOALKANE DEHALOGENASE WITH HALIDE IONS: STUDIES WITH HALIDE COMPOUNDS REVEAL A HALIDE BINDING SITE IN THE ACTIVE SITE
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Deposited on : 1993-05-13
Resolution : 2.19 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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

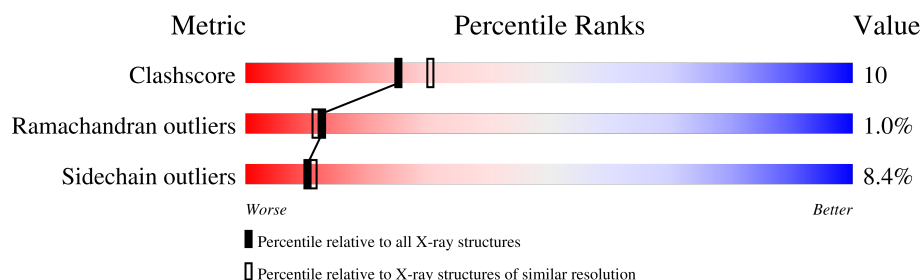
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2652 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 HALOALKANE DEHALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2479	1596	406	462	15			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

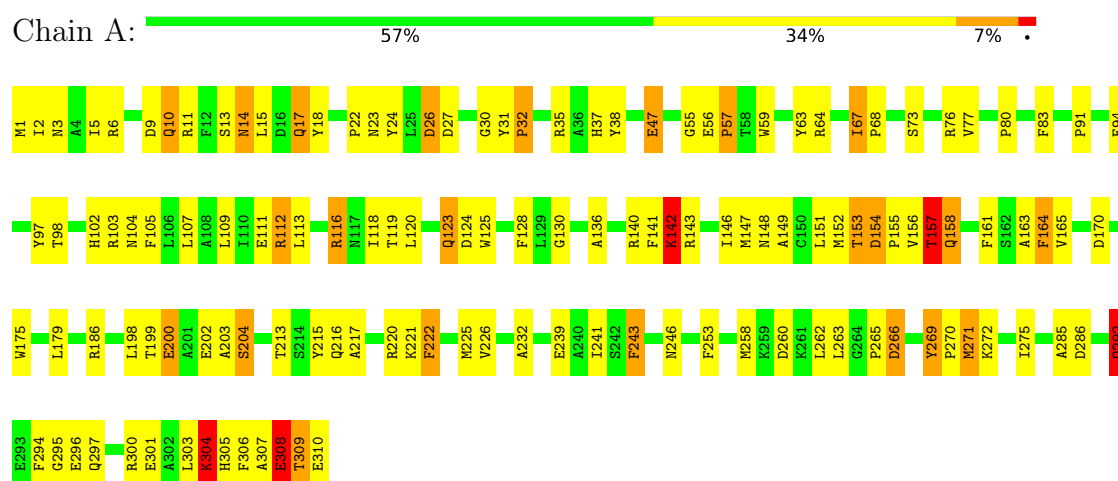
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total	O	0	0
			172	172		

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. 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.

Note EDS was not executed.

• Molecule 1: HALOALKANE DEHALOGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.40 Å 72.50 Å 41.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.19	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2652	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	1.00	0/2552	2.20	115/3470 (3.3%)

