Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 06:19 PM EDT

PDB ID	:	8E3D
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 (i) 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 (i)) were used in the production of this report:

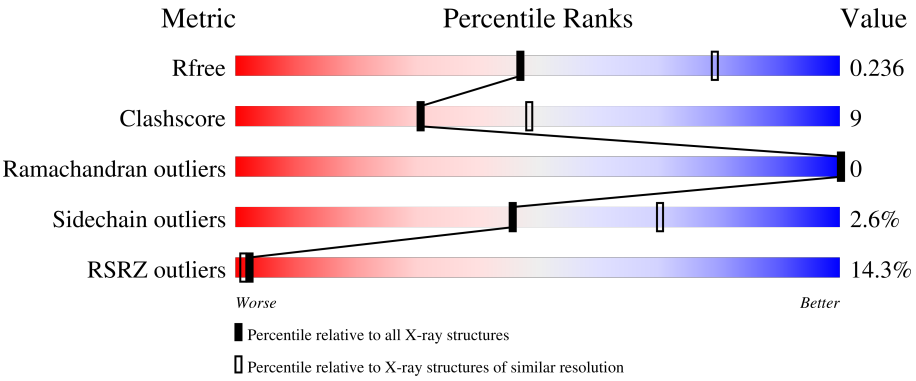
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (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 <=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	2% 65% 17% 17%
1	B	133	3% 71% 14% 14%
1	F	133	41% 69% 14% 17%
2	D	22	64% 36%
2	H	22	23% 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	9% 41% 59%
3	Y	22	23% 77%

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
5	ZN	F	603	-	-	-	X

2 Entry composition (i)

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

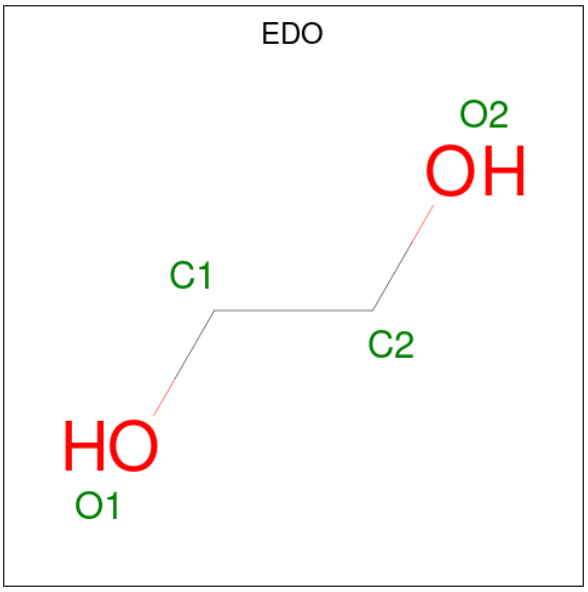
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*TP*TP*GP*GP*GP*GP*AP*GP*GP*GP*GP*TP*CP*TP*TP*TP*AP*AP*CP*C)-3').

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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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 (three-letter code: 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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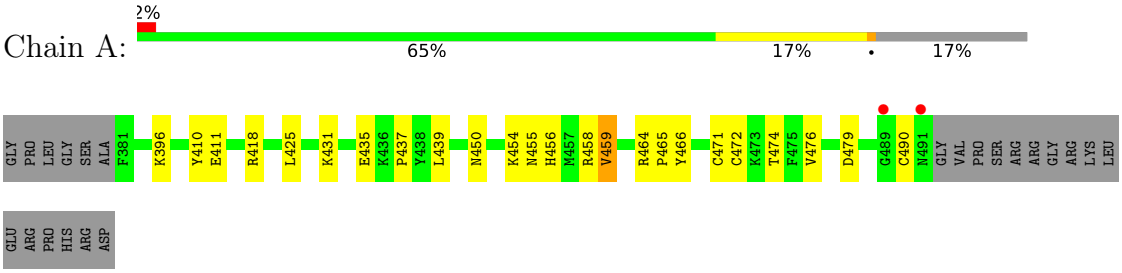
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	7	Total O 7 7	0	0
6	Y	10	Total O 10 10	0	0
6	B	18	Total O 18 18	0	0
6	D	2	Total O 2 2	0	0
6	E	6	Total O 6 6	0	0
6	F	1	Total O 1 1	0	0

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.

