



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:52 AM UTC

PDB ID : 8E3D / pdb_00008e3d
Title : ZBTB7A Zinc Finger Domain Bound to DNA Duplex Containing CAST sequence (#11)
Authors : Horton, J.R.; Ren, R.; Cheng, X.
Deposited on : 2022-08-17
Resolution : 2.62 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

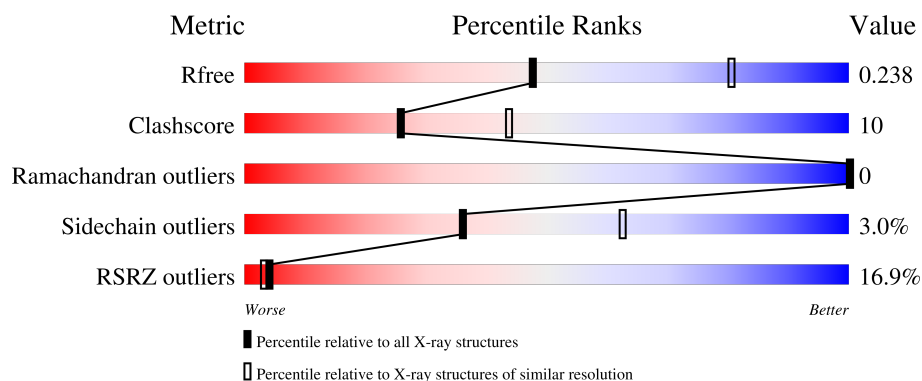
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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 ≥ 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	133	6% 65% 18% • 17%
1	B	133	6% 71% 14% 14%
1	F	133	44% 66% 17% 17%
2	D	22	64% 36%
2	H	22	5% 86% 14%

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Mol	Chain	Length	Quality of chain
2	X	22	41% 59%
3	E	22	55% 45%
3	I	22	14% 41% 59%
3	Y	22	5% 23% 77%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5425 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 Zinc finger and BTB domain-containing protein 7A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			885	549	178	146	12			
1	B	114	Total	C	N	O	S	0	0	0
			892	550	180	150	12			
1	F	111	Total	C	N	O	S	0	0	0
			843	518	171	143	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	GLY	-	expression tag	UNP O95365
A	376	PRO	-	expression tag	UNP O95365
A	377	LEU	-	expression tag	UNP O95365
A	378	GLY	-	expression tag	UNP O95365
A	379	SER	-	expression tag	UNP O95365
A	501	LEU	-	expression tag	UNP O95365
A	502	GLU	-	expression tag	UNP O95365
A	503	ARG	-	expression tag	UNP O95365
A	504	PRO	-	expression tag	UNP O95365
A	505	HIS	-	expression tag	UNP O95365
A	506	ARG	-	expression tag	UNP O95365
A	507	ASP	-	expression tag	UNP O95365
B	375	GLY	-	expression tag	UNP O95365
B	376	PRO	-	expression tag	UNP O95365
B	377	LEU	-	expression tag	UNP O95365
B	378	GLY	-	expression tag	UNP O95365
B	379	SER	-	expression tag	UNP O95365
B	501	LEU	-	expression tag	UNP O95365
B	502	GLU	-	expression tag	UNP O95365
B	503	ARG	-	expression tag	UNP O95365
B	504	PRO	-	expression tag	UNP O95365
B	505	HIS	-	expression tag	UNP O95365
B	506	ARG	-	expression tag	UNP O95365

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Chain	Residue	Modelled	Actual	Comment	Reference
B	507	ASP	-	expression tag	UNP O95365
F	375	GLY	-	expression tag	UNP O95365
F	376	PRO	-	expression tag	UNP O95365
F	377	LEU	-	expression tag	UNP O95365
F	378	GLY	-	expression tag	UNP O95365
F	379	SER	-	expression tag	UNP O95365
F	501	LEU	-	expression tag	UNP O95365
F	502	GLU	-	expression tag	UNP O95365
F	503	ARG	-	expression tag	UNP O95365
F	504	PRO	-	expression tag	UNP O95365
F	505	HIS	-	expression tag	UNP O95365
F	506	ARG	-	expression tag	UNP O95365
F	507	ASP	-	expression tag	UNP O95365