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ASP	CA-CB-CG	-10.65	101.95	112.60
1	A	13	SER	CB-CA-C	-9.76	95.56	110.88
1	A	243	PHE	CA-CB-CG	-9.45	104.35	113.80
1	A	216	GLN	N-CA-C	8.72	123.49	113.02
1	A	269	TYR	CA-CB-CG	-8.47	98.65	113.90
1	A	294	PHE	CA-C-N	7.89	130.01	120.14
1	A	294	PHE	C-N-CA	7.89	130.01	120.14
1	A	295	GLY	N-CA-C	7.89	123.58	113.24
1	A	147	MET	CA-C-O	-7.79	112.13	121.56
1	A	246	ASN	N-CA-C	7.67	123.32	113.88
1	A	297	GLN	N-CA-C	-7.61	102.92	111.07
1	A	246	ASN	CA-CB-CG	7.60	120.20	112.60
1	A	64	ARG	N-CA-C	7.30	121.28	112.38
1	A	83	PHE	CA-CB-CG	-7.22	106.58	113.80
1	A	136	ALA	CA-C-O	6.92	127.89	119.38
1	A	170	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	119	THR	N-CA-C	-6.91	95.75	107.99
1	A	13	SER	N-CA-C	6.89	118.45	111.07
1	A	2	ILE	N-CA-C	-6.89	97.69	108.23
1	A	120	LEU	CB-CA-C	6.74	120.84	109.80
1	A	217	ALA	CA-C-N	6.71	127.43	119.98
1	A	217	ALA	C-N-CA	6.71	127.43	119.98
1	A	266	ASP	CA-CB-CG	-6.70	105.90	112.60
1	A	258	MET	N-CA-C	6.67	119.38	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	GLU	CA-C-O	-6.52	112.73	120.10
1	A	24	TYR	CA-C-O	-6.51	113.51	121.06
1	A	124	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	14	ASN	N-CA-C	6.49	119.90	112.57
1	A	164	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	292	GLN	N-CA-C	6.47	119.16	111.71
1	A	57	PRO	N-CA-C	-6.47	95.27	112.10
1	A	239	GLU	O-C-N	-6.44	114.68	122.22
1	A	153	THR	N-CA-CB	-6.37	101.59	110.38
1	A	59	TRP	N-CA-CB	6.31	121.22	111.24
1	A	55	GLY	CA-C-O	-6.28	115.69	121.72
1	A	111	GLU	N-CA-CB	6.27	119.44	110.16
1	A	304	LYS	CB-CA-C	6.22	120.73	110.90
1	A	164	PHE	N-CA-C	6.15	120.39	113.01
1	A	303	LEU	N-CA-CB	6.13	119.78	110.28
1	A	232	ALA	N-CA-CB	6.11	118.87	110.01
1	A	271	MET	CB-CA-C	-6.11	100.47	110.85
1	A	203	ALA	CA-C-O	6.07	126.98	120.55
1	A	98	THR	CA-CB-OG1	-6.04	100.53	109.60
1	A	204	SER	CB-CA-C	6.01	122.87	110.31
1	A	286	ASP	N-CA-C	5.99	120.59	113.16
1	A	215	TYR	CB-CA-C	-5.92	99.35	110.01
1	A	128	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	3	ASN	N-CA-C	-5.90	101.11	109.96
1	A	294	PHE	N-CA-C	-5.89	103.57	111.87
1	A	47	GLU	CB-CG-CD	5.88	122.59	112.60
1	A	103	ARG	CA-C-O	5.86	126.64	120.42
1	A	67	ILE	CB-CG1-CD1	-5.81	101.60	113.80
1	A	141	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	226	VAL	CA-C-N	5.74	128.45	120.29
1	A	226	VAL	C-N-CA	5.74	128.45	120.29
1	A	18	TYR	CB-CA-C	5.74	120.09	111.14
1	A	124	ASP	CA-C-N	5.73	128.24	120.38