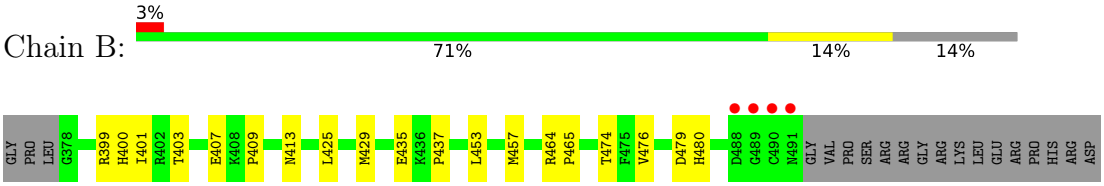
• Molecule 1: Zinc finger and BTB domain-containing protein 7A

Chain A:



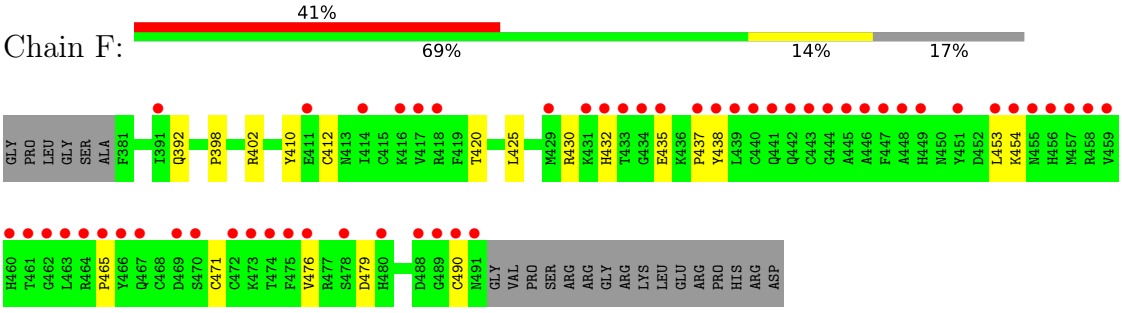
• Molecule 1: Zinc finger and BTB domain-containing protein 7A

Chain B:



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

Chain F:



• 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')

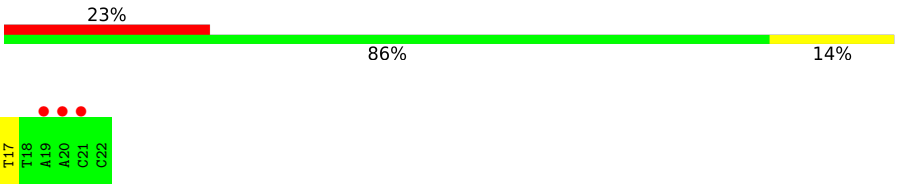
Chain X:

• 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:

• 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:



• Molecule 3: 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')

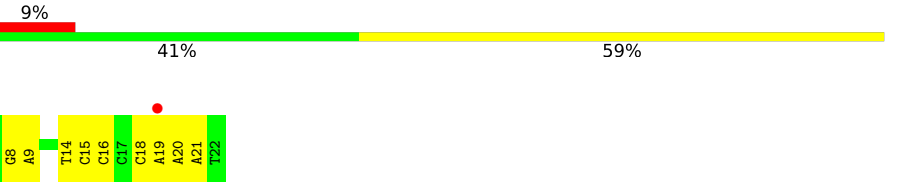
Chain Y:

• Molecule 3: 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')

Chain E:

• Molecule 3: 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')

Chain I:



4 Data and refinement statistics (i)

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 42.47 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.15-2.62) 90.0 (42.47-2.62)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.66 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.237 0.203 , 0.236	Depositor DCC
R_{free} test set	1804 reflections (4.98%)	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)	0.26 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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: EDO, ZN

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	0.24	0/906	0.51	0/1214
1	B	0.25	0/913	0.49	0/1226
1	F	0.23	0/864	0.47	0/1164
2	D	0.54	0/509	0.96	0/786
2	H	0.51	0/509	0.93	0/786
2	X	0.52	0/509	0.95	0/786
3	E	0.58	0/497	0.88	0/763
3	I	0.58	0/500	0.84	0/767
3	Y	0.57	0/500	0.88	0/767
All	All	0.43	0/5707	0.75	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	14	0
1	B	892	0	848	13	0
1	F	843	0	755	10	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	14	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	86	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 9.

All (86) 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
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
1:B:465:PRO:HD2	1:B:476:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:16:DT:H4'	2:X:17:DT:OP1	2.16	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
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 (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	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 (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	94/117 (80%)	91 (97%)	3 (3%)	39	63
1	B	92/117 (79%)	91 (99%)	1 (1%)	73	88
1	F	81/117 (69%)	78 (96%)	3 (4%)	34	58
All	All	267/351 (76%)	260 (97%)	7 (3%)	46	70

All (7) 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
1	F	420	THR
1	F	432	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	GLN