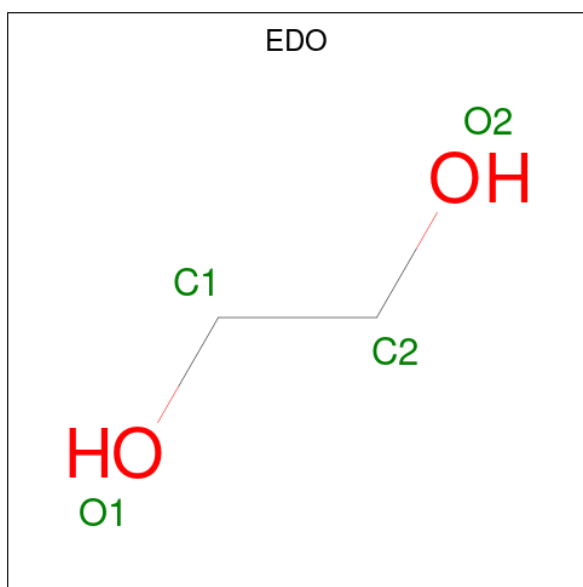
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*TP*TP*GP*GP*GP*GP*AP*GP*GP*GP*TP*CP*TP*TP*TP*AP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	22	Total	C	N	O	P	0	0	0
			454	217	83	133	21			
2	D	22	Total	C	N	O	P	0	0	0
			454	217	83	133	21			
2	H	22	Total	C	N	O	P	0	0	0
			454	217	83	133	21			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*TP*AP*AP*AP*AP*GP*AP*CP*CP*CP*CP*TP*CP*CP*CP*CP*AP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	22	Total	C	N	O	P	0	0	0
			446	212	85	127	22			
3	E	22	Total	C	N	O	P	0	0	0
			443	212	85	125	21			
3	I	22	Total	C	N	O	P	0	0	0
			446	212	85	127	22			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	Y	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Zn 4 4	0	0
5	B	4	Total Zn 4 4	0	0
5	F	4	Total Zn 4 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	0	0

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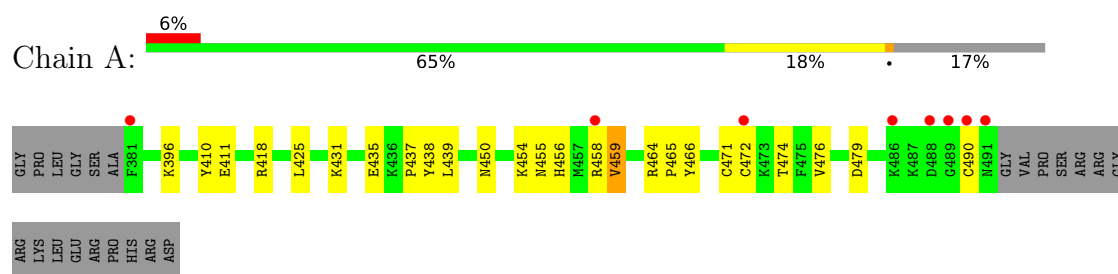
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	X	7	Total 7	O 7	0	0
6	Y	10	Total 10	O 10	0	0
6	B	18	Total 18	O 18	0	0
6	D	2	Total 2	O 2	0	0
6	E	6	Total 6	O 6	0	0
6	F	1	Total 1	O 1	0	0