1	A	124	ASP	C-N-CA	5.73	128.24	120.38
1	A	156	VAL	CA-C-O	5.66	126.85	120.85
1	A	204	SER	CA-CB-OG	-5.64	99.81	111.10
1	A	9	ASP	N-CA-C	5.63	118.19	111.71
1	A	263	LEU	N-CA-C	5.62	117.25	109.54
1	A	266	ASP	N-CA-CB	5.61	119.86	110.32
1	A	10	GLN	CB-CG-CD	5.59	122.11	112.60
1	A	76	ARG	N-CA-C	-5.58	100.61	109.76
1	A	105	PHE	N-CA-C	-5.58	105.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	GLN	N-CA-CB	5.58	118.81	110.22
1	A	112	ARG	CD-NE-CZ	-5.55	116.63	124.40
1	A	102	HIS	CA-CB-CG	5.54	119.34	113.80
1	A	202	GLU	CA-CB-CG	-5.54	103.02	114.10
1	A	146	ILE	CA-C-O	-5.54	114.61	120.48
1	A	130	GLY	CA-C-O	-5.52	115.07	120.75
1	A	116	ARG	NE-CZ-NH2	-5.52	114.24	119.20
1	A	6	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	157	THR	CB-CA-C	5.48	120.17	110.85
1	A	68	PRO	N-CA-CB	5.48	109.33	103.52
1	A	11	ARG	CD-NE-CZ	-5.47	116.74	124.40
1	A	175	TRP	N-CA-CB	-5.40	102.17	110.01
1	A	285	ALA	N-CA-C	5.40	117.86	111.33
1	A	17	GLN	CA-C-N	-5.39	116.62	123.15
1	A	17	GLN	C-N-CA	-5.39	116.62	123.15
1	A	32	PRO	CA-C-O	5.38	126.92	121.27
1	A	253	PHE	N-CA-C	-5.38	99.17	108.69
1	A	120	LEU	N-CA-CB	-5.37	101.31	110.16
1	A	149	ALA	CB-CA-C	-5.37	101.29	110.95
1	A	142	LYS	N-CA-CB	-5.34	103.89	111.00
1	A	198	LEU	CB-CA-C	-5.34	100.85	109.72
1	A	222	PHE	O-C-N	5.34	125.62	120.55
1	A	154	ASP	N-CA-CB	5.33	117.14	109.78
1	A	200	GLU	CB-CG-CD	-5.33	103.54	112.60
1	A	22	PRO	CA-C-O	-5.32	115.36	121.86
1	A	199	THR	CA-CB-OG1	-5.31	101.64	109.60
1	A	26	ASP	CA-C-O	5.30	125.93	119.78
1	A	140	ARG	CB-CA-C	-5.27	99.60	109.72
1	A	163	ALA	N-CA-C	5.25	117.68	111.33
1	A	118	ILE	N-CA-C	5.24	115.81	108.89
1	A	35	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	253	PHE	CA-C-O	-5.21	113.88	120.28
1	A	294	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	149	ALA	CA-C-O	-5.17	115.75	121.28
1	A	306	PHE	N-CA-C	5.16	117.81	111.82
1	A	32	PRO	O-C-N	-5.15	117.36	122.98
1	A	83	PHE	CA-C-N	5.14	131.36	122.05
1	A	83	PHE	C-N-CA	5.14	131.36	122.05
1	A	165	VAL	CA-C-O	-5.12	115.63	120.95
1	A	147	MET	N-CA-C	-5.08	102.26	110.14
1	A	265	PRO	CA-C-O	-5.07	111.27	119.84
1	A	158	GLN	CA-C-O	-5.07	115.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	TYR	N-CA-C	-5.07	106.88	113.16
1	A	260	ASP	CA-C-O	-5.07	114.61	120.49
1	A	37	HIS	O-C-N	-5.06	116.78	123.16
1	A	27	ASP	N-CA-CB	-5.02	104.00	111.43
1	A	23	ASN	N-CA-C	-5.01	100.86	109.24
1	A	179	LEU	N-CA-C	5.01	119.42	112.45
1	A	123	GLN	CA-C-O	-5.01	115.14	120.75