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Mol	Chain	Res	Type
1	A	450	ASN
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 monosaccharides 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	D	101	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	Y	201	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	A	601	-	3,3,3	0.46	0	2,2,2	0.34	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	D	101	-	-	0/1/1/1	-
4	EDO	Y	201	-	-	0/1/1/1	-
4	EDO	A	602	-	-	0/1/1/1	-
4	EDO	B	601	-	-	0/1/1/1	-
4	EDO	A	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, 95^{th} 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%)	0.02	2 (1%) 68 64	40, 55, 94, 165	0
1	B	114/133 (85%)	0.02	4 (3%) 44 37	43, 62, 121, 205	0
1	F	111/133 (83%)	2.71	54 (48%) 0 0	66, 175, 264, 330	0
2	D	22/22 (100%)	-0.14	0 100 100	50, 77, 90, 112	0
2	H	22/22 (100%)	1.18	5 (22%) 0 0	114, 191, 240, 257	0
2	X	22/22 (100%)	-0.04	0 100 100	46, 63, 94, 108	0
3	E	22/22 (100%)	-0.18	0 100 100	56, 79, 103, 105	0
3	I	22/22 (100%)	0.72	2 (9%) 9 6	150, 201, 244, 266	0
3	Y	22/22 (100%)	0.06	0 100 100	49, 65, 100, 118	0
All	All	468/531 (88%)	0.73	67 (14%) 2 1	40, 74, 237, 330	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	440	CYS	14.9
1	F	444	GLY	11.4
1	F	439	LEU	11.4
1	F	441	GLN	10.1
1	F	461	THR	9.7
1	F	445	ALA	8.9
1	F	458	ARG	8.6
1	F	474	THR	6.8
1	F	417	VAL	6.7
1	F	464	ARG	6.4
1	F	459	VAL	6.4
1	F	443	CYS	6.3
1	F	460	HIS	6.2
1	F	446	ALA	6.1
1	F	462	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	F	438	TYR	5.9
2	H	20	DA	5.7
1	F	466	TYR	5.4
1	F	442	GLN	5.3
1	F	475	PHE	5.2
1	B	491	ASN	5.2
1	F	457	MET	5.1
1	F	476	VAL	5.0
1	F	411	GLU	4.8
1	B	490	CYS	4.6
1	F	453	LEU	4.6
1	F	465	PRO	4.4
1	F	491	ASN	4.3
1	F	456	HIS	4.2
1	F	451	TYR	4.2
1	F	437	PRO	4.1
1	B	489	GLY	4.1
1	F	489	GLY	4.1
1	F	455	ASN	4.0
2	H	21	DC	4.0
2	H	1	DA	3.8
1	F	431	LYS	3.7
1	F	433	THR	3.7
1	F	469	ASP	3.7
1	F	488	ASP	3.7
1	F	449	HIS	3.6
1	F	434	GLY	3.5
1	F	416	LYS	3.4
1	F	454	LYS	3.4
1	F	463	LEU	3.4
1	A	491	ASN	3.3
1	F	470	SER	3.3
1	F	418	ARG	3.3
1	F	429	MET	3.2
3	I	4	DA	3.1
1	F	467	GLN	3.0
1	F	447	PHE	3.0
1	F	391	ILE	2.6
1	F	472	CYS	2.5
1	A	489	GLY	2.5
3	I	19	DA	2.4
1	F	448	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	480	HIS	2.3
1	F	432	HIS	2.3
1	B	488	ASP	2.3
1	F	473	LYS	2.2
2	H	19	DA	2.1
1	F	490	CYS	2.1
1	F	414	ILE	2.0
1	F	435	GLU	2.0
1	F	478	SER	2.0
2	H	5	DG	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 monosaccharides 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, 95^{th} 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	0.22	0.75	311,311,311,311	0
4	EDO	D	101	4/4	0.78	0.20	67,74,76,91	0
4	EDO	Y	201	4/4	0.82	0.27	84,95,97,103	0
5	ZN	F	604	1/1	0.86	0.23	250,250,250,250	0
5	ZN	A	606	1/1	0.89	0.12	63,63,63,63	0
4	EDO	A	601	4/4	0.90	0.21	73,82,83,89	0
4	EDO	A	602	4/4	0.91	0.28	51,52,54,68	0
4	EDO	B	601	4/4	0.94	0.20	43,44,50,67	0
5	ZN	B	605	1/1	0.96	0.09	81,81,81,81	0
5	ZN	F	601	1/1	0.96	0.06	189,189,189,189	0
5	ZN	A	604	1/1	0.97	0.15	46,46,46,46	0
5	ZN	B	603	1/1	0.97	0.15	59,59,59,59	0
5	ZN	B	604	1/1	0.98	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	F	602	1/1	0.98	0.11	69,69,69,69	0
5	ZN	A	603	1/1	0.99	0.19	59,59,59,59	0
5	ZN	A	605	1/1	0.99	0.12	59,59,59,59	0
5	ZN	B	602	1/1	1.00	0.14	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.