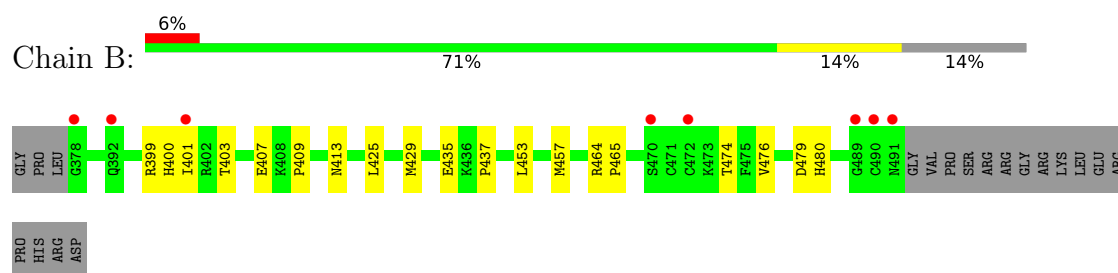
3 Residue-property plots [i](#)

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.

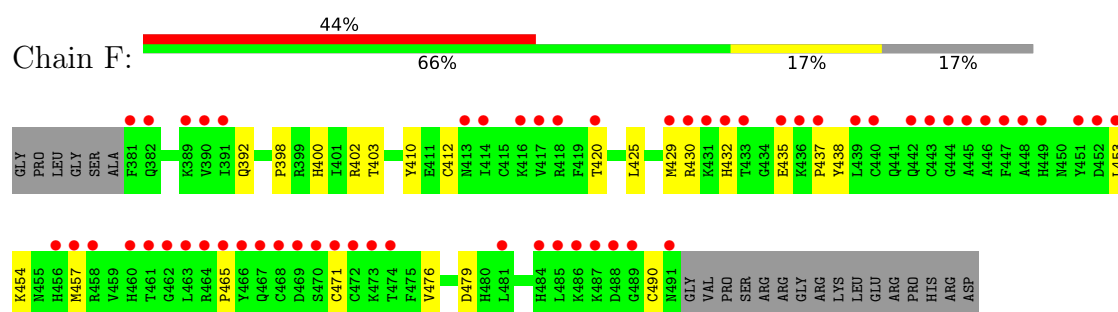
- Molecule 1: Zinc finger and BTB domain-containing protein 7A



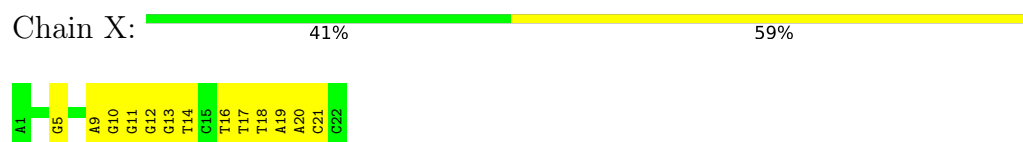
- Molecule 1: Zinc finger and BTB domain-containing protein 7A



- Molecule 1: Zinc finger and BTB domain-containing protein 7A

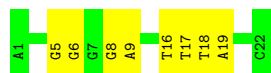


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*GP*GP*GP*GP*AP*GP*GP*GP*TP*CP*TP*TP*TP*AP*AP*CP*C)-3')



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

Chain D:  64% 36%



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

Chain H:  5% 86% 14%



- Molecule 3: DNA (5'-D(P*GP*GP*TP*AP*AP*AP*AP*GP*AP*CP*CP*CP*CP*TP*CP*CP*CP*AP*AP*AP*T)-3')

Chain Y:  5% 23% 77%



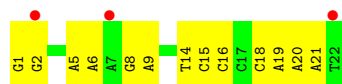
- Molecule 3: DNA (5'-D(P*GP*GP*TP*AP*AP*AP*AP*GP*AP*CP*CP*CP*CP*TP*CP*CP*CP*AP*AP*AP*T)-3')

Chain E:  55% 45%



- Molecule 3: DNA (5'-D(P*GP*GP*TP*AP*AP*AP*AP*GP*AP*CP*CP*CP*CP*TP*CP*CP*CP*AP*AP*AP*T)-3')