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	2479	0	2379	47	0
2	A	1	0	0	0	0
3	A	172	0	0	5	1
All	All	2652	0	2379	47	1

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 10.

All (47) 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:292:GLN:HE21	1:A:292:GLN:H	1.06	1.01
1:A:142:LYS:HG2	1:A:143:ARG:HG3	1.66	0.77
1:A:292:GLN:HE21	1:A:292:GLN:N	1.83	0.75
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.58	0.67
1:A:292:GLN:H	1:A:292:GLN:NE2	1.87	0.64
1:A:152:MET:HA	1:A:152:MET:HE2	1.82	0.61
1:A:17:GLN:HG3	3:A:413:HOH:O	2.04	0.58
1:A:112:ARG:HG3	1:A:112:ARG:NH1	2.16	0.57
1:A:154:ASP:HB2	1:A:155:PRO:HD2	1.88	0.56
1:A:296:GLU:O	1:A:300:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:OD1	1:A:157:THR:HG23	2.08	0.53
1:A:262:LEU:HD23	3:A:539:HOH:O	2.10	0.52
1:A:309:THR:O	1:A:309:THR:HG22	2.09	0.52
1:A:104:ASN:ND2	3:A:415:HOH:O	2.40	0.51
1:A:26:ASP:N	1:A:26:ASP:OD1	2.30	0.51
1:A:125:TRP:CH2	1:A:225:MET:HE2	2.45	0.51
1:A:142:LYS:HG2	1:A:143:ARG:CG	2.38	0.51
1:A:307:ALA:C	1:A:309:THR:H	2.21	0.49
1:A:243:PHE:CD2	1:A:243:PHE:C	2.91	0.49
1:A:97:TYR:HB2	1:A:221:LYS:HG2	1.95	0.49
1:A:151:LEU:HD13	1:A:241:ILE:HG13	1.95	0.49
1:A:67:ILE:HG12	1:A:77:VAL:HG11	1.94	0.49
1:A:269:TYR:HB2	1:A:270:PRO:HD3	1.94	0.48
1:A:272:LYS:O	1:A:272:LYS:HG2	2.13	0.48
1:A:308:GLU:O	1:A:308:GLU:HG3	2.15	0.47
1:A:309:THR:O	1:A:310:GLU:HB2	2.16	0.46
1:A:153:THR:HG21	1:A:158:GLN:HB2	1.98	0.46
1:A:142:LYS:O	1:A:143:ARG:HG2	2.16	0.45
1:A:154:ASP:CG	1:A:157:THR:HG23	2.41	0.45
1:A:38:TYR:CB	1:A:80:PRO:HA	2.47	0.44
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.78	0.44
1:A:30:GLY:C	1:A:32:PRO:HD2	2.43	0.43
1:A:266:ASP:HB2	3:A:426:HOH:O	2.18	0.43
1:A:5:ILE:HD13	1:A:5:ILE:HG21	1.49	0.43
1:A:310:GLU:O	1:A:310:GLU:HG2	2.18	0.43
1:A:56:GLU:HA	1:A:57:PRO:HA	1.95	0.42
1:A:220:ARG:HD3	3:A:449:HOH:O	2.19	0.42
1:A:269:TYR:CB	1:A:270:PRO:HD3	2.50	0.42
1:A:125:TRP:CH2	1:A:225:MET:CE	3.03	0.41
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.84	0.41
1:A:161:PHE:CD1	1:A:161:PHE:N	2.88	0.41
1:A:164:PHE:CD1	1:A:164:PHE:C	2.98	0.41
1:A:301:GLU:OE1	1:A:304:LYS:HD2	2.21	0.41
1:A:31:TYR:N	1:A:32:PRO:CD	2.84	0.41
1:A:154:ASP:OD1	1:A:157:THR:CG2	2.68	0.41
1:A:30:GLY:O	1:A:32:PRO:HD2	2.21	0.40
1:A:305:HIS:O	1:A:308:GLU:HG2	2.21	0.40

All (1) 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)
3:A:569:HOH:O	3:A:569:HOH:O[2_685]	2.10	0.10

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	308/310 (99%)	293 (95%)	12 (4%)	3 (1%)	12 11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	309	THR
1	A	308	GLU

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	262/262 (100%)	240 (92%)	22 (8%)	10 11

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	GLN
1	A	14	ASN

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Mol	Chain	Res	Type
1	A	15	LEU
1	A	47	GLU
1	A	73	SER
1	A	91	PRO
1	A	109	LEU
1	A	113	LEU
1	A	116	ARG
1	A	123	GLN
1	A	142	LYS
1	A	157	THR
1	A	186	ARG
1	A	200	GLU
1	A	204	SER
1	A	213	THR
1	A	222	PHE
1	A	271	MET
1	A	292	GLN
1	A	304	LYS
1	A	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	43	ASN
1	A	104	ASN
1	A	123	GLN
1	A	251	GLN
1	A	292	GLN

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 [i](#)

There are no oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.