Chain I:  14% 41% 59%



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	196.18Å 196.18Å 54.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.15 – 2.62 46.15 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.15-2.62) 90.0 (46.15-2.62)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.237 0.204 , 0.238	Depositor DCC
R_{free} test set	1804 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: ZN, EDO

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	0.12	0/906	0.28	0/1214
1	B	0.12	0/913	0.26	0/1226
1	F	0.08	0/864	0.23	0/1164
2	D	0.21	0/509	0.50	0/786
2	H	0.19	0/509	0.41	0/786
2	X	0.20	0/509	0.46	0/786
3	E	0.23	0/497	0.47	0/763
3	I	0.22	0/500	0.40	0/767
3	Y	0.22	0/500	0.46	0/767
All	All	0.17	0/5707	0.38	0/8259

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	885	0	863	15	0
1	B	892	0	848	13	0
1	F	843	0	755	12	0
2	D	454	0	251	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	454	0	251	3	0
2	X	454	0	251	10	0
3	E	443	0	247	8	0
3	I	446	0	246	10	0
3	Y	446	0	246	15	0
4	A	8	0	12	0	0
4	B	4	0	6	2	0
4	D	4	0	6	0	0
4	Y	4	0	6	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	F	4	0	0	0	0
6	A	32	0	0	1	0
6	B	18	0	0	0	0
6	D	2	0	0	0	0
6	E	6	0	0	0	0
6	F	1	0	0	0	0
6	X	7	0	0	0	0
6	Y	10	0	0	0	0
All	All	5425	0	3988	89	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 10.

All (89) 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:471:CYS:HB3	1:A:490:CYS:SG	1.86	1.16
1:F:471:CYS:HB3	1:F:490:CYS:SG	2.31	0.69
3:Y:5:DA:H2'	3:Y:6:DA:C8	2.26	0.69
3:I:5:DA:H2'	3:I:6:DA:C8	2.31	0.66
2:X:9:DA:H2'	2:X:10:DG:H8	1.64	0.62
2:X:9:DA:H2'	2:X:10:DG:C8	2.39	0.58
3:E:13:DC:H2'	3:E:14:DT:C6	2.39	0.57
2:D:18:DT:H2''	2:D:19:DA:C8	2.39	0.56
3:E:8:DG:H2''	3:E:9:DA:O5'	2.04	0.56
3:I:18:DC:H2''	3:I:19:DA:C8	2.40	0.56
1:A:464:ARG:NH2	2:X:5:DG:OP1	2.39	0.55
3:Y:8:DG:H2''	3:Y:9:DA:O5'	2.07	0.55
1:A:450:ASN:HD21	1:A:454:LYS:HE3	1.70	0.55
3:Y:21:DA:H2''	3:Y:22:DT:O5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLU:HG2	1:B:409:PRO:HD3	1.89	0.55
1:B:435:GLU:HG2	1:B:437:PRO:HD3	1.90	0.54
2:X:18:DT:H2''	2:X:19:DA:C8	2.44	0.53
2:X:20:DA:H2''	2:X:21:DC:H5''	1.91	0.53
1:F:435:GLU:HG2	1:F:437:PRO:HD3	1.91	0.53
1:F:430:ARG:HD3	1:F:437:PRO:HG3	1.92	0.52
1:A:435:GLU:HG2	1:A:437:PRO:HD3	1.92	0.52
3:E:20:DA:H2''	3:E:21:DA:O5'	2.10	0.52
2:D:5:DG:H4'	2:D:6:DG:OP1	2.09	0.51
2:X:18:DT:H2''	2:X:19:DA:N7	2.25	0.51
3:I:8:DG:H2''	3:I:9:DA:O5'	2.10	0.51
1:B:413:ASN:OD1	4:B:601:EDO:O1	2.29	0.50
1:F:465:PRO:HD2	1:F:476:VAL:HA	1.92	0.50
3:Y:20:DA:H4'	3:Y:21:DA:OP1	2.11	0.49
1:B:480:HIS:HE1	2:D:5:DG:H2'	1.78	0.49
3:I:20:DA:H4'	3:I:21:DA:OP1	2.11	0.49
1:A:396:LYS:NZ	6:A:703:HOH:O	2.42	0.49
2:X:11:DG:H2''	2:X:12:DG:H8	1.78	0.48
1:B:399:ARG:O	1:B:403:THR:HG23	2.13	0.48
1:F:438:TYR:HB3	1:F:453:LEU:HD22	1.93	0.48
1:A:411:GLU:HB2	1:A:418:ARG:HD2	1.95	0.48
3:Y:12:DC:H2'	3:Y:13:DC:C6	2.49	0.47
2:H:16:DT:H4'	2:H:17:DT:OP1	2.13	0.47
1:B:429:MET:HG3	4:B:601:EDO:H21	1.96	0.47
1:B:480:HIS:CE1	2:D:5:DG:H2'	2.50	0.47
1:A:465:PRO:HD2	1:A:476:VAL:HA	1.97	0.47
3:Y:12:DC:H2'	3:Y:13:DC:H6	1.80	0.47
3:Y:15:DC:H2'	3:Y:16:DC:C6	2.50	0.47
3:Y:21:DA:H4'	3:Y:22:DT:OP1	2.15	0.46
2:D:16:DT:H2'	2:D:17:DT:H72	1.97	0.46
3:E:20:DA:H4'	3:E:21:DA:OP1	2.14	0.46
3:E:5:DA:H2''	3:E:6:DA:C8	2.50	0.46
3:I:8:DG:H2'	3:I:9:DA:C8	2.51	0.46
1:F:410:TYR:HB3	1:F:425:LEU:HD22	1.98	0.46
1:A:438:TYR:OH	3:Y:11:DC:OP2	2.32	0.45
2:D:8:DG:H2''	2:D:9:DA:H8	1.81	0.45
1:F:479:ASP:OD1	1:F:479:ASP:N	2.49	0.45
3:Y:11:DC:H2'	3:Y:12:DC:C6	2.51	0.45
1:B:425:LEU:O	1:B:429:MET:HG2	2.16	0.45
3:E:5:DA:H4'	3:E:6:DA:OP1	2.16	0.45
3:Y:20:DA:H2''	3:Y:21:DA:O5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:PRO:HD2	1:B:476:VAL:HA	1.99	0.45
2:X:16:DT:H4'	2:X:17:DT:OP1	2.16	0.45
1:F:429:MET:HE2	1:F:429:MET:HA	1.99	0.45
1:A:479:ASP:OD1	1:A:479:ASP:N	2.50	0.44
1:A:464:ARG:HD3	1:A:474:THR:OG1	2.16	0.44
1:F:398:PRO:O	1:F:402:ARG:HG3	2.17	0.44
1:A:431:LYS:HB2	1:A:431:LYS:HE3	1.75	0.44
3:Y:14:DT:H2''	3:Y:15:DC:H6	1.82	0.44
2:D:16:DT:H4'	2:D:17:DT:OP1	2.17	0.44
1:B:464:ARG:HE	1:B:474:THR:HG23	1.83	0.44
1:B:479:ASP:OD1	1:B:479:ASP:N	2.51	0.43
3:Y:8:DG:H4'	3:Y:9:DA:OP1	2.18	0.43
2:D:17:DT:H1'	2:D:18:DT:H5'	2.01	0.43
3:I:8:DG:H4'	3:I:9:DA:OP1	2.19	0.43
2:X:11:DG:H2''	2:X:12:DG:C8	2.54	0.43
1:A:456:HIS:O	1:A:459:VAL:HB	2.18	0.43
3:Y:18:DC:H2''	3:Y:19:DA:C8	2.54	0.43
3:E:16:DC:H1'	3:E:17:DC:H5'	2.00	0.43
3:I:14:DT:H2''	3:I:15:DC:H6	1.85	0.42
1:B:400:HIS:O	1:B:403:THR:OG1	2.22	0.42
3:Y:3:DT:H2''	3:Y:4:DA:C8	2.55	0.42
2:X:13:DG:H2'	2:X:14:DT:C7	2.50	0.41
1:F:454:LYS:HA	1:F:454:LYS:HD3	1.81	0.41
1:A:410:TYR:HB3	1:A:425:LEU:HD22	2.03	0.41
1:A:465:PRO:HG2	1:A:466:TYR:CD1	2.56	0.41
3:I:15:DC:C2	3:I:16:DC:C4	3.09	0.41
1:B:453:LEU:O	1:B:457:MET:HG2	2.20	0.41
1:F:392:GLN:NE2	2:H:13:DG:H3'	2.36	0.41
1:F:400:HIS:O	1:F:403:THR:OG1	2.32	0.41
3:I:1:DG:H2''	3:I:2:DG:C8	2.56	0.41
1:A:455:ASN:O	1:A:458:ARG:HG2	2.21	0.40
3:E:8:DG:H4'	3:E:9:DA:OP1	2.22	0.40
3:I:1:DG:H2''	3:I:2:DG:H8	1.87	0.40
2:H:16:DT:C6	2:H:17:DT:H72	2.55	0.40

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	109/133 (82%)	106 (97%)	3 (3%)	0	100	100
1	B	112/133 (84%)	110 (98%)	2 (2%)	0	100	100
1	F	109/133 (82%)	106 (97%)	3 (3%)	0	100	100
All	All	330/399 (83%)	322 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	94/117 (80%)	91 (97%)	3 (3%)	34	60
1	B	92/117 (79%)	91 (99%)	1 (1%)	65	83
1	F	81/117 (69%)	77 (95%)	4 (5%)	22	44
All	All	267/351 (76%)	259 (97%)	8 (3%)	36	62

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	LEU
1	A	459	VAL
1	A	472	CYS
1	B	401	ILE
1	F	412	CYS

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Mol	Chain	Res	Type
1	F	420	THR
1	F	432	HIS
1	F	457	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	GLN
1	A	450	ASN
1	B	482	HIS
1	F	392	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	$\# Z > 2$
4	EDO	Y	201	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	A	601	-	3,3,3	0.43	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	602	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	D	101	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	B	601	-	3,3,3	0.42	0	2,2,2	0.38	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
4	EDO	Y	201	-	-	0/1/1/1	-
4	EDO	A	601	-	-	0/1/1/1	-
4	EDO	A	602	-	-	0/1/1/1	-
4	EDO	D	101	-	-	0/1/1/1	-
4	EDO	B	601	-	-	0/1/1/1	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	EDO	2	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 ⓘ

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	111/133 (83%)	0.45	8 (7%) 21 18	40, 55, 94, 165	0
1	B	114/133 (85%)	0.61	8 (7%) 22 18	43, 62, 121, 205	0
1	F	111/133 (83%)	2.11	58 (52%) 0 0	66, 175, 264, 330	0
2	D	22/22 (100%)	0.16	0 100 100	50, 77, 90, 112	0
2	H	22/22 (100%)	1.16	1 (4%) 38 33	114, 191, 240, 257	0
2	X	22/22 (100%)	-0.13	0 100 100	46, 63, 94, 108	0
3	E	22/22 (100%)	0.06	0 100 100	56, 79, 103, 105	0
3	I	22/22 (100%)	1.01	3 (13%) 7 5	150, 201, 244, 266	0
3	Y	22/22 (100%)	0.06	1 (4%) 38 33	49, 65, 100, 118	0
All	All	468/531 (88%)	0.86	79 (16%) 4 3	40, 74, 237, 330	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	ASN	6.1
1	F	448	ALA	5.7
1	F	472	CYS	5.2
1	F	458	ARG	4.9
1	B	491	ASN	4.8
1	F	451	TYR	4.7
1	F	449	HIS	4.6
1	F	439	LEU	4.3
1	F	464	ARG	4.1
1	F	431	LYS	4.1
1	F	452	ASP	4.1
1	F	440	CYS	4.0
1	F	463	LEU	3.9
1	F	465	PRO	3.7
1	A	489	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	466	TYR	3.6
1	F	462	GLY	3.5
1	F	381	PHE	3.5
1	B	470	SER	3.4
1	F	445	ALA	3.3
1	F	446	ALA	3.3
1	F	491	ASN	3.3
1	B	490	CYS	3.3
1	F	473	LYS	3.3
1	F	489	GLY	3.2
1	F	488	ASP	3.2
1	A	488	ASP	3.1
1	F	471	CYS	3.1
1	F	456	HIS	3.0
1	F	444	GLY	3.0
1	F	481	LEU	3.0
1	F	435	GLU	2.9
1	F	433	THR	2.9
1	F	416	LYS	2.9
1	F	453	LEU	2.9
1	F	414	ILE	2.8
1	F	417	VAL	2.8
1	F	486	LYS	2.8
1	A	490	CYS	2.8
1	F	436	LYS	2.8
1	F	461	THR	2.7
1	F	485	LEU	2.7
1	F	487	LYS	2.6
1	F	420	THR	2.6
1	F	469	ASP	2.6
1	B	489	GLY	2.6
1	F	443	CYS	2.6
1	F	484	HIS	2.5
1	F	447	PHE	2.5
1	F	413	ASN	2.4
1	B	378	GLY	2.4
3	Y	1	DG	2.4
2	H	20	DA	2.4
1	A	458	ARG	2.3
1	F	457	MET	2.3
1	F	470	SER	2.3
1	F	467	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	486	LYS	2.3
1	F	429	MET	2.3
1	F	437	PRO	2.3
1	A	381	PHE	2.3
1	F	474	THR	2.2
1	F	390	VAL	2.2
1	F	432	HIS	2.2
1	F	430	ARG	2.2
3	I	22	DT	2.2
1	B	472	CYS	2.1
1	F	382	GLN	2.1
1	B	401	ILE	2.1
1	F	418	ARG	2.1
1	F	389	LYS	2.1
1	F	468	CYS	2.1
1	F	391	ILE	2.1
1	F	442	GLN	2.1
1	A	472	CYS	2.1
1	F	460	HIS	2.1
1	B	392	GLN	2.0
3	I	2	DG	2.0
3	I	7	DA	2.0

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
5	ZN	F	603	1/1	0.40	0.22	311,311,311,311	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	F	604	1/1	0.69	0.18	250,250,250,250	0
4	EDO	D	101	4/4	0.75	0.20	67,74,76,91	0
4	EDO	Y	201	4/4	0.84	0.16	84,95,97,103	0
4	EDO	A	601	4/4	0.86	0.22	73,82,83,89	0
4	EDO	B	601	4/4	0.91	0.15	43,44,50,67	0
4	EDO	A	602	4/4	0.96	0.12	51,52,54,68	0
5	ZN	F	601	1/1	0.97	0.08	189,189,189,189	0
5	ZN	B	605	1/1	0.98	0.05	81,81,81,81	0
5	ZN	A	606	1/1	0.98	0.05	63,63,63,63	0
5	ZN	B	603	1/1	0.99	0.04	59,59,59,59	0
5	ZN	F	602	1/1	0.99	0.03	69,69,69,69	0
5	ZN	B	604	1/1	0.99	0.03	57,57,57,57	0
5	ZN	A	604	1/1	0.99	0.03	46,46,46,46	0
5	ZN	A	603	1/1	1.00	0.06	59,59,59,59	0
5	ZN	B	602	1/1	1.00	0.04	60,60,60,60	0
5	ZN	A	605	1/1	1.00	0.02	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.